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A LINEAR LEAST-SQUARES FITTING PROGRAM
FOR THE ANALYSIS OF GAMMA-RAY SPECTRA
INCLUDING A GAIN-SHIFT ROUTINE

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ABSTRACT

A computer program is described which is intended for use in the analysis of complex gamma-ray spectra obtained with scintillation spectrometers. Given a composite spectrum and a set of up to 25 component spectra, the program determines the intensities of these components in the composite by carrying out a linear, least-squares fit. Several options are available to adapt the program to spectral analysis. These include the ability to subtract backgrounds, fix the intensities of selected components, fix the relative intensity of any two components, reject negative intensities, vary the number of data points used in the fit, and use different weighting functions. In order to correct for drift in the electronic system, the gain of the spectra may be changed by a gain-shift subroutine. Cycling options are available to expedite the processing of large numbers of composite spectra. Results of four problems are discussed to illustrate the use of the program. Input formats are given along with a sample output listing. Complete FORTRAN listings are included for versions used on IBM-7040 and 7094 computers.

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I. INTRODUCTION

The computer program described herein was developed for use in the analysis of gamma-ray spectra obtained with NaI(Tl) scintillation spectrometers. Such spectra represent the radiations, characteristic of one radioactive isotope or a combination of several. One may desire to analyze the composite spectrum either to obtain the intensities of the isotopic components or to obtain the intensities of the individual gamma rays. This computer program can be applied to either problem.

If one considers a complex spectrum of unknown isotopic composition, the analysis would be very difficult. Fortunately, this is usually not the case. More often the spectrum will exhibit characteristic peaks which permit the identification of components by either energy, relative intensity, half-life, or chemical properties. The problem is then reduced to that of determining the relative intensities. This may be done by a linear least-squares method.

The mathematical treatment of the two types of problems, isotopic and gamma-ray analysis, is the same. In either case the mathematical model assumes that the spectrum to be analyzed (i.e., the composite) is an exact linear combination of a set of component spectra, except for random statistical errors. These component spectra must then represent the response of the scintillation spectrometer to the elements of the composite under the same experimental conditions. This means that the pulse-height versus energy (gain) scales for the composite and all component spectra must be identical. It also assumes that the component spectra are known exactly (i.e., no random or systematic errors in the data points).

These mathematical conditions cannot be entirely satisfied for either of the two classes of problems. For isotopic analysis the component spectra are empirically determined and contain statistical fluctuations in the data points. Also, even when the utmost care is taken to establish a standard pulse-height scale, there will be small but finite variations in gain between the spectra. To minimize this problem, it is necessary to establish well-defined calibration procedures. Methods in general use at this laboratory are described in References 1 through 4. In the analysis of spectra to obtain intensities of individual gamma rays, a component will be a pulse-height distribution calculated by means of a computer program developed for this purpose [4]. These gamma-ray shapes will contain some systematic error.

To reduce the uncertainty which would be produced in the least-squares fit by a difference in pulse-height scales between the composite and component spectra, a routine has been included which can change the gain of a given spectrum. This is accomplished by a parabolic interpolation method which is described in Section IV.

In the fitting program, it is assumed that the components of a given spectrum are known and a set of standard spectra representing the instrumental response to these constituents is available. The problem is to determine then the intensities of these components. Let the components be labeled by an index, j , and the channels of the analyzer by i . The count in channel i of a given component is then y_{ji} and that of the composite, y_i . If β_j is the intensity of the j th component,

then the total contribution in channel i from all the components is

$$\bar{y}_i = \sum_{j=1}^J \beta_j y_{ji} \quad (1)$$

where J is the number of components.

The problem is then to determine the β_j so that the calculated spectrum $\bar{y}_i$ is the "best" possible approximation to the experimental spectrum y_i . The least-squares criterion is taken as the definition of the "best" intensities. That is, the β_j are calculated which minimize the expression

$$R^2 = \sum_i w_i (y_i - \bar{y}_i)^2 \quad (2)$$

where w_i is a set of weights. The sum is over the channels of interest.

Various options are provided in the program to assist in the analysis in particular cases. These will be discussed in the following sections as they arise.

This program has been used on IBM-7094 and 7040 computers. Although the program does not represent any new technique in the field of least-squares fitting, it does provide a compact package with special options for spectral analysis, especially the gain-shift routine. The authors have in use a pair of more advanced programs which treat gamma-ray energies or spectral gains as a parameter in the fit. These programs will be reported when they have been refined to a more useable form.

II. MATHEMATICS OF LEAST-SQUARES FITTING

1. DEFINITIONS

In this report, the following notation is used:

y_i = experimental count of composite spectrum in channel i

y_{B_i} = experimental count of background spectrum in channel i

y_{ji} = count in channel i of j th component spectrum

α = intensity of background

β_j = intensity of j th component (parameters to be calculated)

y_i^* = $y_i - \alpha y_{B_i}$ = net experimental count in channel i

σ_i = $\sqrt{y_i}$ = standard deviation associated with y_i

σ_{B_i} = $\sqrt{y_{B_i}}$ = standard deviation associated with y_{B_i}

σ_i^* = $\sqrt{y_i + \alpha^2 y_{B_i}}$ = standard deviation associated with y_i^*

σ_j = estimated uncertainty associated with β_j

$\bar{y}_i = \sum_{j=1}^J \beta_j y_{ji}$ = calculated count in channel i

CH1 = first channel used in fit

CH2 = last channel used in fit

n = number of channels used in fit

m = number of independently varying β_j computed in fit

χ^2 = chi-squared = minimum value of $\sum_{i=CH1}^{CH2} w_i (y_i^* - \bar{y}_i)^2$

Q.F. = $\frac{\chi^2}{n-m}$ = a quality of fit number which should, under certain assumptions, be about 1.

2. BASIC METHOD

As the spectra are read into the computer they can be gain-shifted. The options related to this process and the method used are discussed in Section IV.

Before the fit is carried out, a background spectrum can be subtracted. That is, $y_i^* = y_i - \alpha y_{B_i}$ is calculated. (In fact five such "backgrounds" can be subtracted so that $y_i^* = y_i - \sum_{k=1}^5 \alpha_k y_{B_{ki}}$.)

If all of the β_j are to be determined independently (i.e., not fixed or related), the mathematical procedures are as follows. The "best" β_j are defined as those which minimize the function

$$R^2 = \sum_{i=CH1}^{CH2} w_i (y_i^* - \bar{y}_i)^2. \quad (3)$$

Since the β_j occur linearly in $\bar{y}_i = \sum_{j=1}^J \beta_j y_{ji}$, the "best" β_j are obtained by solving the J linear equations

$$\frac{\partial R^2}{\partial \beta_j} = 0. \quad (4)$$

These equations can be written in the form $A\vec{\beta} = \vec{Y}$ where A is a $J \times J$ symmetric matrix, $\vec{\beta}$ is the column vector $(\beta_1, \beta_2, \dots, \beta_J)$ and $\vec{Y}$ is a column vector

with components $Y_j = 2 \sum_{i=CH1}^{CH2} w_i y_i^* y_{ji}$. The solution can then be written $\vec{\beta} = B \vec{Y}$ where the matrix B is inverse of A , $B = A^{-1}$.

The weighting function w_i can be taken as any one of three sets of values. By input control option, one can set

$$w_i = 1, \text{ for all } i, \text{ or} \quad (5a)$$

$$w_i = \frac{1}{\sigma_i^{*2}} \text{ where } \sigma_i^{*2} = y_i + \sum_{k=1}^5 \alpha_k^2 y_{B_{ki}}, \text{ or} \quad (5b)$$

$$w_i = \text{list of values provided as input.} \quad (5c)$$

In equation (5b), the formula for σ_i^* assumes that any error in α_k is negligible.

At the end of the calculations, the values of the β_j are printed, along with estimates of the estimated uncertainties associated with the β_j . These estimates are as follows:

$$\sigma_j \approx \sqrt{\frac{\chi^2}{n-m} B_{jj}} \quad (6)$$

where B_{jj} is the j th diagonal element of the inverse matrix obtained in the process of computing the β_j . The derivation of this error estimate is based on the assumptions of the mathematical model as noted in Section I. Care should be exercised, therefore, in the interpretation of these numbers [5].

3. FIXED INTENSITIES OF COMPONENTS

In some cases, a certain β_j may be restricted to a given value. If this intensity is called β_ℓ , the following function is minimized.

$$R^2 = \sum_{i=CH1}^{CH2} w_i \left[(y_i^* - \beta_\ell y_{\ell i}) - \sum_{j \neq \ell, j=1}^J \beta_j y_{ji} \right]^2 \quad (7)$$

The w_i have the values given in equation (6). [If the w_i are all equal (eq. (5a)), there is no difference between a background and a fixed-intensity spectrum. However, if equation (5b) is used, the backgrounds affect the weights while the fixed-intensity spectra do not.] This option is often used to reduce the number of variable parameters in preliminary fits or in cases where the intensities can be calculated from other data. Up to ten fixed-intensity components can be handled at once.

4. FIXED RATIOS FOR INTENSITIES

The program provides the option of fixing the ratio of any two β_j . Let the two component spectra involved by y_{ri} and y_{si} where β_r/β_s is known. The sum

$(y_{ri} + \frac{\beta_s}{\beta_r} y_{si})$ is then computed and used as a single component in the fit. If

the computed intensity for this combination is β'_r , the required intensities are

$\beta_r = \beta'_r$ and $\beta_s = (\beta'_r \frac{\beta_s}{\beta_r})$. The estimated uncertainties are then $\sigma_{\beta_r} =$

$\sigma_{\beta'_r}$ (computed in fit) and $\sigma_{\beta_s} = (\frac{\beta'_r \beta_s}{\beta_r}) \sigma_{\beta'_r}$. This option is used, for example,

in cases where the relative intensity of two gamma rays can be determined more accurately from the analysis of another spectrum.

III. DISCUSSION OF OPTIONS AND INPUT FORMAT

In addition to the binary program deck two sets of cards are needed, as shown in Figure 1. The cards in the first set are numbered 100 through 170 and are used to control the fitting process. The second group consists of 180, 181, and 500 cards and the cards on which the spectra appear. The card formats are shown in Figure 2.

Fig. 1 Arrangement of input card deck.

1. GENERAL CONTROL INFORMATION

The first set of cards, 100-170, are as follows:

Card

100 Any alphanumeric title which the user wishes printed on the output.

110 Contains a set of integers used for control information,

CH1 = first channel used in fit

CH2 = last channel used in fit ($CH1 < CH2 < 400$)

NS1 = total number of spectra to be read in (≤ 26)

NB = number of background spectra to be subtracted (≤ 5)

NF = number of spectra to have fixed intensities (≤ 10)

0000000000	1111111111	2222222222	3333333333	4444444444	5555555555	6666666666	7777777777	8888888888
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
100	XXXXX	ALPHANUMERIC TITLE CARD						XXXXX
110	CH1	CH2	NS1	NB	NF	NR	NS2	NCO
	XXX	XXX	XX	XX	XX	XX	XX	XX
120	COMPOSITE IDENTIFICATION							
	XXXXXXXXXX							
130	BACKGROUND IDENTIFICATIONS							
	XXXXXXXXXX XXXXXXXX XXXXXXXX XXXXXXXX							
131	BACKGROUND INTENSITIES α_k							
	XXX XXXX X XXXXXXX XX XXXXX XXXXXXX XXX XXXX							
140	COMPONENT IDENTIFICATIONS							
	XXXXXXXXXX XXXXXXXX XXXXXXXX XXXXXXXX XXXXXXXX XXXXXXXX							
140	XXXXXXXXXX XXXXXXXX ETC							
150	IDENTIFICATIONS OF FIXED INTENSITY SPECTRA							
	XXXXXXXXXX XXXXXXXX ETC							
152	INTENSITIES β_j OF FIXED-INTENSITY SPECTRA							
	XX XXXXX X XXXXXXX ETC							
160	IDENTIFICATIONS OF RELATED-INTENSITY SPECTRA							
	XXXXXXXXXX XXXXXXXX ETC							
162	INTENSITIES OF RELATED-INTENSITY SPECTRA							
	XX XXXXX X XXXXXXX ETC							
170	CHANNELS BETWEEN CH1 & CH2 OMITTED FROM FIT							
	XXX XXX XXX XXX XXX XXX ETC							
180	SPECTRUM IDENTIFICATION							
	XXXXXXXXXX FCH LCH X_1 X_2 GSC							
	XXXXXXXXXX XXX XXX XXX XXX X							
181	X_1 A a b r							
	XXXX XX XX XXXXX X XXXXXXX XXX XXXX XXX XXXX							
00	CARD COUNT SPECTRAL DATA							
	XXXXXXXX XXXXXX XXXXXX XXXXXX XXXXXX XX XXXX XXXXXX XXXXXX XXXXXX XXXXXX (NOT READ)							
01	XXXXXXXX ETC							
500	TRANSFER CARD							
0000000000	1111111111	2222222222	3333333333	4444444444	5555555555	6666666666	7777777777	8888888888
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

Fig. 2 Card formats.

NR = number of spectra involved in pairs with fixed relative intensities (≤ 10 and even)

NS2 = number of component spectra used in fit (NS2 = NS1 - NB - 1)

NCO = number of channels between CH1 and CH2 to be omitted from fit (≤ 20)

WC = weighting option control (0, 1, 2)

RC = option for recycle on negative intensity (0, 1)

OC = output option control (0, 1, 2)

IC = input option control (0, 1, 2).

The options related to the 110 card are as follows:

The choice of values should be clear for the constants CH1 through NS2.

The NCO option allows deletion from the fit one or more channels in the fitting range. That is, these channels are omitted in the summation to compute R^2 [equation (3)]. This option is to provide a method of deleting points which appear to be incorrect due to systematic error.

The weights in the expression for R^2 are taken as

$$\begin{array}{ll} \frac{1}{\sigma_i^{*2}} & \text{if } WC = 0 \\ 1 & \text{if } WC = 1 \\ \text{input list} & \text{if } WC = 2 \end{array}$$

If $WC = 2$, the values of $1/w_i$ must be on cards in the same format as the spectra, and they must precede all spectra and be followed by a 500 card. (That is, this group of cards must follow the 170 card with no intervening 180 card.) It should be emphasized that the derivation of the estimated uncertainties in the β_j assumes that the weights used are $\frac{1}{\sigma_i^{*2}}$ where σ_i^* is a good estimate of the standard deviation associated with y_i^* . This requirement is even more important for the interpretation of χ^2 or $\chi^2/(n-m)$. If the assumptions of the mathematical model are valid, the value of $\chi^2/(n-m)$ should be very close to unity. Thus, if the weights are so chosen, it can often be concluded from a "large" value of $\chi^2/(n-m)$ that either there are other components present in the composite or the gains are not all the same. If other weights are used, the value of $\chi^2/(n-m)$ has no simple interpretation.

The RC option is used to prevent the appearance of negative intensities in those situations where such a value is not physically allowable. This is often the case. If $RC = 1$ and a computed intensity is negative, the program sets this β_j equal to zero, fixes it, and repeats the fit. This process continues until all the intensities are positive or zero. If $RC = 0$, the computed negative intensities are accepted.

The value of OC determines the length of the output. The regular or short form ($OC = 0$) is shown along with one of the examples in Section V. This output includes the β_j , σ_j , χ^2 , $\chi^2/(n-m)$, and a channel-by-channel listing of y_i , σ_i , y_i^* , σ_i^* , $\bar{y}_i$, $y_i^* - \bar{y}_i$, and $\sqrt{w_i}(y_i^* - y_i)$. The medium form ($OC = 1$) includes a listing of the original data after successively subtracting each component (i.e., y_i^{**} , $y^* - \beta_1 y_{1i}$, $y^* - \beta_1 y_{1i} - \beta_2 y_{2i}$, ...). The long form ($OC = 2$) includes the matrix product (AB)

If IC = 0, the complete input deck as outlined here must be present. This is always the case for the first problem in a set. If IC = 1, the deck includes only the control cards (100-170 cards), and all the same spectra are used. If IC = 2, the deck includes only the control cards (100-170 cards) and the composite spectrum (180 and 181 cards, data, and two 500 cards); the same component and background spectra will be used. This option is often used to process a series of spectra with the same components. It should be emphasized that only the gain-shifted spectra are stored in the computer, so that in subsequent fits the shifted spectra must be used, or else all of the input data must be read in again.

The remaining general control cards are as follows:

- 120 Identification (eight numeric digits) of composite spectrum.
- 130 Identifications of any background spectra.
- 132 Intensities of the background spectra (α_k).
- 140 Identification of all spectra used but not listed on 120 or 130 cards (NS2 of them on up to 4 cards).
- 150 Identifications of any spectra that are to have fixed intensities. (If there are more than 5, use two cards.)
- 152 Intensities of the spectra on the 150 cards. (If there are two 152 cards, both follow the two 150 cards.)
- 160 Identification of spectra to have fixed relative intensities. The first two listed will be related, etc.
- 162 Intensities of related pairs. The magnitudes of the intensities have no significance since only the ratio will be used. (If there are more than three pairs, the two 160 cards precede the two 162 cards.)
- 170 List of channels between CH1 and CH2 which are to be omitted from the fit.

Of the above cards, 100, 110, 120, and 140 must be present for each problem run. The others are present only if they are used. If a 130 card is present, the accompanying 132 must also be present, similarly for 150 and 152, and 160 and 162. On the 130 and 132 cards, the first intensity on 132 applies to the spectrum whose identification is first on the 130 card, etc. This applies to the 150 and 160 cards also.

Data Deck

The second set of cards includes the spectral data; it is as follows:

Card

- 180 This card contains the identification of spectrum that follows and gives the first (FCH) and last (LCH) channel of data that are to be used. The identification must match one of those on a 120, 130, or 140 card. The constant GSC is 1 if the spectrum is to be gain-shifted and 0 if it is not. The remaining information refers to the gain-shift and is discussed in Section IV.
- 181 If GSC = 1 this card is present and gives additional gain-shift information. If GSC = 0 this card is not present.

Data

The 180 or 181 card is followed by a set of data in the form of counts per channel with ten channels per card in the format which is shown in Figure 2. The data start with channel 0 which is the live-time for all analyzers used in this laboratory. The first real count then is in channel 1.

500 The last data card is followed by a "500" card which signifies the end of a spectrum. The last spectrum in a problem is followed by two 500 cards.

It should be noted that the program does not check the card numbers quoted above, except for the 500. They are for convenience in assembling decks only. Therefore, the user must make certain the cards are in the proper order. Also, it is recommended that the data decks appear in the following order: composite, backgrounds, fixed-intensity spectra, related-intensity spectra, and independently varying intensity spectra. This order should also be used on the 140 cards.

IV. GAIN-SHIFT ROUTINE

The mathematical procedure for carrying out a change in the gain of a spectrum is as follows. Assume that there is to be no shift in the zero of the spectrum, then, if channel x' in the new spectrum corresponds to channel x in the original spectrum,

$$x' = r x \quad (8)$$

where r is called the "gain-shift ratio". If the independent variables x and x' were continuous, the count $y'(x')$ at x' could be computed as

$$y'(x') = \frac{1}{r} y(x). \quad (9)$$

The factor $\frac{1}{r}$ is introduced so the area under the curve (i.e., the total number of counts), is $\frac{1}{r}$ conserved.

Since the original spectrum, $y(x)$, is represented by a set of discrete points, some method of interpolation must be used. Given a channel x' (an integer), the corresponding pulse height x (not an integer in general) is computed from equation (8). The three channels nearest x are chosen. (That is, x is rounded to the nearest integer, x_ℓ , and $x_\ell-1$, x_ℓ , and $x_\ell+1$ are selected.) These three data points are fitted with the function, $y = a + bx + cx^2$, to determine the parameters a , b , and c . Then, for nonintegral x values, $y(x)$ is calculated by evaluating this polynomial at x , and $y'(x')$ is computed from equation (9).

Since there are three parameters and three data points, the function, $a + bx + cx^2$, fits these points exactly. Thus, this procedure is not intended to be a smoothing process.

If it is desired that the zero as well as the gain of the pulse-height scale be changed, equation (8) becomes

$$x' = r(x - A) \quad (10)$$

where A is the desired shift in the zero. Equation (9) remains unchanged.

Although this program is intended for use with small gain shifts (e.g., $0.9 < r < 1.1$), it can be used for larger shifts. As an extreme example, Figure 3 shows two Cs-137 spectra, one measured at 5 keV/channel and the other at 10 keV/channel and shifted ($r \approx 2.0$) to 5 keV/channel. The agreement is considered excellent for such a large scale change. The finite channel widths cause the broader, lower peaks on the shifted 10-keV spectrum. This result indicates that the distortion for small shifts should be very small. Other tests have been made to determine the effect of a shift on the shape of a photopeak. These results indicate that the effects are negligible.

In the computer program, there are two different ways of making a shift. The first method is to supply r and A in the format shown in Figure 2 on the 181 card. On the 180 card, GSC must be 1. In this case the values of x_1 , x_2 , x_t , a , and b should be zero (i.e., left blank).

The second gain-shift method allows the shifting of a well defined peak to a known channel without knowing its position in the experimental spectrum. In

Fig. 3 Comparison of Cs-137 spectrum measured at 5 keV per channel with one taken at 10 keV per channel and gain-shifted to 5 keV.

this case r must be zero and GSC is 1. The program then computes the parameters y_0 , x_0 , and b_0 in the function

$$g(x) = y_0 e^{-\frac{(x-x_0)^2}{b_0}} + a + bx$$
 such that $g(x)$ gives the best fit to the data points from x_1 to x_2 , inclusive. This determines the position x_0 of the experimental peak. A value of r is then computed such that this peak will be shifted to channel x_t [i.e., $r = x_t/(x_0 - A)$]. The line $a + bx$ is used to approximate the contribution of the spectral background underlying the peak of interest. The parameters a and b are not computed in the fit; they must be supplied as input. The values of y_0 , x_0 , and b_0 are computed by an unweighted least-squares fit after linearizing the forms of the parameters. That is,

$$\ln(y - a - bx) \approx \ln(g - a - bx) = \left[\ln y_0 - \frac{x_0^2}{b_0} \right] + \left[\frac{2x_0}{b_0} \right] x + \left[-\frac{1}{b_0} \right] x^2.$$

The quantities in the brackets are computed in the fit and then x_0 is determined from these values.

V. EXAMPLES OF RESULTS

The following examples are included to show the types of problems for which the program has been used and the quality of fits that can be obtained.

The result of an isotopic analysis problem with five components is shown in Figure 4. In this case, the five component spectra were each measured individually for a given counting time. Then the sources were placed together and the composite spectrum was measured for the same time. The calculated intensities then should be very close to 1.00. As shown in the figure, the intensities differ from 1.0 by 1-1/2 percent at most, with calculated errors which are the correct order of magnitude. The residuals $(y_i^* - \bar{y}_i)$ are shown at the

bottom of the figure in the form $\left(\frac{y_i^* - \bar{y}_i}{\sigma_i^*} \right)$. This is an idealized isotopic analysis

problem since the same sources were used for the composite and the components. However, the results indicate the accuracy that can be obtained.

Another isotopic analysis problem is indicated in Figure 5 in which the amount of Ru-103 and Ru-106 present in a sample is to be determined. Again, the composite sources consisted of separate Ru-103 and Ru-106 sources stacked together. By measuring the spectra of the individual samples, the "correct" answers were determined. In each composite source, a Hg-203 sample was also included in order to provide a well-defined peak to use for gain normalization.

The results of the analyses of three spectra are shown in Figure 6. A least-squares fit was carried out for several different gain shifts of the composite. (The Hg-203 peak was shifted to a set of "true channels", x_t , as shown on the abscissa.) The quality of fit number, $\chi^2/(n-m)$, is plotted along with the two intensities, β_{103} and β_{106} . For each sample, the gain of the composite spectrum corresponding to the "correct" values of the intensities and the best fit are marked by the three vertical lines. Ideally, these three lines should coincide and also be the same for all three problems; however the following useful observations can be made.

- (1) A shift of 0.01 channels or 0.03 percent makes a significant change in the results.
- (2) All correct values and minima in $\chi^2/(n-m)$ occur within a range of 0.03 channels for x_t .
- (3) The "correct" values of β_{106} and β_{103} correspond to values of $\chi^2/(n-m)$ which are no more than about 50 percent above the minimum value of $\chi^2/(n-m)$.

Two other facts should be taken into account in considering these results. Although considerable care was taken in gain-shifting the components to the same gain scale, the fits could undoubtedly be improved by varying the gain of one of the components. Second, as the Ru-103 intensity becomes small, it becomes indeterminate since its peaks are not distinguishable from the Ru-106 peaks. The reverse is not the case since the 1.2-MeV peak in the Ru-106 is always resolved from the Ru-103 spectrum. This case illustrates the impor-

Fig. 4 Results of least-squares fit of a spectrum with five components.

tance of considering the "interference" between major features of component spectra in assessing the error to be expected in the analysis of a given isotopic mixture.

A listing of the input deck and output information for one of these fits appears at the end of this Section.

The third example (Figure 7) shows the analysis of a Nb-94m spectrum into its constituent gamma rays. Here the component spectra are shapes of single gamma rays which have been calculated with the aid of a computer program [4]. As shown, fits were carried out with one and two gamma rays. The residuals for the former case indicate the improvement obtained with the second gamma ray. The accuracy of the calculated gamma-ray shapes is good enough to allow the conclusion that the 0.703-MeV gamma ray is present. The existence of this gamma ray also was verified by gamma-gamma coincidence measurements.

Fig. 6 Results of fits to three Ru-103 + Ru-106 mixtures as a function of the gain of the composite spectrum.

Another example of the determination of gamma-ray intensities is that of Nb-94 shown in Figure 8. In this case, there are only two transitions and their intensities are known to be equal. Since the two gamma rays are in cascade, there is also coincidence summing. The two gamma-ray shapes were generated and the sum spectrum was calculated [4]. The composite was then fitted with these three components. The resulting intensities were $\beta_{703} = 2.097 \pm 0.006$, $\beta_{874} = 2.123 \pm 0.006$, $\beta_{\text{sum}} = 2.82 \pm 0.05$. These results are really a check on the intensity normalization procedure of the program that generates the single gamma-ray shapes. In this case, the accuracy of the normalization is indicated to be 1 to 2 percent. In this fit, the quality of fit number was 2.0 when all channels above 5 were used. The accuracy of shapes to this low channel is especially satisfying. In order to obtain the best fit, it was necessary in this case to generate the gamma-ray shapes at the correct channel to within about 0.01 channels.

Fig. 7 Results of least-squares fits to Nb-94m spectrum.

Fig. 8 Results of fit to Nb-94 spectrum (two calculated gamma-ray shapes and sum spectrum).

EXAMPLE OF INPUT FORMAT
LINEAR LEAST SQUARES SPECTRUM FITTING PROGRAM

```

$JOB      P PLC11400-C28  400035          L.S.G.F.
100      RU-103+106  SPECTRUM 1          02-13-64
110          040  121   3                  2          1          0
120          05172001
140          C5167103  05167106
180          05172001  001  130  025  C32  1
181          28.495          11000.0
00 580000 019735 048602 068453 067937 065802 060006 081037 154106 098014      2001
01 054466 043035 043242 044074 044564 041550 039516 041358 043268 042257      2001
02 039614 037652 036972 037280 038116 041769 069368 163463 283830 285910      2001
03 163812 062443 026775 019341 016535 014352 013361 012541 012560 012214      2001
04 011932 011863 011394 010779 009969 009535 010435 015705 030123 057367      2001
05 091828 117490 117419 089975 053144 025265 011856 007915 009830 016914      2001
06 027355 038508 045771 043575 034058 021635 011788 006177 003553 002510      2001
07 002013 001918 001765 001735 001608 001650 001613 001676 001585 001595      2001
08 001576 001472 001496 001655 001714 001923 001981 002068 001949 001634      2001
09 001311 001155 001024 000877 000783 000747 000655 000738 000928 001213      2001
10 001578 002232 002801 003168 003304 003078 002751 002240 001943 001662      2001
11 001659 001697 001700 001658 001672 001462 001337 001066 000865 000626      2001
12 000455 000347 000280 000245 000205 000191 000210 000195 000201 000190      2001
13 000187 000148 000180 000180 000138 000158 000140 000151 000122 000125      2001
14 000105 000114 000120 000134 000123 000137 000158 000191 000197 000236      2001
15 000267 000268 000243 000264 000279 000255 000219 000189 000170 000143      2001
50
180          05167103  001   68
00 580000 003106 011160 011209 005693 005964 006944 006002 005488 005567      7103
01 005575 005880 005971 005976 006039 006332 006937 008177 008794 007832      7103
02 006650 006184 005810 006025 006171 006360 006345 006651 006824 007270      7103
03 007169 006865 005626 004326 003416 002926 002769 002514 002286 002210      7103
04 002168 002285 002244 002282 002679 003690 007427 016955 033199 052557      7103
05 062491 056975 038853 020137 008036 003039 001405 001075 001243 001874      7103
06 002487 002965 002735 002119 001305 000625 000277 000111 000056 000013      7103
07 000020 000013 000025 000017 000030 000019 000035 000003 000023 000011      7103
08 000011 000013 000020 000019 000020 000018 999996 999989 000006 000018      7103
09 999989 999999 000005 000004 999994 000002 000001 999996 000008 000003      7103
10 999995 000010 999996 999995 000011 000001 999999 000006 000004 000007      7103
11 000002 999984 999993 999984 000002 999988 999993 999996 000019 999988      7103
12 999989 999992 999991 999992 999996 000001 000010 000000 999978 000005      7103
13 999993 999995 999999 000005 000001 000002 999988 999996 000000 999995      7103
14 999993 000000 000002 999994 999998 000004 000005 999998 000000 999994      7103
15 00000
50
180          05167106  001  121
00 000000 000000 000000 050059 046372 040778 039643 037775 036000 033728
01 032329 030833 029617 028508 027310 026808 027080 028907 030612 029068
02 025777 023664 022180 021523 021109 020719 020509 020637 020615 020633
03 020717 020522 019857 017919 015467 013661 012907 012080 011885 011581
04 011370 011261 010844 010059 009288 008699 009136 013537 025864 051077
05 084223 111418 113920 087786 052476 025334 011555 007406 009356 016039
06 026659 038077 045073 043844 033937 021536 011591 006184 003500 002378
07 001875 001748 001664 001576 001530 001638 001486 001594 001450 001442
08 001465 001392 001485 001549 001706 001898 002010 002053 001838 001618
09 001334 001051 000929 000778 000714 000733 000675 000626 000870 001158
10 001562 002223 002733 003234 003389 003267 002755 002283 001797 001690
11 001626 001585 001600 001699 001610 001493 001277 001068 000855 000574
12 000468 000345
50
50

```

EXAMPLE OF OUTPUT FORMAT 7040 LINEAR LEAST SQUARES FITTING PROGRAM

```

RU-103+106 SPECTRUM 1                                02-13-64
PROBLEM CONTROL PARAMETERS
COMPOSITE SPECTRUM IDENTIFICATION - 5172001
FITTING LIMITS IN CHANNEL NUMBER
A. LOWER - 40
B. UPPER - 121
NUMBER OF SPECTRA IN PROBLEM - 3
A. BACKGROUND - -0
B. FIXED INTENSITY - -0
C. FIXED RATIO - -0
D. VARIABLE PARAMETERS - 2
WEIGHTED BY 1/Y
CONTROL CARD LISTING
110 40 121 3 -0 -0 -0 2 -0 0 1 0 0
120 5172001
140 5167103 5167106
180 5172001 1 130 25 32 1
181 28.495 -0. 11000.0000 -0. -0.
LISTING OF GAIN SHIFTED SPECTRA
0 0 1 2 3 4 5 6 7 8 9
0 0. 19717. 48514. 68364. 67880. 65760. 59910. 80664. 153900. 98335. 5172001
1 54669. 43053. 43197. 44026. 44540. 41547. 39482. 41292. 43221. 42250. 5172001
2 39620. 37644. 36943. 37235. 38033. 41381. 67879. 160678. 281967. 287194. 5172001
3 166732. 64353. 27393. 19480. 16598. 14391. 13379. 12544. 12554. 12215. 5172001
4 11928. 11862. 11405. 10797. 9986. 9518. 10300. 15277. 29195. 55942. 5172001
5 90262. 116759. 117035. 91427. 54702. 76398. 12302. 7969. 2591. 16432. 5172001
6 26740. 37954. 45572. 43860. 34664. 22281. 12251. 6429. 3667. 2558. 5172001
7 2031. 1925. 1770. 1739. 1610. 1649. 1611. 1676. 1587. 1594. 5172001
8 1579. 1474. 1489. 1645. 1703. 1911. 1974. 2067. 1965. 1659. 5172001
9 1331. 1166. 1035. 887. 789. 752. 656. 726. 907. 1183. 5172001
10 1532. 2174. 2754. 3141. 3304. 3102. 2789. 2219. 1970. 1676. 5172001
11 1656. 1694. 1701. 1659. 1680. 1479. 1356. 1091. 888. 649. 5172001
12 471. 357. 286. 249. 209. 191. 210. 196. 201. 191. 5172001
13 187. 1. 1. 1. 1. 1. 1. 1. 1. 1. 5172001
180 5167103 1 68 -0 -0 0
180 5167106 1 121 -0 -0 0

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RU-103+106 SPECTRUM 1                                02 13 64
RESULTS FOR SPECTRA USED IN FITTING SUBROUTINE
SPECTRA      IDENTITY      INTENSITY      STANDARD DEVIATION
COMPOSITE    5172001
STANDARD     5167103      0.07773641     0.00707839
STANDARD     5167106      1.01867032     0.00329559
CHI-SQUARED  =      0.41427211E 03
DEGREES OF FREEDOM = 79
QUALITY OF FIT NUMBER = 5.244

```

WEIGHTED FIT - QUALITY OF FIT NUMBER SHOULD BE APPROXIMATELY 1.0
QUALITY OF FIT NUMBER INDICATES A POOR FIT.

EXAMPLE OF OUTPUT FORMAT
7040 LINEAR LEAST SQUARES FITTING PROGRAM (Continued)

RU-103+106 SPECTRUM 1				02-13-64			
CHAN.	Y	SIGMA	Y-BKG	YCALC.	SIGMA Y-BKG	RESIDUAL	R/SG.Y-BKG
1	19716.96	140.417	19716.96	242.47	140.417	19474.4917	138.690
2	48513.06	220.257	48513.06	868.56	220.257	47644.5054	216.313
3	68363.86	261.465	68363.86	51864.96	261.465	16498.8970	63.102
4	67879.73	260.537	67879.73	47680.33	260.537	20199.3945	77.530
5	65759.92	256.437	65759.92	42002.96	256.437	23756.9604	92.642
6	59909.81	244.765	59909.81	40922.95	244.765	18986.8608	77.572
7	80663.18	284.013	80663.18	38946.84	284.013	41716.3359	146.882
8	153899.62	392.300	153899.62	37098.75	392.300	116800.8760	297.733
9	98334.33	313.583	98334.33	34790.47	313.583	63543.8613	202.638
10	54668.60	233.813	54668.60	33365.97	233.813	21302.6318	91.110
11	43052.63	207.491	43052.63	31865.75	207.491	11186.8801	53.915
12	43196.82	207.838	43196.82	30634.12	207.838	12562.6931	60.445
13	44025.84	209.823	44025.84	29504.81	209.823	14521.0322	69.206
14	44539.11	211.043	44539.11	28289.34	211.043	16249.7751	76.997
15	41546.69	203.830	41546.69	27800.74	203.830	13745.9468	67.438
16	39481.69	198.700	39481.69	28124.85	198.700	11356.8425	57.156
17	41291.07	203.202	41291.07	30082.35	203.202	11208.7214	55.160
18	43220.67	207.896	43220.67	31867.15	207.896	11353.5161	54.612
19	42249.83	205.548	42249.83	30219.54	205.548	12030.2871	58.528
20	39619.96	199.048	39619.96	26775.21	199.048	12844.7483	64.531
21	37643.16	194.018	37643.16	24586.54	194.018	13056.6189	67.296
22	36942.14	192.203	36942.14	23045.76	192.203	13896.3826	72.300
23	37234.02	192.961	37234.02	22393.20	192.961	14840.8191	76.911
24	38032.63	195.020	38032.63	21982.82	195.020	16049.8081	82.298
25	41380.33	203.422	41380.33	21600.23	203.422	19780.0920	97.237
26	67878.39	260.535	67878.39	21385.15	260.535	46493.2466	178.453
27	160677.24	400.846	160677.24	21539.32	400.846	139137.9121	347.111
28	281966.51	531.005	281966.51	21530.36	531.005	260436.1445	490.459
29	287193.73	535.905	287193.73	21581.37	535.905	265610.3555	495.630
30	166731.20	408.327	166731.20	21661.09	408.327	145070.1113	355.279
31	64352.12	253.677	64352.12	21438.81	253.677	42913.3076	169.165
32	27392.56	165.507	27392.56	20665.08	165.507	6727.4805	40.648
33	19479.74	139.570	19479.74	18589.84	139.570	889.8982	6.376
34	16597.65	128.832	16597.65	16021.32	128.832	576.3245	4.473
35	14390.22	119.959	14390.22	14143.51	119.959	246.7045	2.057
36	13378.65	115.666	13378.65	13363.23	115.666	15.4218	0.133
37	12543.55	111.998	12543.55	12500.97	111.998	42.5798	0.380
38	12553.97	112.045	12553.97	12284.60	112.045	269.3724	2.404
39	12214.06	110.517	12214.06	11969.02	110.517	245.0421	2.217
FIT OF DATA BEGINS WITH THE NEXT CHANNEL							
40	11927.65	109.214	11927.65	11750.81	109.214	176.8331	1.619
41	11861.95	108.913	11861.95	11648.87	108.913	213.0734	1.956
42	11404.27	106.791	11404.27	11220.90	106.791	183.3652	1.717
43	10796.98	103.909	10796.98	10424.20	103.909	372.7775	3.588
44	9985.19	99.926	9985.19	9669.67	99.926	315.5225	3.158
45	9517.84	97.559	9517.84	9148.26	97.559	369.5780	3.788
46	10299.76	101.438	10299.76	9883.92	101.438	415.8433	4.097
47	15276.52	123.598	15276.52	15107.76	123.598	168.7616	1.365
48	29194.54	170.864	29194.54	28927.66	170.864	266.8782	1.562
49	55941.07	236.519	55941.07	56116.22	236.519	-175.1494	-0.741
50	90362.20	300.603	90362.20	90653.29	300.603	-291.0986	-0.968
51	116757.67	341.698	116757.67	117927.24	341.698	-1169.5693	-3.423
52	117934.59	343.416	117934.59	119067.21	343.416	-1132.6211	-3.298
53	91436.34	302.384	91436.34	90990.37	302.384	445.9687	1.475
54	54701.95	233.884	54701.95	54080.43	233.884	621.5166	2.657
55	26297.44	162.165	26297.44	26743.23	162.165	254.2041	1.568
56	12301.24	110.911	12301.24	11879.96	110.911	421.2897	3.798
57	7968.33	89.266	7968.33	7627.84	89.266	340.4953	3.814
58	9590.10	97.929	9590.10	9627.31	97.929	-37.2054	-0.380
59	16431.28	128.185	16431.28	16484.13	128.185	-52.8528	-0.412
60	26739.41	163.522	26739.41	27350.06	163.522	-610.6528	-3.734
61	37953.77	194.817	37953.77	39018.40	194.817	-1064.6245	-5.465
62	45571.30	213.474	45571.30	46127.14	213.474	-555.8325	-2.604
63	43859.87	209.427	43859.87	44827.30	209.427	-967.4346	-4.619
64	34663.10	186.180	34663.10	34627.06	186.180	-8.9634	-0.048
65	22280.74	149.267	22280.74	21986.67	149.267	294.0696	1.970
66	12250.92	110.684	12250.92	11828.94	110.684	421.9752	3.812
67	6428.87	80.180	6428.87	6308.09	80.180	120.7819	1.506
68	3666.68	60.553	3666.68	3569.70	60.553	96.9771	1.602
69	2557.30	50.570	2557.30	2422.40	50.570	134.9028	2.668
70	2030.92	45.066	2030.92	1913.01	45.066	120.9084	2.683
71	1924.16	43.865	1924.16	1780.64	43.865	143.5276	3.272
72	1769.67	42.067	1769.67	1695.07	42.067	74.5986	1.773
73	1738.43	41.694	1738.43	1605.42	41.694	133.0065	3.190
74	1609.79	40.122	1609.79	1558.57	40.122	51.2232	1.277
75	1648.13	40.597	1648.13	1668.58	40.597	-20.4474	-0.504

EXAMPLE OF OUTPUT FORMAT
7040 LINEAR LEAST SQUARES FITTING PROGRAM (Continued)

CHAN.	Y	SIGMA	Y-BKG	YCALC.	SIGMA Y-BKG	RESIDUAL	R/SG.Y-BKG
76	1610.86	40.136	1610.86	1513.74	40.136	97.1180	2.420
77	1675.07	40.928	1675.07	1623.76	40.928	51.3123	1.254
78	1586.69	39.833	1586.69	1477.07	39.833	109.6169	2.752
79	1593.79	39.922	1593.79	1468.92	39.922	124.8682	3.128
80	1578.82	39.734	1578.82	1492.35	39.734	86.4691	2.176
81	1473.97	38.392	1473.97	1417.99	38.392	55.9787	1.458
82	1488.16	38.577	1488.16	1512.73	38.577	-24.5675	-0.637
83	1644.94	40.558	1644.94	1577.92	40.558	-67.0160	-1.652
84	1702.60	41.263	1702.60	1737.85	41.263	-35.2531	-0.854
85	1910.42	43.708	1910.42	1933.44	43.708	-23.0124	-0.526
86	1973.58	44.425	1973.58	2047.53	44.425	-73.9435	-1.664
87	2066.74	45.461	2066.74	2091.33	45.461	-24.5883	-0.541
88	1964.04	44.317	1964.04	1872.32	44.317	91.7229	2.070
89	1650.41	40.724	1650.41	1640.21	40.724	10.2003	0.250
90	1330.05	36.470	1330.05	1358.91	36.470	-28.8575	-0.791
91	1165.96	34.146	1165.96	1070.62	34.146	95.3341	2.792
92	1034.69	32.167	1034.69	946.34	32.167	88.3414	2.746
93	886.62	29.776	886.62	792.53	29.776	94.0969	3.160
94	788.08	28.073	788.08	727.33	28.073	60.7491	2.164
95	751.66	27.416	751.66	746.69	27.416	4.9746	0.181
96	655.46	25.602	655.46	687.60	25.602	-32.1397	-1.255
97	725.65	26.938	725.65	708.99	26.938	16.6579	0.618
98	906.27	30.104	906.27	906.62	30.104	-0.3442	-0.011
99	1182.84	34.392	1182.84	1179.62	34.392	3.2155	0.093
100	1531.21	39.131	1531.21	1591.16	39.131	-59.9547	-1.532
101	2173.19	46.617	2173.19	2264.50	46.617	-91.3128	-1.959
102	2753.96	52.478	2753.96	2784.03	52.478	-30.0614	-0.573
103	3140.42	56.039	3140.42	3294.38	56.039	-153.9563	-2.747
104	3303.62	57.477	3303.62	3452.27	57.477	-148.6558	-2.586
105	3101.23	55.689	3101.23	3328.00	55.689	-226.7631	-4.072
106	2788.18	52.803	2788.18	2806.44	52.803	-18.2534	-0.346
107	2278.45	47.733	2278.45	2325.62	47.733	-47.1778	-0.988
108	1969.81	44.383	1969.81	1830.55	44.383	139.2585	3.138
109	1675.98	40.939	1675.98	1721.55	40.939	-45.5707	-1.113
110	1655.93	40.693	1655.93	1656.36	40.693	-0.4258	-0.010
111	1693.19	41.148	1693.19	1614.59	41.148	78.5986	1.910
112	1700.21	41.234	1700.21	1629.87	41.234	70.3336	1.706
113	1658.23	40.721	1658.23	1733.12	40.721	-72.4420	-1.780
114	1679.45	40.981	1679.45	1640.06	40.981	39.3885	0.961
115	1478.72	38.454	1478.72	1520.87	38.454	-42.1575	-1.096
116	1355.94	36.823	1355.94	1300.84	36.823	55.0970	1.496
117	1090.65	33.025	1090.65	1087.94	33.025	2.7067	0.082
118	887.70	29.794	887.70	870.96	29.794	16.7364	0.562
119	648.11	25.458	648.11	584.72	25.458	63.3934	2.490
120	470.25	21.685	470.25	476.74	21.685	-6.4883	-0.299
121	356.61	18.884	356.61	351.44	18.884	5.1661	0.274
FIT OF DATA ENDS WITH THE PRECEEDING CHANNEL							
122	285.63	16.901	285.63	0.	16.901	285.6273	16.901
123	248.96	15.778	248.96	0.	15.778	248.9568	15.778
124	208.04	14.423	208.04	0.	14.423	208.0362	14.423
125	190.76	13.811	190.76	0.	13.811	190.7552	13.811
126	209.35	14.469	209.35	0.	14.469	209.3514	14.469
127	195.49	13.982	195.49	0.	13.982	195.4852	13.982
128	200.99	14.177	200.99	0.	14.177	200.9919	14.177
129	190.71	13.810	190.71	0.	13.810	190.7064	13.810
130	186.77	13.666	186.77	0.	13.666	186.7666	13.666

OPTION FOR RESIDUALS PRINTOUT NOT SPECIFIED

END OF PROBLEM

END-OF-DATA ENCOUNTERED ON SYSTEM INPUT FILE.

L.S.G.F. PAT CHASE

\$IBSYS

\$JOBTHM P PLC11400-C28 400J35 02.298 02.316 00.017 052564
*LINES = 00217, CARDS = 00002

VI. REFERENCES

1. R. L. Heath, Scintillation Spectrometry -- Gamma-Ray Spectrum Catalogue, 2nd Ed., Vol. I, IDO-16880 (August 1964).
2. R. L. Heath, "Scintillation Spectrometry -- The Experimental Problem", in G. D. O'Kelley, ed., Proceedings of a Symposium on Applications of Computers to Nuclear and Radiochemistry, Gatlinburg, 1962, National Research Council, Nuclear Science Series, Radiochemical Techniques 3107.
3. D. F. Crouch and R. L. Heath, Routine Testing and Calibration Procedures for Multichannel Pulse Analyzers and Gamma-Ray Spectrometers, IDO-16923 (November 1963).
4. R. L. Heath, "Recent Developments in Scintillation Spectrometry", IRE Trans. on Nuclear Sci. NS-9, No. 3 (June 1962) pp 294-304.
5. R. H. Moore and R. K. Zeigler, The Solution of the General Least Squares Problem with Special Reference to High-Speed Computers, LA-2367 (October 1959).

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APPENDIX

FORTRAN LISTINGS

The complete FORTRAN listings for this program for compilation on the IBM-7040 and 7094 computers are given in the following. Although considerable effort has been expended to check all options and calculations, some errors may still exist in these programs.

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C      LINEAR LEAST SQUARES GAMMA SPECTRUM FITTING PROGRAM
C      IN FORTRAN II LANGUAGE FOR THE IBM-7090 COMPUTER
C      USING DOUBLE PRECISION MATRIX INVERSION
C      D. D. METCALF, PHILLIPS PETROLEUM CO., A.E.O.
C      NATIONAL REACTOR TESTING STATION, IDAHO FALLS, IDAHO
C
C      DIMENSION SPECT(400,26),SIGMA(400),SIGMAS(400),ID(2,26),
1      ISPLTS(2,26),IPPLTS(2,26),JFS(26),ID1(2,10),ID2(2,10),
2      JFST(20),RSDL(20),INCLO(20),TITLE(11),FIXINT(10),FIXRT(10),
3      IFI(10),IRI(10),IRID(10),BETA(10),BETR(10),BGINT(6)
D      DIMENSION A(20,20),B(20,20),C(20,20),DATA(400),DET(1)
COMMON SPECT,SIGMA,SIGMAS,ID,ISPLTS,IPPLTS,JFS,ID1,ID2,JFST,
1      RSDL,INCLO,TITLE,FIXINT,FIXRT,IFI,IRI,IRID,BETA,BETR,
2      BGINT,A,B,C,DATA,DET,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,
3      JNCLO,JMT,JOPT1,JOPT2,JRC,IPAGE,IFS,KLOW,KHIGH
C
500  IPAGE=0
      CALL INPUT
      CALL PAGE(IPAGE)
      WRITE OUTPUT TAPE 6,960,(TITLE(I),I=1,11)
C
C      OBTAIN SPECTRA IDENTITY NUMBERS FOR STANDARDS
C      USED IN FITTING.
C
      DO 502 K=1,26
502   JFS(K)=0
      N=JSUB+2
      DO 505 K=N,JN
505   JFS(K)=K
      KLOW=ISPLTS (1,1)
      KHIGH=ISPLTS (2,1)
C
C      SET AREA FOR IDENTITY OF FIXED INTENSITY SPECTRA
C      TO ZERO
C
504  DO 507 K=1,10
      IRI(K)=0
517  IRID(K)=0
      BETR(K)=0
530  BETA(K)=0
507  IFI(K)=0
      DO 508 K=1,20
508  JFST(K)=0
C
C      OBTAIN IDENTITY NUMBERS FOR FIXED INTENSITY SPECTRA
C
      IF (JNFI) 510,520,510
510  DO 511 K=1,JNFI
      DO 512 L=N,JN
      IF(ID(1,L)-ID1(1,K)) 512,514,512
514  IF(ID(2,L)-ID1(2,K)) 512,515,512
515  IFI(K)=L
      JFS(L)=0
512  CONTINUE
511  CONTINUE

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C      SUBTRACT OFF FIXED INTENSITY SPECTRA
C
      IF(JRC-1) 571,572,571
572  DO 573 K=KLOW,KHIGH
573  SPECT(K,1)=DATA(K)
      IF(JSUB) 574,571,574
574  JSUB1=JSUB+1
      DO 577 J=2,JSUB1
      DO 576 K=1,KHIGH
      SPECT(K,1)=SPECT(K,1)-RGINT(J)*SPECT(K,J)
576  CONTINUE
577  CONTINUE
571  DO 575 K=1,JNFI
      IFI(K)=IFI(K)
      FIXINK=FIXINT(K)
      DO 580 M=JX1,JX2
580  SPECT(M,1)=SPECT(M,1)-SPECT(M,IFI(K))*FIXINK
575  CONTINUE
C
C      OBTAIN IDENTITY NUMBERS FOR RELATED INTENSITY SPECTRA
C
520  IF (JNRI) 521,583,521
521  DO 524 K=1,JNRI
      DO 525 L=N,JN
      IF(ID(1,L)-ID2(1,K)) 525,528,525
528  IF(ID(2,L)-ID2(2,K)) 525,529,525
529  IRI(K)=L
525  CONTINUE
524  CONTINUE
C
C      COMBINE PAIRS OF RELATED INTENSITY SPECTRA
C
      MARX=0
      JNRI1 = JNRI - 1
540  DO 550 K=1,JNRI1,2
      N=IRI(K)
      N1=IRI(K+1)
      IF(FIXRT(K)-FIXRT(K+1))552,552,553
552  BETA(K+1)=FIXRT(K+1)/FIXRT(K)
      IF(MARX) 555,554,555
554  JFS(N1)=0
      IRID(K)=IRI(K)
555  DO 560 M=JX1,JX2
560  SPECT(M,N)=SPECT(M,N)+BETA(K+1)*SPECT(M,N1)
      GO TO 550
553  BETA(K)=FIXRT(K)/FIXRT(K+1)
      IF(MARX) 563,561,563
561  JFS(N)=0
      IRID(K+1)=IRI(K+1)
563  DO 564 M=JX1,JX2
564  SPECT(M,N1)=SPECT(M,N1)+BETA(K)*SPECT(M,N)
550  CONTINUE
C
C      CONDENSE STANDARD IDENTITY NUMBERS IN AREA JFS
C

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583 JINDX=1
584 L=1
DO 586 K=1,JN
IF (JFS(K)) 585,586,585
585 JFS(L)=JFS(K)
IF (L-K) 587,588,587
587 JFS(K)=0
588 L=L+1
586 CONTINUE
JSFTD=L-1
IF (JSFTD) 605,820,605
C
C      COMPUTE THE SIGMA FOR THE WEIGHTING FUNCTION
C
605 IF(JWT-1) 610,620,617
610 IF(JSUB) 611,615,611
611 JSUB1=JSUB+1
612 DO 614 K=KLOW,KHIGH
SIGMA(K)=0.0
DO 616 J=2,JSUB1
616 SIGMA(K)=SIGMA(K)+BGINT(J)*2.*SPECT(K,J)
SIGMA(K)=SIGMA(K)+DATA(K)
614 CONTINUE
GO TO 620
617 IF(JSUB) 621,620,621
621 JSUB1 = JSUB + 1
DO 622 K=KLOW,KHIGH
DO 623 J=2,JSUB1
623 SIGMA(K)=SIGMA(K)+BGINT(J)*2.0*SPECT(K,J)
622 CONTINUE
GO TO 620
615 DO 618 K=KLOW,KHIGH
618 SIGMA(K)=SIGMA(K)
C
C      CALCULATE MATRIX ELEMENTS FOR MATRIX INVERSE SUBROUTINE
C
620 DO 632 I=1,JSFTD
JFSI=JFS(I)
DO 635 J=1,JSFTD
JFSJ=JFS(J)
SUM=0.0
SUM1=0.0
DO 638 M=JX1,JX2
IF(JNCLO) 639,642,639
639 DO 640 L=1,JNCLO
IF(INCLO(L)-M) 640,638,640
640 CONTINUE
642 IF(JWT)645,643,645
643 SUM=SUM+(SPECT(M,JFSI)/SIGMA(M))*SPECT(M,JFSJ)
IF(J=JSFTD) 638,641,638
641 SUM1=SUM1+(SPECT(M,1)/SIGMA(M))*SPECT(M,JFSI)
GO TO 638
645 SUM=SUM+(SPECT(M,JFSI)/SIGMA(M))*SPECT(M,JFSJ)
IF(J=JSFTD) 638,644,638
644 SUM1=SUM1+(SPECT(M,1)/SIGMA(M))*SPECT(M,JFSI)
638 CONTINUE
D A(I,J)= 0.0

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```

D B(I,J)= 0.0
D C(I,J)= 0.0
A(I,J)=SUM
C(I,J)=SUM
B(I,1)=SUM1
635 CONTINUE
632 CONTINUE
C
C      SCALE THE MATRIX BEFORE INVERTING
DO 652 M=1,JSFTD
652 SCALE(M)=SQRT(A(M,M))
DO 655 I=1,JSFTD
B(I,1)=B(I,1)/SCALE(I)
DO 655 M=1,JSFTD
655 A(M,I)=A(M,I)/(SCALE(M)*SCALE(I))
D 680 CALL DMAINV (JSFTD,1)
C      RESTORE MATRIX INVERSION TO SCALE
DO 662 I=1,JSFTD
B(I,1)=B(I,1)/SCALE(I)
DO 662 M=1,JSFTD
662 A(M,I)=A(M,I)/(SCALE(I)*SCALE(M))
C
C      TEST FOR SINGULAR MATRIX
C
C      IF (IFS) 820,805,820
C
C      OUTPUT OF FITTING PROGRAM RESULTS
C
820 WRITE OUTPUT TAPE 6,822
822 FORMAT(51H0 RESULTS FOR SPECTRA USED IN FITTING SUBROUTINE)
WRITE OUTPUT TAPE 6,823
823 FORMAT (69H0 SPECTRA IDENTITY INTENSITY STA
INRDARD DEVIATION)
824 WRITE OUTPUT TAPE 6,826,ID(1,1),ID(2,1)
826 FORMAT (23H0 COMPOSITE ,I4,I4)
C
C      OBTAIN THE SUM OF THE SQUARED RESIDUALS
C
R=0.0
SUM=0.0
DO 830 M=JX1,JX2
IF (JNCLO) 825,828,825
825 DO 827 L=1,JNCLO
IF (INCLO(L)-M) 827,830,827
827 CONTINUE
828 DO 829 I=1,JSFTD
JFSI=JFS(I)
SUM=SUM+(SPECT(M,JFSI)*B(I,1))
829 CONTINUE
SUM1=(SPECT(M,1)-SUM)*2
SUM=0.0
IF (JWT) 831,832,831
831 R=R+(SUM1/SIGMA(M))
GO TO 830
832 R=R+(SUM1/SIGMA(M))
830 CONTINUE
IDOF=(JX2-JX1-JNCLO-JSFTD)

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DOF=IDOF
ZERO=0.0
C
840 IF (JSUB) 841,845,841
841 DO 842 J=2,JSUB1
842 WRITE OUTPUT TAPE 6,843,ID(1,J),ID(2,J),BGINT(J),ZERO
843 FORMAT (18H0 BACKGROUND,5X,I4,I4,6X,F11.8,6X,F10.8)
C
C WRITE OUT INDEX FOR FIXED INTENSITY SPECTRA
C
845 IF (JNFI) 847,850,847
847 DO 848 J=1,JNFI
848 WRITE OUTPUT TAPE 6,849,ID(1,J),ID(2,J),FIXINT(J),ZERO
849 FORMAT (18H0 FIXED INT.,5X,I4,I4,6X,F11.8,6X,F10.8)
C
C WRITE OUT INDEX FOR RELATED INTENSITY SPECTRA
C
C
850 IF (JNRI) 851,885,851
851 DO 860 K=1,JNRI1,2
IRIK=IRI(K)
IRIK1=IRI(K+1)
L=(K+1)/2
IF (IRI(K)-IRID(K)) 852,854,852
854 DO 856 M=JX1,JX2
856 SPECT(M,IRIK)=SPECT(M,IRIK)-SPECT(M,IRIK1)*BETA(K+1)
BETA(K)=B(L,1)
BETA(K+1)=BETA(K)*BETA(K+1)
GO TO 860
852 DO 858 M=JX1,JX2
858 SPECT(M,IRIK1)=SPECT(M,IRIK1)-SPECT(M,IRIK)*BETA(K)
BETA(K+1)=B(L,1)
BETA(K)=BETA(K+1)*BETA(K)
860 CONTINUE
C
C CALCULATE THE DEVIATIONS FOR RELATED SPECTRA
C
ISUB = 1
DO 870 K=1,JNRI1,2
IF (BETA(K)-BETA(K+1)) 868,868,372
868 BETR(K)=SQRTF((R/DOF)*ABSF(A(ISUB,ISUB)))
BETR(K+1)=BETR(K) * (BETA(K+1)/BETA(K))
GO TO 869
872 BETR(K+1)=SQRTF((R/DOF)*ABSF(A(1*UB,ISUB)))
BETR(K)= BETR(K+1)* (BETA(K)/BETA(K+1))
869 ISUB =ISUB + 1
870 CONTINUE
C
DO 873 K=1,JNRI
873 WRITE OUTPUT TAPE 6,875,ID2(1,K),ID2(2,K),BETA(K),BETR(K)
875 FORMAT (20H0 RELATED INT.,5X,I4,I4,6X,F12.8,6X,F10.8)
C
C WRITE OUT INDEX FOR ALL OTHER STANDARDS USED IN FIT
C
DO 876 K=1,JSFTD
DO 877 M=1,JNRI
IF (IRI(M)-JFS(K)) 877,876,877

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877 CONTINUE
JFSK=JFS(K)
RDOF=SQRTF((R/DOF)*ABSF(A(K,K)))
880 WRITE OUTPUT TAPE 6,890,ID(1,JFSK),ID(2,JFSK),B(K,1),RDOF
876 CONTINUE
882 FORMAT (18H0 STANDARD ,5X,I4,I4,5X,F12.8,6X,F10.8)
GO TO 883
885 DO 887 K=1,JSFTD
JFSK=JFS(K)
RDOF=SQRTF((R/DOF)*ABSF(A(K,K)))
887 WRITE OUTPUT TAPE 6,890,ID(1,JFSK),ID(2,JFSK),B(K,1),RDOF
890 FORMAT (18H0 STANDARD ,5X,I4,I4,6X,F11.8,6X,F10.8)
883 WRITE OUTPUT TAPE 6,881,R
881 FORMAT(39H0 CHI-SQUARED = ,F14.8)
WRITE OUTPUT TAPE 6,884,IDOF
884 FORMAT(37H0 DEGREES OF FREEDOM = ,I3)
QOFN = R/DOF
WRITE OUTPUT TAPE 6,886,QOFN
886 FORMAT(34H0 QUALITY OF FIT NUMBER =,F10.3)
C
WRITE OUTPUT TAPE 6,888
888 FORMAT(1H0)
IF (JMT-1) 891,906,891
891 WRITE OUTPUT TAPE 6,892
892 FORMAT(80H0 WEIGHTED FIT - QUALITY OF FIT NUMBER SHO
IULD BE APPROXIMATELY 1.0)
IF (QOFN-25.0) 894,894,893
893 WRITE OUTPUT TAPE 6,895
895 FORMAT(63H0 QUALITY OF FIT NUMBER INDICATES A VERY P
OOR FIT.)
GO TO 907
894 IF (QOFN-5.0) 897,897,896
896 WRITE OUTPUT TAPE 6,898
898 FORMAT(58H0 QUALITY OF FIT NUMBER INDICATES A POOR F
IT.)
897 IF (QOFN-1.2) 902,907,907
900 WRITE OUTPUT TAPE 6,901
901 FORMAT(58H0 QUALITY OF FIT NUMBER INDICATES A GOOD F
IT.)
GO TO 907
902 IF (QOFN-0.7) 899,899,900
899 IF (QOFN-0.1) 903,907,907
903 WRITE OUTPUT TAPE 6,904
904 FORMAT(42H0 SIGMA VALUES ARE TOO LARGE.)
GO TO 907
906 WRITE OUTPUT TAPE 6,909
909 FORMAT (91H0 UNWEIGHTED FIT - CHI SQUARED AND QUALIT
Y OF FIT NUMBER HAVE NO SIGNIFICANCE.)
C
C TEST FOR NEGATIVE INTENSITIES AND OBTAIN IDENTITY
C NUMBERS FOR NEGATIVE OR ZERO INTENSITIES
907 IF (JOPT1) 950,950,908
908 L=JINDX
DO 920 I=1,JSFTD
IF (B(I,1)) 922,922,920
922 JFST(I)=JFS(I)
JFS(I)=0

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```

L=L+1
920 CONTINUE
IF (L-JNDX) 926,950,926
926 L=L-1
JNDX=L
JSFTD=JSFTD-JNDX
KFLAG=0
IF(JNRI) 927,944,927
927 JTAB=JNRI
DO 930 K=1,L
DO 929 J=1,JNRI
IF (JFST(K)-IRI(J)) 929,928,929
928 KFLAG=KFLAG+1
IRI(J)=0
929 CONTINUE
930 CONTINUE
IF(KFLAG) 932,941,932
932 JNRI=JNRI-2
KFLAG=KFLAG-1
IF (KFLAG) 932,933,932
933 DO 938 K=1,JTAB,2
IF (IRI(K)) 935,936,935
935 IF (IRI(K+1)) 938,936,938
936 IRI(K)=0
IRI(K+1)=0
938 CONTINUE
M=1
DO 940 J=1,JTAB
IF (IRI(J)) 942,943,942
942 IRI(M)=IRI(J)
IRID(M)=IRID(J)
FIXRT(M)=FIXRT(J)
BETA(M)=BETA(J)
M=M+1
940 CONTINUE
941 CALL PAGE(IPAGE)
WRITE OUTPUT TAPE 6,946
946 FORMAT(58H0 PROBLEM RECYCLE ELIMINATES NEGATIVE INTENSITY SPEC
1TRA)
MARX=1
GO TO 540
944 CALL PAGE(IPAGE)
WRITE OUTPUT TAPE 6,946
GO TO 583
950 CALL PRINT
GO TO 500
905 WRITE OUTPUT TAPE 6,910
910 FORMAT(45H0MATRIX IS SINGULAR, NO SOLUTION IS POSSIBLE.)
960 FORMAT(15H0 ,11A6)
970 GO TO 500
END

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SUBROUTINE INPUT
C
C DATA INPJT ROUTINE FOR PARAMETERS AND SPECTRA
C
1 DIMENSION SPECT(400,26),SIGMA(400),SIGMAS(400),ID(2,26),
2 ISPLTS(2,26),IPPLTS(2,26),JFS(26),ID1(2,10),ID2(2,10),
3 JFST(20),RSDL(20),INCLO(20),TITLE(11),FIXINT(10),FIXRT(10),
4 IFI(10),IRI(10),IRID(10),BETA(10),BETR(10),BGINT(6)
D DIMENSION A(20,20),B(20,20),C(20,20),DATA(400),DET(1)
COMMON SPECT,SIGMA,SIGMAS,ID,ISPLTS,IPPLTS,JFS,ID1,ID2,JFST,
1 RSDL,INCLO,TITLE,FIXINT,FIXRT,IFI,IRI,IRID,BETA,BETR,
2 BGINT,A,B,C,DATA,DET,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,
3 JNCLO,JWT,JOPT1,JOPT2,JRC,IMAGE,IFS,KLOW,KHIGH
ODIMENSION ISIGMA(10),IDATA(10),IPAT(2,10),SSIGMA(10),DAT(10)
C
READ INPUT TAPE 5,3,ICTYP,(TITLE(I),I=1,11)
CALL PAGE(IPAGE)
3 FORMAT(13,3X,11A6)
WRITE OUTPUT TAPE 6,100,(TITLE(I),I=1,11)
100 FORMAT(15H0 ,11A6)
WRITE OUTPUT TAPE 6,184
184 FORMAT(32H0 PROBLEM CONTROL PARAMETERS)
4 READ INPUT TAPE 5-110,ICTYP,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,JNCLO,
1 JWT,JOPT1,JOPT2,JRC
110 FORMAT(13,7X,2(13-2X),6(12,3X),4(11,4X))
DO 103 J=1,2
DO 103 K=1,10
ID1(J,K)=0
103 ID2(J,K)=0
DO 104 J=1,2
DO 104 K=1,26
104 ID(J,K)=0
READ INPUT TAPE 5,120,ICTYP,ID3,ID4
120 FORMAT(13,7X,214)
8 WRITE OUTPUT TAPE 6,102,ID3,ID4
102 FORMAT(51H0 COMPOSITE SPECTRUM IDENTIFICATION - 214)
ID(1,1)=ID3
ID(2,1)=ID4
JVBP=JN-JSUB-JNFI-(JNRI/2)-1
7 WRITE OUTPUT TAPE 6,101,JX1,JX2,JN,JSUB,JNFI,JNRI,JVBP
101 FORMAT(44H0 FITTING LIMITS IN CHANNEL NUMBER//
1 27H A. LOWER - 13//
2 27H B. UPPER - 13//
3 43H NUMBER OF SPECTRA IN PROBLEM - 12//
4 43H A. BACKGROUND - 12//
5 43H B. FIXED INTENSITY - 12//
6 43H C. FIXED RATIO - 12//
7 43H D. VARIABLE PARAMETERS - 12)
IF(JWT-1) 301,303,305
301 WRITE OUTPUT TAPE 5,302
302 FORMAT(28H0 WEIGHTED BY 1/Y)
GO TO 308
303 WRITE OUTPUT TAPE 5,304
304 FORMAT(31H0 FIT IS NOT WEIGHTED)
GO TO 309
305 WRITE OUTPUT TAPE 5,306
306 FORMAT(38H0 WEIGHTED BY VALUES READ IN)

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308 WRITE OUTPUT TAPE 6,307
307 FORMAT(32H3          CONTROL CARD LISTING)
   WRITE OUTPUT TAPE 6,310,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,JNCLO,
1   JMT,JOPT1,JOPT2,JRC
310 FORMAT(4H0110,7X,2(I3,2X),6(I2,3X),4(I1,4X))
   WRITE OUTPUT TAPE 6,320,ICTYP,ID3,ID4
320 FORMAT(1H ,I3,7X,2I4)
   IF(JSUB)9,11,9
9   K=JSUB+1
   READ INPUT TAPE 5,130,ICTYP,((ID(I,J),I=1,2),J=2,K)
   FORMAT(I3,7X,6(2I4,2X))
   WRITE OUTPUT TAPE 6,330,ICTYP,((ID(I,J),I=1,2),J=2,K)
330 FORMAT(1H ,I3,7X,6(2I4,2X))
   READ INPUT TAPE 5,131,ICTYP,(BGINT(I),I=2,K)
331 FORMAT(I3,7X,6(F8.6,2X))
   WRITE OUTPUT TAPE 6,331,ICTYP,(BGINT(I),I=2,K)
331 FORMAT(1H ,I3,7X,6(F8.6,2X))
C
C      READ STANDARD IDENTIFICATION
C
11  K=JSUB+2
   L=JNST+K-1
   K1=K
   GO TO 12
14  K1=K1+6
12  K2=K1+5
   IF(K2-L)13,13,15
15  K2=L
13  READ INPUT TAPE 5,130,ICTYP,((ID(I,J),I=1,2),J=K1,K2)
   WRITE OUTPUT TAPE 6,330,ICTYP,((ID(I,J),I=1,2),J=K1,K2)
16  IF(K2-L)14,17,14
17  IF(JNFI)18,19,18
18  L=JNFI
   K=1
   K1=K
   GO TO 20
21  K1=K1+6
20  K2=K1+5
   IF(K2-L)22,22,23
23  K2=L
22  READ INPUT TAPE 5,130,ICTYP,((ID1(I,J),I=1,2),J=K1,K2)
   WRITE OUTPUT TAPE 6,330,ICTYP,((ID1(I,J),I=1,2),J=K1,K2)
24  IF(K2-L)21,25,21
25  L=JNFI
   K=1
   K1=K
   GO TO 26
27  K1=K1+6
26  K2=K1+5
   IF(K2-L)28,28,29
29  K2=L
28  READ INPUT TAPE 5,131,ICTYP,(FIXINT(I),I=K1,K2)
   WRITE OUTPUT TAPE 5,331,ICTYP,(FIXINT(I),I=K1,K2)
30  IF(K2-L)27,19,27
19  IF(JNRI)31,44,31
31  L=JNRI
   K=1

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```

K1=K
GO TO 32
33  K1=K1+6
32  K2=K1+5
   IF(K2-L)34,34,35
35  K2=L
34  READ INPUT TAPE 5,130,ICTYP,((ID2(I,J),I=1,2),J=K1,K2)
   WRITE OUTPUT TAPE 6,330,ICTYP,((ID2(I,J),I=1,2),J=K1,K2)
36  IF(K2-L)33,37,33
37  L=JNRI
   K=1
   K1=K
   GO TO 39
40  K1=K1+6
39  K2=K1+5
   IF(K2-L)41,41,42
42  K2=L
41  READ INPUT TAPE 5,131,ICTYP,(FIXRT(I),I=K1,K2)
   WRITE OUTPUT TAPE 6,331,ICTYP,(FIXRT(I),I=K1,K2)
43  IF(K2-L)40,44,40
44  IF(JNCLO)45,46,45
45  IF(JNCLO-10) 47,47,49
47  READ INPUT TAPE 5,170,ICTYP,((INCLO(I),I=1,JNCLO)
   WRITE OUTPUT TAPE 6,370,ICTYP,((INCLO(I),I=1,JNCLO)
   GO TO 46
49  READ INPUT TAPE 5,170,ICTYP,((INCLO(I),I=1,10)
   READ INPUT TAPE 5,170,ICTYP,((INCLO(I),I=11,JNCLO)
   WRITE OUTPUT TAPE 6,370,ICTYP,((INCLO(I),I=1,10)
   WRITE OUTPUT TAPE 6,370,ICTYP,((INCLO(I),I=11,JNCLO)
170 FORMAT(I3,7X,10(I3,2X))
370 FORMAT(1H ,I3,7X,10(I3,2X))
46  IF(JWT-1)50,51,52
52  NCDS=0
58  READ INPUT TAPE 5,190,IC,(SSIGMA(J),J=1,10)
   IF(IC-50) 53,50,53
53  IF(NCDS) 55,56,55
56  DO 57 I=1,9
57  SIGMA(I)=SSIGMA(I+1)
   NCDS=NCDS+1
   GO TO 58
55  DO 60 J=1,10
   JS=10*NCDS-I+J
60  SIGMA(JS)=SSIGMA(J)
   NCDS=NCDS+1
   GO TO 58
51  DO 62 J=1,400
62  SIGMA(J)=1.0
50  ITEST=0
   IF(JRC-1) 54,315,54
315 WRITE OUTPUT TAPE 6,316
316 FORMAT(38H      PROBLEM RECYCLES ON PREVIOUS DATA)
   READ INPUT TAPE 5,120,ICTYP
   RETURN
54  DO 63 L=1,JN
   READ INPUT TAPE 5,180,ICTYP,ID7,ID8,ISPILL,ISPUL,IPPLL,IPPUL,IGCTL
180 FORMAT(I3,7X,2I4,4(I2X,I3),2X,I1)
   WRITE OUTPUT TAPE 6,380,ICTYP,ID7,ID8,ISPILL,ISPUL,IPPLL,IPPUL,

```

```

1 IGCTL
380 FORMAT(1H ,13,7X,214,4(2X,13),2X,11)
      IF(IGCTL) 350,64,350
350 READ INPUT TAPE 5,181,ICTYP,TRUE,AS,AL,BL,RATIO
181 FORMAT(13,7X,F8.3,2X,F8.4,2X,2F10.4,F10.6)
      WRITE OUTPUT TAPE 6,381,ICTYP,TRUE,AS,AL,BL,RATIO
381 FORMAT(1H ,13,7X,F8.3,2X,F8.4,2X,2F10.4,F10.6)

      READ DATA

64 NCDS=0
78 READ INPUT TAPE 5,190,IC,(DAT(I),I=1,10),AD1,AD2
190 FORMAT(12,10F7.0,2A4)
      IF(IC=50) 69,311,69
69 IF(NCDS)71,72,71
72 DO 73 K=1,9
73 DATA(K)=DAT(K+1)
      NCDS=NCDS+1
      GO TO 78
71 DO 79 J=1,10
      JS=10*NCDS-1+J
79 DATA(JS)= DAT(J)
      NCDS=NCDS+1
      GO TO 78

      CHECK DATA FOR CONSISTANCY

311 IF(IGCTL) 70,70,312
312 CALL GSHIFT(ISPUL,IPPLL,IPPUL,TRUE,AS,AL,BL,RATIO)
      WRITE OUTPUT TAPE 6,394
394 FORMAT(41H LISTING OF GAIN SHIFTED SPECTRA)
      WRITE OUTPUT TAPE 6,392
392 FORMAT(1H 6X1H06X1H16X1H26X1H36X1H46X1H56X1H66X1H76X1H86X1H9)
      JS=0
      NCDS=0
84 DO 85 I=1,10
85 DAT(I)=0.0
      IF (NCDS) 86,87,86
87 DO 89 I=1,9
89 DAT(I+1)=DATA(I)+0.5
95 WRITE OUTPUT TAPE 6,390,NCDS,(DAT(I),I=1,10),ID7,ID8
      IF(JS=ISPUL) 92,70,70
86 DO 94 I=1,10
      JS=10*NCDS-1+I
94 DAT(I)=DATA(JS)+0.5
      GO TO 95
92 NCDS=NCDS+1
      GO TO 84
390 FORMAT(1H ,12,10F7.0,2X,214)
70 DO 210 K=1,ISPUL
      IF (DATA(K)) 202,202,210
202 DATA(K)=1.0
210 CONTINUE

```

```

C
C
C
      STORE DATA
DO 80 M=1,JN

```

```

      IF(ID7-ID(1,M)) 80,82,80
82 IF(ID8-ID(2,M)) 80,83,80
83 MARK=M
      GO TO 203
80 CONTINUE
203 DO 206 K=1,ISPUL
206 SPECT(K,MARK)=DATA(K)
      ISPLTS(1,MARK)=ISPUL
      ISPLTS(2,MARK)=ISPUL
      ISPUL=ISPUL+1
      DO 239 K=ISPUL,400
239 SPECT(K,MARK)=0.0
      IF(JRC-1) 63,63,75
63 CONTINUE
75 READ INPUT TAPE 5,120,ICTYP

      PRESERVE ORIGINAL SPECTRA IN AREA (DATA)

      KLOW=ISPLTS (1,1)
      XHIGH=ISPLTS (2,1)
      DO 249 K=KLOW,KHIGH
249 DATA(K)=SPECT(K,1)

      SUBTRACT BACKGROUND SPECTRA

      IF (JSUB) 213,154,213
213 JSUB1=JSUB+1
      DO 216 J=2,JSUB1
      DO 217 K=1,KHIGH
      SPECT(K,1)=SPECT K,1)-BGINT(J)*SPECT(K,J)
217 CONTINUE
216 CONTINUE
154 IF (JWT) 155,88,155
88 DO 90 K=1,KHIGH
90 SIGMA(K)=SPECT(K,1)
      GO TO 156
155 DO 153 K=1,KHIGH
153 SIGMA(K)=SPECT(K,1)
156 RETURN
      END

```

```

SUBROUTINE PRINT
  DIMENSION SPECT(400,26),SIGMA(400),SIGMAS(400),ID(2,26),
1    ISPLTS(2,26),IPPLTS(2,26),JFS(26),ID1(2,101),ID2(2,101),
2    JFST(20),RSDL(20),INCLO(20),TITLE(11),FIXINT(10),FIXRT(10),
3    IFI(10),IRI(10),IRID(10),BETA(10),BETR(10),BGINT(6)
D  DIMENSION A(20,20),B(20,20),C(20,20),DATA(400),DET(1)
COMMON SPECT,SIGMA,SIGMAS,ID,ISPLTS,IPPLTS,JFS,ID1,ID2,JFST,
1    RSDL,INCLO,TITLE,FIXINT,FXPT,IFI,IRI,IRID,BETA,BETR,
2    BGINF,A,B,C,DATA,DET,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,
3    JNCLO,JWT,JOPT1,JOPT2,JRC,I*PAGE,IFS,KLOW,KHIGH
CALL PAGE(IPAGE)

C  WRITE OUTPUT TAPE 6,114,(TITLE(I),I=1,11)
  WRITE OUTPUT TAPE 6,4
4  FORMAT(109H0CHAN.      Y      SIGMA      Y-BKG
1  YCALC.      SIGMA Y-BKG      RESIDUAL      R/SG.Y-BKG)

C  ILOW=ISPLTS(1,1)
  IHIGH=ISPLTS(2,1)
  ITEST = 51
  DO 50 K=ILOW,IHIGH
    IF (K-ITEST) 1,46,1
46  CALL PAGE(IPAGE)
    ITEST = ITEST + 50
    WRITE OUTPUT TAPE 6,4
    1  IF (K-JX1) 5,2,5
    2  WRITE OUTPUT TAPE 6,3
    3  FORMAT(46H          FIT OF DATA BEGINS WITH THE NEXT CHANNEL)
    5  IF (K-(JX2+1)) 9,6,9
    6  WRITE OUTPUT TAPE 6,7
    7  FORMAT(50H          FIT OF DATA END* WITH THE PRECEEDING CHANNEL)
    9  IF (JNCLO) 10,15,10
10  DO 14 M=1,JNCLO
    IF (INCLO(M)-K) 14,11,14
11  WRITE OUTPUT TAPE 6,12
12  FORMAT(48H          THE NEXT CHANNEL WAS OMITTED FROM THE FIT)
14  CONTINUE
15  YI=DATA(K)
    SIGYI=SQRTF(YI)
    IF (JWT) 16,18,16
16  YISTR=SIGMAS(K)
    SYISTR=ABSF(SQRTF(SIGMA(K)))
    GO TO 20
18  YISTR=SIGMA(K)
    SYISTR=ABSF(SQRTF(SIGMAS(K)))

C  CALCULATE YBAR
C
C  20 YBAR=0.0
    IF (JNRI) 21,28,21
    21 DO 22 L=1,JNRI
      IRIK=IRI(L)
    22 YBAR=YBAR+SPECT(K,IRIK)*BETA(L)
    IF ((JNRI/2)-JSFTD) 24,32,24
    24 DO 25 I=1,JSFTD
      DO 26 M=1,JNRI
        IF (IRI(M)-JFS(I)) 26,25,26

```

```

26 CONTINUE
  JFSK=JFS(I)
  YBAR=YBAR+SPECT(K,JFSK)*B(I,1)
25 CONTINUE
  GO TO 32
28 DO 30 I=1,JSFTD
  JFSI=JFS(I)
  YBAR=YBAR+SPECT(K,JFSI)*B(I,1)
30 CONTINUE
32 IF (JNFI) 33,35,33
33 DO 34 J=1,JNFI
  IFIK=IFI(J)
34 YBAR=YBAR+SPECT(K,IFIK)*FIXINT(J)
35 RES=YISTR-YBAR
  IF (SYISTR) 36,38,36
36 QUAN=RES/SYISTR

C  37 WRITE OUTPUT TAPE 6,39,K,YI,SIGYI,YISTR,YBAR,SYISTR,RES,QUAN
39 FORMAT(2X,13,5X,F11.2,5X,F9.3,4X,F11.2,4X,F11.2,4X,F9.3,4X,F13.4,
14X,F9.3)
  GO TO 50
38 WRITE OUTPUT TAPE 6,40,K,YI,SIGYI,YISTR,YBAR,SYISTR,RES
40 FORMAT(2X,13,5X,F11.2,5X,F9.3,4X,F11.2,4X,F11.2,4X,F9.3,4X,F13.4,
14X,5HBLANK)
50 CONTINUE
  IF (IHIGH-JX2) 43,47,43
47 WRITE OUTPUT TAPE 6,7
43 IF (JOPT2-1) 42,51,51
42 WRITE OUTPUT TAPE 6,45
45 FORMAT(46H0 OPTION FOR RESIDUALS PRINTOUT NOT SPECIFIED//
1 32H0          END OF PROBLEM)
  RETURN

C  PRINT OUT THE RESIDUALS OF THE FIT.
C
C  51 CALL PAGE(IPAGE)
  WRITE OUTPUT TAPE 6,114,(TITLE(I),I=1,11)
  WRITE OUTPUT TAPE 6,52
52 FORMAT(52H0 RESIDUALS OF THE FIT IN ORDER OF RESULT LISTING//
166H CHAN.      Y-BKG.      YCALC.      ALL RESIDUALS OF THE
FIT)
  ITEST = 51
  DO 100 K=ILOW,IHIGH
    IF (K-ITEST) 56,115,56
115 CALL PAGE(IPAGE)
    ITEST = ITEST + 50
    WRITE OUTPUT TAPE 6,52
    56 IF (JWT) 53,54,53
    53 YISTR=SIGMAS(K)
    GO TO 55
    54 YISTR=SIGMA(K)
    55 YBAR=0.0
    IF (JNRI) 61,68,61
    61 DO 62 L=1,JNRI
      IRIK=IRI(L)
    62 YBAR=YBAR+SPECT(K,IRIK)*BETA(L)
    IF ((JNRI/2)-JSFTD) 64,72,64

```

```

64 DO 65 I=1,JSFTD
DO 66 M=1,JNRI
IF (IRI(M)-JFS(I)) 66,65,66
66 CONTINUE
JFSK=JFS(I)
YBAR=YBAR+SPECT(K,JFSK)*B(I,1)
65 CONTINUE
GO TO 72
68 DO 70 J=1,JSFTD
JFSK=JFS(J)
70 YBAR=YBAR+SPECT(K,JFSK)*B(J,1)
72 IF (JNFI) 73,77,73
73 DO 74 J=1,JNFI
IFIK=IFI(J)
74 YBAR=YBAR+SPECT(K,IFIK)*FIXINT(2)
77 DEC=0.0
DO 76 M=1,20
76 RSOL(M)=0.0
M=J
IF (JNFI) 75,80,75
75 DO 78 M=1,JNFI
IFIK=IFI(M)
DEC=DEC+SPECT(K,IFIK)*FIXINT(M)
78 RSOL(M)=YISTR-DEC
M=JNFI
80 IF (JNRI) 79,85,79
DO 81 I=1,JNRI
IRIK=IRI(I)
DEC=DEC+SPECT(K,IRIK)*BETA(I)
MI=M+I
81 RSOL(MI)=YISTR-DEC
M=M+JNRI
IF ((JNRI/2)-JSFTD) 82,90,82
82 JNRI21=(JNRI/2)+1
ISUB = M - (JNRI/2)
DO 84 L=JNRI21,JSFTD
JFSK=JFS(L)
DEC=DEC+SPECT(K,JFSK)*B(L,1)
ISUBL=ISUB+L
84 RSOL(ISUBL)=YISTR-DEC
M=M+JSFTD-(JNRI/2)
GO TO 90
85 IF (JSFTD) 86,90,86
DO 88 J=1,JSFTD
JFSK=JFS(J)
DEC=DEC+SPECT(K,JFSK)*B(J,1)
MJ=M+J
88 RSOL(MJ)=YISTR-DEC
M=M+JSFTD
90 WRITE OUTPUT TAPE 6,92,M,YISTR,YBAR,(RSOL(L),L=1,7)
92 FORMAT(3X,13,6X,5F12.2)
IF(M-7) 100,100,94
94 WRITE OUTPUT TAPE 6,96,(RSOL(L),L=8,14)
96 FORMAT(36H ,7F12.2)
IF(M-14) 100,100,98
98 WRITE OUTPUT TAPE 6,99,(RSOL(L),L=15,21)
99 FORMAT(36H ,7F12.2)

```

```

100 CONTINUE
IF(JOPT2-2) 104,103,103
104 WRITE OUTPUT TAPE 6,116
116 FORMAT(54H0 END OF PROBLEM
GO TO 102

```

```

C
C
C      MATRIX MULTIPLY ROUTINE FOR MATRIX CHECKING
103 CALL PAGE(IPAGE)
WRITE OUTPUT TAPE 6,114,(TITLE(I),I=1,11)
105 WRITE OUTPUT TAPE 6,107
107 FORMAT (42H0 ELEMENTS OF THE MATRIX PRODUCT,A X A-1.)
DO 109 I=1,JSFTD
DO 109 J=1,JSFTD
108 B(I,J)=0.0
DO 109 K=1,JSFTD
109 B(I,J)=B(I,J)+A(I,K)*C(K,J)
IF(JSFTD-10) 110,110,113
110 K=1
111 WRITE OUTPUT TAPE 6,112,(B(K,I),I=1,JSFTD)
K=K+1
IF(K-JSFTD-1) 111,102,102
113 K=1
106 WRITE OUTPUT TAPE 6,112,(B(K,I),I=1,10)
WRITE OUTPUT TAPE 6,112,(B(K,I),I=11,JSFTD)
K=K+1
IF(K-JSFTD-1) 106,117,117
117 WRITE OUTPUT TAPE 6,116
112 FORMAT(2H0 ,F10.7,9(2X,F10.7))
114 FORMAT(15H0 ,11A6)
102 RETURN
END
C
C
C      OUTPUT SUBROUTINE FOR NUMBERING PAGES

```

မ

```

SUBROUTINE DMAINV(M,N)
C      DOUBLE PRECISION DOUBLE PIVOTAL MATRIX INVERSION SUBROUTINE
C      D.H. GIPSON      PHILLIPS PETROLEUM CO.      JUNE, 1962
C
C
C

```

```

1 DIMENSION SPECT(400,26),SIGMA(400),SIGMAS(400),ID(2,26),
2 ISPLTS(2,26),IPLPTS(2,26),JFS(26),ID1(2,10),ID2(2,10),
3 JFST(10),RSDL(20),INCLD(20),TITLE(11),FIXINT(10),FIXRT(10),
4 IFI(10),IRI(10),IRID(10),BETA(10),BETR(10),BGINT(6)
D DIMENSION A(20,20),B(20,20),C(20,20),DATA(400),DET(1)
COMMON SPECT,SIGMA,SIGMAS,ISPLTS,IPLPTS,JFS,ID1,ID2,JFST,
1 RSDL,INCLD,TITLE,FIXINT,FXPT,IFI,IRI,IRID,BETA,BETR,
2 BGINT,A,B,C,DATA,DET,JX1,JX2,JN,JSUB,JNF1,JNR1,JNST,
3 JNCLD,JWT,JOPT1,JOPT2,JRC,1*AGE,IFS,KLOW,KHIGH
DIMENSION IROW(20),JCOL(20)

```

```

C
C
C      INITIALIZATION
C
C      1 DO 2 I=1,M
C        IROW(I)=0
C      2 JCOL(I)=0
C      DET=1.0
C      IFS=1
C      DO 23 K=1,M

```

```

C
C      FIND THE PIVOT ELEMENT
C
D 3  PIVOT= 0.
   DO 8 J=1,M
   IF(JCOL(J))8,4,8
4  DO 7 I=1,M
   IF(IROW(I))7,5,7
D 5  X=ABSF(A(I,J))
D   IF(X-PIVOT) 7,6,6
D 6  PIVOT=X
   JP=J
   IP=I
7  CONTINUE
8  CONTINUE

```

```

C          TEST TO SEE IF MATRIX IS SINGULAR                                PART (2)
C
C          PIVOT=A(IP,JP)
D          DET=DET*PIVOT
D          IF(PIVOT) 10,9,10
D          9  IFS=0
D          RETURN

```

```

C
C      REMEMBER LOCATION OF THE PIVOT ELEMENT
C
C      PART (2)
10  IROW(IP)=JP
    JCOL(JP)=IP

```

[illegible]


```

      DO 12 I=1,M
      IF(I-IP)11,12,11
D 11  A(I,JP)=-A(I,JP)/PIVOT
      12 CONTINUE

```

```

C      ARITHMETIC OPERATIONS ON OTHER COLUMNS OF (A)      PART (4)
C

```

```

      DO 17 J=1,M
      IF(J-JP)13,17,13
D 13  IF(A(IP,J)) 14,17,14
D 14  ALPHA=A(IP,J)
      A(IP,J)=ALPHA/PIVOT
      DO 16 I=1,M
      IF(I-IP)15,16,15
D 15  A(I,J)=A(I,J)+ALPHA*A(I,JP)
      16 CONTINUE
      17 CONTINUE

```

```

C      ARITHMETIC OPERATIONS ON THE COLUMNS OF (B)      PART (4)
C

```

```

      IF(N)18,23,18
      DO 22 J=1,N
      IF(B(IP,J)) 19,22,19
D 19  ALPHA=B(IP,J)
      B(IP,J)=ALPHA/PIVOT
      DO 21 I=1,M
      IF(I-IP)20,21,20
D 20  B(I,J)=B(I,J)+ALPHA*B(I,JP)
      21 CONTINUE
      22 CONTINUE
      23 CONTINUE

```

```

C      ROW PERMUTATIONS      PART (5)
C

```

```

      DO 30 K=1,M
      I=IROW(K)
      IF(I-K)25,30,25
D 25  DET=-DET
      DO 26 J=1,M
      TEMP=A(I,J)
      A(I,J)=A(K,J)
D 26  A(K,J)=TEMP
      IF(N)27,29,27
      DO 28 J=1,N
      TEMP=B(I,J)
      B(I,J)=B(K,J)
D 28  B(K,J)=TEMP
      IROW(K)=IROW(I)
      IROW(I)=I
      GO TO 24
      30 CONTINUE

```

```

C      COLUMN PERMUTATIONS      PART (6)
C

```

```

      DO 34 K=1,M
      J=JCOL(K)
      IF(J-K)32,34,32

```

```

      32 DO 33 I=1,M
      TEMP=A(I,J)
      A(I,J)=A(I,K)
D 33  A(I,K)=TEMP
      JCOL(K)=JCOL(J)
      JCOL(J)=J
      GO TO 31
      34 CONTINUE
      RETURN
      END

```

```

SUBROUTINE GSHIFT(ISPUL,IPPLL,IPPUL,TRUE,AS,AL,BL,RATIO)
  C      GAIN SHIFT SUBROUTINE
  C      G.A.CAZIER PHILLIPS PETROLEUM CO.  NOVEMBER 1962
  C
  DIMENSION SPECT(400,26),SIGMA(400),SIGMAS(400),ID(2,26),
1  ISPLTS(2,26),IPPLTS(2,26),JFS(26),ID1(2,10),ID2(2,10),
2  JFST(20),RSDL(20),INCLO(20),TITLE(11),FIXINT(10),FIXRT(10),
3  IFI(10),IRI(10),IRID(10),BETA(10),BETR(10),BGINT(6)
  D  DIMENSION A(20,20),B(20,20),C(20,20),DATA(400),DET(1)
  COMMON SPECT,SIGMA,SIGMAS,ID,ISPLTS,IPPLTS,JFS,ID1,ID2,JFST,
1  RSDL,INCLO,TITLE,FIXINT,FIXRT,IFI,IRI,IRID,BETA,BETR,
2  BGINT,A,B,C,DATA,DET,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,
3  JNCLO,JWT,JOPT1,JOPT2,JRC,IPAGE,IFS,KLOW,KHIGH
  D  DIMENSION C2(400)
  C
  C      INITIALIZATION
  C
  IF(RATIO)307,306,307
  D 306 W=100.0*DATA(IPPLL)*.2
  DO 308 J=1,3
  DO 308 I=1,3
  D 308 A(J,I)=0.0
  DO 500 I=1,3
  D 500 B(I,I)=0.0
  D  XN=0.0
  DO 400 I=1,400
  D 400 C2(I)=0.0
  C
  C      SUBTRACT STRAIGHT LINE AL+BL*CHANNEL NUMBER
  C
  IF(AL+BL)350,410,350
  D 410 DO 415 I=1,ISPUL
  D 415 C2(I)=DATA(I)
  GO TO 309
  D 350 DO 353 J=IPPLL,IPPUL
  D  X1=J
  D 353 C2(J)=DATA(J)-AL-BL*X1
  C
  C      FORM SOLUTION MATRIX
  C
  D 309 DO 310 K=IPPLL,IPPUL
  D  KN2=XN*XN
  D  XN3=XN2*XN
  D  XN4=XN3*XN
  D  P=C2(K)*C2(K)/W
  D  ZN=LOGF(C2(K))
  D  A(1,1)=A(1,1)+P*XN4
  D  A(1,2)=A(1,2)+P*XN3
  D  A(1,3)=A(1,3)+P*XN2
  D  A(2,3)=A(2,3)+P*XN
  D  A(3,3)=A(3,3)+P
  D  B(1,1)=B(1,1)+XN2*P*ZN
  D  B(2,1)=B(2,1)+XN*P*ZN
  D  B(3,1)=B(3,1)+P*ZN
  D 310 XN=XN+1.0
  D  A(2,1)=A(1,2)
  D  A(3,1)=A(1,3)

```

```

  D  A(2,2)=A(1,3)
  D  A(3,2)=A(2,3)
  C
  C      CALCULATE THE POSITION OF THE PHOTO PEAK
  C
  D  CALL DMINV(3,1)
  C
  D 329 PPLL=IPPLL
  D  X0=(-B(2,1)/(2.0*B(1,1)))+PPLL
  D  RATIO=TRUE/(X0-AS)
  D 307 X=0.0
  D  I1=0
  D  SPUL=ISPUL
  D  ISPULM=SPUL*RATIO+0.5
  C
  C      TEST DATA FOR ZERO COUNTS IN CHANNELS 1,2,3
  C
  IF(DATA(1)) 312,313,312
  D 313 IF(DATA(2)) 314,315,314
  D 315 IF(DATA(3)) 316,318,316
  C
  D 314 DATA(1)=DATA(2)
  D  GO TO 312
  D 316 DATA(1)=DATA(3)
  D  DATA(2)=DATA(3)
  D  GO TO 312
  D 318 DATA(1)=DATA(4)
  D  DATA(2)=DATA(4)
  D  DATA(3)=DATA(4)
  C
  C      FIT 3 POINTS OF DATA WITH PARABOLA AND EVALUATE
  C
  D 312 X=X+1.0
  D  I1=I1+1
  D 317 XP=(X/RATIO)+AS
  D  IF(XP-1.1600,600,603
  D 603 IF(XP-2.1601,319,319
  D 600 C2(I1)=DATA(I1)/RATIO
  D  GO TO 312
  D 601 X1=1.0
  D  X2=2.0
  D  X3=3.0
  D  Y1=DATA(I1)
  D  Y2=DATA(I2)
  D  Y3=DATA(I3)
  D  GO TO 604
  D 319 IX2=XP+0.5
  D  IF(IX2-ISPUL)320,323,323
  D 320 IX1=IX2-1
  D  IX3=IX2+1
  D  Y1=DATA(IX1)
  D  Y2=DATA(IX2)
  D  Y3=DATA(IX3)
  D 602 X1=IX1
  D  X2=IX2
  D  X3=IX3
  D 604 AA=(Y3-2.0*Y2+Y1)/2.0

```

```

D      BB=(-Y3*(X2+X1)+2.0*Y2*(X1+X3)-Y1*(X3+X2))/2.0
D      CC=((X1*X2*Y3)-2.0*(X1*X3*Y2)+(X2*X3*Y1))/2.0
D 323  C2(I1)=(AA*XP*XP+BB*XP+CC)/RATIO
      IF(ISPULM-I1:322,322,312
322  DO 324  I=1,400
324  DATA(I)=0.0
331  DO 330  I=1,ISPULM
330  DATA(I)=C2(I1)
      ISPUL=ISPULM
      RETURN
      END

```

C
C
C
C
C
C

7040 LINEAR LEAST SQUARES SPECTRUM FITTING PROGRAM
WITH DOUBLE PRECISION DOUBLE PIVOTAL MATRIX INVERSE
ROUTINE WRITTEN IN MAP SYMBOLIC LANGUAGE.
D. D. METCALF, PHILLIPS PETROLEUM COMPANY

```

0 DIMENSION SPECT(400,26),ID(2,26),TITLE(11),ISPLTS(2,26),
1 IPPLTS(2,26),ID1(2,10),FIXINT(10),ID2(2,10),FIXRT(10),
2 INCLD(20),SIGMA(400),BGINT(6),JFS(26),JNIS(26),IFI(10),
3 IRI(10),IRID(10),BETA(10),BETR(10),SIGMAS(400),XICB(20),
4 JFST(20),RSDL(20),A(40,20),B(40,20),C(40,20),DATA(400)
0 COMMON SPECT,ID,TITLE,ISPLTS,IPPLTS,ID1,FIXINT,ID2,FIXRT,
1 INCLD,SIGMA,BGINT,JFS,JNIS,IFI,IRI,IRID,BETA,BETR,SIGMAS,
2 XICB,JFST,RSDL,A,B,C,DATA,JSFTD,YFS,JN,JNFI,JNRI,JX1,JX2,
3 JSUB,JWT,JNCLO,JGPT1,JOPT2,JNST,PAGE
DIMENSION ISIGMA(10),IDATA(10),IPAT(2,10),SSIGMA(10),DAT(10)
IPAGE=0
400 READ (5,3)ICTYP,(TITLE(I),I=1,11)
3 FORMAT(13,3X,11A6)
CALL PAGE(IPAGE)
WRITE (6,100)(TITLE(I),I=1,11)
100 FORMAT(15H0 ,11A6)
WRITE(6,184)
184 FORMAT(32H0 PROBLEM CONTROL PARAMETERS)
4 READ (5,110)ICTYP,JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,JNCLO,JWT,JOPT1
1,JOPT2,JRC
110 FORMAT(13,7X,2(13,2X),6(12,3X),4(11,4X))
DO 103 J=1,2
DO 103 K=1,10
ID1(J,K)=0
103 ID2(J,K)=0
DO 104 J=1,2
DO 104 K=1,26
ID(J,K)=0
104 READ (5,120)ICTYP,ID3,ID4
120 FORMAT(13,7X,2I4)
8 WRITE (6,102)ID3,ID4
102 FORMAT(51H0 COMPOSITE SPECTRUM IDENTIFICATION - 214)
ID(1,1)=ID3
ID(2,1)=ID4
JVB=JN-JSUB-JNFI-(JNRI/2)-1
7 WRITE (6,101)JX1,JX2,JN,JSUB,JNFI,JNRI,JVB
101 FORMAT(44H0 FITTING LIMITS IN CHANNEL NUMBER//
1 27H A. LOWER - 13//
2 27H B. UPPER - 13//
3 43H NUMBER OF SPECTRA IN PROBLEM - 12//
4 43H A. BACKGROUND - 12//
5 43H B. FIXED INTENSITY - 12//
6 43H C. FIXED RATIO - 12//
7 43H D. VARIABLE PARAMETERS - 12)
IFI(JWT-1) 301,303,305
301 WRITE (6,302)
302 FORMAT(28H0 WEIGHTED BY 1/Y)
GO TO 308
303 WRITE (6,304)
304 FORMAT(31H0 FIT IS NOT WEIGHTED)
GO TO 308

```

```

305 WRITE (6,306)
306 FORMAT(38H0 WEIGHTED BY VALUES READ IN)
308 WRITE (6,307)
307 FORMAT(32H0 CONTROL CARD LISTING)
WRITE (6,310)JX1,JX2,JN,JSUB,JNFI,JNRI,JNST,JNCLO,JWT,JOPT1,
1 JOPT2,JRC
310 FORMAT(4H0110,7X,2(13,2X),6(12,3X),4(11,4X))
WRITE (6,320)ICTYP,ID3,ID4
320 FORMAT(1H ,13,7X,2I4)
IFI(JSUB)9,11,9
9 K=JSUB+1
READ (5,130)ICTYP,((ID(I,J),I=1,2),J=2,K)
130 FORMAT(13,7X,6(2I4,2X))
WRITE (6,330)ICTYP,((ID(I,J),I=1,2),J=2,K)
330 FORMAT(1H ,13,7X,6(2I4,2X))
READ (5,131)ICTYP,(BGINT(I),I=2,K)
131 FORMAT(13,7X,6(F8.6,2X))
WRITE (6,331)ICTYP,(BGINT(I),I=2,K)
331 FORMAT(1H ,13,7X,6(F8.6,2X))
C
C READ STANDARD IDENTIFICATION
C
11 K=JSUB+2
L=JNST+K-1
K1=K
GO TO 12
14 K1=K1+6
12 K2=K1+5
IFI(K2-L)13,13,15
15 K2=L
13 READ (5,130)ICTYP,((ID(I,J),I=1,2),J=K1,K2)
WRITE (6,330)ICTYP,((ID(I,J),I=1,2),J=K1,K2)
16 IF(K2-L)14,17,14
17 IF(JNFI)18,19,18
18 L=JNFI
K=1
K1=K
GO TO 20
21 K1=K1+6
20 K2=K1+5
IFI(K2-L)22,22,23
23 K2=L
22 READ (5,130)ICTYP,((ID(I,J),I=1,2),J=K1,K2)
WRITE (6,330)ICTYP,((ID(I,J),I=1,2),J=K1,K2)
24 IF(K2-L)21,25,21
25 L=JNFI
K=1
K1=K
GO TO 26
27 K1=K1+6
26 K2=K1+5
IFI(K2-L)28,28,29
29 K2=L
28 READ (5,131)ICTYP,(FIXINT(I),I=K1,K2)
WRITE (6,331)ICTYP,(FIXINT(I),I=K1,K2)
30 IF(K2-L)27,19,27
19 IF(JNRI)31,44,31

```

```

31 L=JNRI
   K=1
   K1=K
   GO TO 32
33 K1=K1+6
32 K2=K1+5
   IF(K2-L)34,34,35
35 K2=L
34 READ (5,130)ICTYP,((ID2(I,J),I=1,2),J=K1,K2)
   WRITE (6,330)ICTYP,((ID2(I,J),I=1,2),J=K1,K2)
36 IF(K2-L)33,37,33
37 L=JNRI
   K=L
   K1=K
   GO TO 39
40 K1=K1+6
39 K2=K1+5
   IF(K2-L)41,41,42
42 K2=L
41 READ (5,131)ICTYP,(FIXRT(I),I=K1,K2)
   WRITE (6,331)ICTYP,(FIXRT(I),I=K1,K2)
43 IF(K2-L)40,44,40
44 IF(JNCLO)45,46,45
45 IF(JNCLO-10)47,47,49
47 READ (5,170)ICTYP,(INCLO(I),I=1,JNCLO)
   WRITE (6,370)ICTYP,(INCLO(I),I=1,JNCLO)
   GO TO 46
49 READ (5,170)ICTYP,(INCLO(I),I=1,10)
   READ (5,170)ICTYP,(INCLO(I),I=11,JNCLO)
   WRITE (6,370)ICTYP,(INCLO(I),I=1,10)
   WRITE (6,370)ICTYP,(INCLO(I),I=11,JNCLO)
170 FORMAT(13,7X,10(13,2X))
370 FORMAT(1H,13,7X,10(13,2X))
46 IF(JMT-1150,51,52)
52 NCDS=0
58 READ (5,190) IC,(SSIGMA(J),J=1,10)
   IF(IC-50)53,50,53
53 IF(NCDS)55,56,55
56 DO 57 I=1,9
57 SIGMA(I)=SSIGMA(I+1)
   NCDS=NCDS+1
   GO TO 58
55 DO 60 J=1,10
   JS=10*NCDS-1+J
60 SIGMA(JS)=SSIGMA(J)
   NCDS=NCDS+1
   GO TO 58
51 DO 62 J=1,400
62 SIGMA(J)=1.0
50 ITEST=0
   IF(JRC-1)54,315,54
315 WRITE (6,316)
316 FORMAT(38H PROBLEM RECYCLES ON PREVIOUS DATA)
   READ (5,120)ICTYP
   CALL LSGFIT
   GO TO 400
54 DO 63 L=1,JN

```

```

   READ(5,180)ICTYP,ID7,ID8,ISPULL,ISPUL,IPPLL,IPPUL,IGNCON
180 FORMAT(13,7X,214,4(2X,13),2X,11)
   WRITE (6,380)ICTYP,ID7,ID8,ISPULL,ISPUL,IPPLL,IPPUL,IGNCON
380 FORMAT(1H,13,7X,214,4(2X,13),2X,11)
   IF(IGNCON)353,64,350
350 READ (5,181)ICTYP,TRUE,AS,AL,BL,RATIO
181 FORMAT(13,7X,F8.3,2X,F8.4,2X,2F10.4,F10.6)
   WRITE (6,381)ICTYP,TRUE,AS,AL,BL,RATIO
381 FORMAT(1H,13,7X,F8.3,2X,F8.4,2X,2F10.4,F10.6)

```

C
C
C

READ DATA

```

64 NCDS=0
78 READ (5,190) IC,(DAT(I),I=1,10),AD1,AD2
190 FORMAT(12,10F7.0,2A4)
   IF(IC-50)69,311,69
69 IF(NCDS)71,72,71
72 DO 73 K=1,9
73 DATA(K)=DAT(K+1)
   NCDS=NCDS+1
   GO TO 78
71 DO 79 J=1,10
   JS=10*NCDS-1+J
79 DATA(JS)=DAT(J)
   NCDS=NCDS+1
   GO TO 78

```

C
C
C

CHECK DATA FOR CONSISTANCY

```

311 IF(IGNCON)70,70,312
312 CALL GSHIFT(ISPUL,IPPLL,IPPUL,TRUE,AS,AL,BL,RATIO)
   WRITE (6,394)
394 FORMAT(41H LISTING OF GAIN SHIFTED SPECTRA)
   WRITE (6,392)
392 FORMAT(1H 6X1H06X1H16X1H26X1H36X1H46X1H56X1H66X1H76X1H86X1H9)
   JS=0
   NCDS=0
84 DO 85 I=1,10
85 DAT(I)=0.0
   IF (NCDS)86,87,86
87 DO 89 I=1,9
89 DAT(I+1)=DATA(I)+0.5
95 WRITE(6,390)NCDS,(DAT(I),I=1,10),ID7,ID8
   IF(JS-ISPUL)92,70,70
86 DO 94 I=1,10
   JS=10*NCDS-1+I
94 DAT(I)=DATA(JS)+0.5
   GO TO 95
92 NCDS=NCDS+1
   GO TO 34
390 FORMAT(1H,12,10F7.0,2X,214)
70 DO 210 K=1,ISPUL
   IF (DATA(K))202,202,210
202 DATA(K)=1.0
210 CONTINUE

```

C
C

STORE DATA


```

SUBROUTINE SSGFIT
0 DIMENSION SPECT(400,26),ID1(2,26),TITLE(11),ISPLTS(2,26),
1   IPPLTS(2,26),ID1(2,10),FIXINT(10),ID2(2,10),FIXRT(10),
2   INCLQ(20),SIGMA(400),BGINT(6),JFS(26),JNIS(26),IFI(10),
3   IRI(10),IRID(10),BETA(10),BETR(10),SIGMAS(400),XICB(20),
4   JFST(20),RSDL(20),A(40,20),B(40,20),C(40,20),DATA(400)
0 COMMON SPECT,ID,TITLE,ISPLTS,IPPLTS,ID1,FIXINT,ID2,FIXRT,
1   INCLQ,SIGMA,BGINT,JFS,JNIS,IFI,IRI,IRID,BETA,BETR,SIGMAS,
2   XICB,JFST,RSDL,A,B,C,DATA,JSFTD,IFS,JN,JNF1,JNRI,JX1,JX2,
3   JSUB,JWT,JNCLO,JOPT1,JOPT2,JNST,IPAGE
   DIMENSION SCALE(20)

CALL PAGE(IPAGE)
WRITE (6,960)(TITLE(I),I=1,11)

      OBTAIN SPECTRA IDENTITY NUMBERS FOR STANDARDS
      USED IN FITTING.

DO 502 L=1,26
502 JFS(K)=0
N=JSUB+2
DO 505 E=N,JN
505 JFS(K)=L
KLOW=ISPLTS (1,1)
KHIGH=ISPLTS (2,1)

      SET AREA FOR IDENTITY OF FIXED INTENSITY SPECTRA
      TO ZERO

504 DO 507 E=1,10
   IRI(K)=0
517 IRID(K)=0
   BETR(K)=0
530 BETA(K)=0
507 IFI(K)=0
   DO 508 K=1,20
508 JFST(K)=0

      OBTAIN IDENTITY NUMBERS FOR FIXED INTENSITY SPECTRA

   IF (JNF1) 510,520,510
510 DO 511 K=1,JNF1
   DO 512 L=N,JN
   IF(ID(1,L)-ID1(1,K)) 512,514,512
514 IF(ID(2,L)-ID1(2,K)) 512,515,512
515 IFI(K)=L
   JFS(L)=0
512 CONTINUE
511 CONTINUE

      SUBTRACT OFF FIXED INTENSITY SPECTRA

   IF(JRC-1) 571,572,571
572 DO 573 K=KLOW,KHIGH
573 SPECT(K,1)=DATA(K)
   IF(JSUB) 574,571,574

```

```

C
DO 80 M=1,JN
  IF(ID7-ID(1,M)) 80,32,80
82  IF(ID8-ID(2,M)) 80,83,8C
83  MARK=M
    GO TO 203
80  CONTINUE
203  DO 206 K=1,ISPUL
206  SPECT(K,MARK)=DATA(K)
    ISPLTS(1,MARK)=ISPLL
    ISPLTS(2,MARK)=ISPUL
    ISPUL1=ISPUL+1
    DO 239 K=ISPUL1,400
239  SPECT(K,MARK)=0.0
    IF(JRC-1) 63,63,75
63  CONTINUE
75  READ (5,120)ICTYP

      PRESERVE ORIGINAL SPECTRA IN AREA (DATA)

KLOW=ISPLTS (1,1)
KHIGH=ISPLTS (2,1)
DO 249 K=KLOW,KHIGH
249 DATA(K)=SPECT(K,1)

      SUBTRACT BACKGROUND SPECTRA

  IF (JSUB) 213,154,213
213 JSUB1=JSUB+1
    DO 216 J=2,JSUB1
    DO 217 K=1,KHIGH
      SPECT(K,1)=SPECT(K,1)-BGINT(J)*SPECT(K,J)
217 CONTINUE
216 CONTINUE
154 IF (JWT) 155,88,155
88 DO 90 K=1,KHIGH
90 SIGMA(K)=SPECT(K,1)
    GO TO 156
155 DO 153 K=1,KHIGH
153 SIGMAS(K)=SPECT(K,1)
156 CALL LSGFIT
    GO TO 400
END

```

```

574 JSUB1=JSUB+1
DO 577 J=2,JSUB1
DO 576 K=1,KHIGH
SPECT(K,1)=SPECT(K,1)-BGINT(J)+SPECT(K,J)
576 CONTINUE
577 CONTINUE
571 DO 575 K=1,JNF1
IFIK=IFI(K)
FIXINK=FIXINT(K)
DO 580 M=JX1,JX2
SPECT(M,1)=SPECT(M,1)-SPECT(M,FIK)*FIXINK
575 CONTINUE

```

C
C
C OBTAIN IDENTITY NUMBERS FOR RELATED INTENSITY SPECTRA

```

520 I= (JNRI) 521,593,521
521 DO 524 K=1,JNRI
DO 525 L=N,JN
IF(ID(1,L)-ID2(1,K)) 525,528,525
528 IF(ID(2,L)-ID2(2,K)) 525,529,525
529 IRI(K)=L
525 CONTINUE
524 CONTINUE

```

C
C
C COMBINE PAIRS OF RELATED INTENSITY SPECTRA

```

MARX=0
JNRI1 = JNRI - 1
540 DO 550 K=1,JNRI1,2
N=IRI(K)
N1=IRI(K+1)
IF(FIXRT(K)-FIXRT(K+1))552,552,553
552 BETA(K+1)=FIXRT(K+1)/FIXRT(K)
IF(MARX) 555,554,555
554 JFS(N1)=0
IRID(K)=IRI(K)
555 DO 560 M=JX1,JX2
560 SPECT(M,N)=SPECT(M,N)+BETA(K+1)*SPECT(M,N1)
GO TO 550
553 BETA(K)=FIXRT(K)/FIXRT(K+1)
IF(MARX) 563,561,563
561 JFS(N)=0
IRID(K+1)=IRI(K+1)
563 DO 564 M=JX1,JX2
564 SPECT(M,N1)=SPECT(M,N1)+BETA(K)*SPECT(M,N)
550 CONTINUE

```

C
C
C CONDENSE STANDARD IDENTITY NUMBERS IN AREA JFS

```

583 JINDX=1
584 L=1
DO 586 K=1,JN
IF (JFS(K)) 585,586,585
585 JFS(L)=JFS(K)
IF (L-K) 587,588,587

```

```

587 JFS(K)=0
588 L=L+1
586 CONTINUE
JSFTD=L-1
IF (JSFTD) 605,620,605

```

C
C
C COMPUTE THE SIGMA FOR THE WEIGHTING FUNCTION

```

605 IF(JWT-1) 610,620,617
610 IF(JSUB) 611,615,611
611 JSUB1=JSUB+1
612 DO 614 K=KLOW,KHIGH
SIGMAS(K)=0.0
DO 616 J=2,JSUB1
616 SIGMAS(K)=SIGMAS(K)+BGINT(J)**2.0*SPECT(K,J)
SIGMAS(K)=SIGMAS(K)+DATA(K)
614 CONTINUE
GO TO 620
617 IF(JSUB) 621,620,621
621 JSUB1 = JSUB + 1
DO 622 K=KLOW,KHIGH
DO 623 J=2,JSUB1
623 SIGMA(K)=SIGMA(K)+BGINT(J)**2.0*SPECT(K,J)
622 CONTINUE
GO TO 620
615 DO 618 K=KLOW,KHIGH
618 SIGMAS(K)=SIGMA(K)

```

C
C
C CALCULATE MATRIX ELEMENTS FOR MATRIX INVERSE SUBROUTINE

```

620 DO 632 I=1,JSFTD
JFSI=JFS(I)
DO 635 J=1,JSFTD
JFSJ=JFS(J)
SUM=0.0
SUM1=0.0
DO 638 M=JX1,JX2
IF(JNCLO) 639,642,639
639 DO 640 L=1,JNCLO
IF(INCLO(L)-M) 640,638,640
640 CONTINUE
642 IF(JWT)645,643,645
643 SUM=SUM+(SPECT(M,JFSI)/SIGMAS(M))*SPECT(M,JFSJ)
IF(J-JSFTD) 638,641,638
641 SUM1=SUM1+SPECT(M,1)/SIGMAS(M)*SPECT(M,JFSI)
GO TO 638
645 SUM=SUM+(SPECT(M,JFSI)/SIGMA(M))*SPECT(M,JFSJ)
IF(J-JSFTD) 638,644,638
644 SUM1=SUM1+SPECT(M,1)/SIGMA(M)*SPECT(M,JFSI)
638 CONTINUE
A(I,J)=SUM
C(I,J)=SUM
B(I,1)=SUM1
635 CONTINUE
632 CONTINUE

```

C
C
C SCALE THE MATRIX BEFORE INVERTING

```

DO 652 M=1,JSFTD
652 SCALE(M)=SQRT(A(M,M))
DO 655 I=1,JSFTD
  B(I,1)=B(I,1)/SCALE(I)
DO 655 M=1,JSFTD
655 A(M,1)=A(M,1)/(SCALE(M)*SCALE(I))
  DET=0.0
680 CALL MAINS(A,JSFTD,B,1,DET,IFS)
  RESTORE MATRIX INVERSION TO SCALE
DO 662 I=1,JSFTD
  B(I,1)=B(I,1)/SCALE(I)
DO 662 M=1,JSFTD
662 A(M,1)=A(M,1)/(SCALE(I)*SCALE(M))

  TEST FOR SINGULAR MATRIX
  IF (IFS) 820,905,820

  OUTPUT OF FITTING PROGRAM RESULTS
820 WRITE (6,822)
822 FORMAT(51H0 RESULTS FOR SPECTRA USED IN FITTING SUBROUTINE)
  WRITE (6,823)
823 FORMAT(59H0 SPECTRA IDENTITY INTENSITY STA
  INDARD DEVIATION)
824 WRITE (6,826) ID(1,1),ID(2,1)
826 FORMAT(23H0 COMPOSITE ,I4,I4)

  OBTAIN THE SUM OF THE SQUARED RESIDUALS
R=0.0
SUM=0.0
DO 830 M=JX1,JX2
  IF (JNCLO) 825,828,825
825 DO 827 L=1,JNCLO
  IF (INCLO(L)-M) 827,830,827
827 CONTINUE
828 DO 829 I=1,JSFTD
  JFSI=JFS(I)
  SUM=SUM+(SPECT(M,JFSI)*B(I,1))
829 CONTINUE
  SUM1=(SPECT(M,1)-SUM)* * 2
  SUM=0.0
  IF (JMT) 831,832,831
831 R=R+(SUM1/SIGMA(M))
  GO TO 830
832 R=R+(SUM1/SIGMA(M))
830 CONTINUE
  IDOF=(JX2-JX1-JNCLO-JSFTD)
  DOF=IDOF
  ZERO=0.0

840 IF (JSUB) 841,845,841
841 DO 842 J=2,JSUB1
842 WRITE (6,843) ID(1,J),ID(2,J),BGINT(J),ZERO
843 FGRMAT (18H0 BACKGROUND,5X,I4,I4,6X,F11.8,6X,F10.8)

```

```

C WRITE OUT INDEX FOR FIXED INTENSITY SPECTRA
C
845 IF (JNFI) 847,850,847
847 DO 848 J=1,JNFI
848 WRITE (6,849) ID(1,J),ID(2,J),FIXINT(J),ZERO
849 FORMAT (18H0 FIXED INT.,5X,I4,I4,6X,F11.8,6X,F10.8)

C WRITE OUT INDEX FOR RELATED INTENSITY SPECTRA
C
C
850 IF (JNRI) 851,885,851
851 DO 860 K=1,JNRI1,2
  IRIK=IRI(K)
  IRIK1=IRI(K+1)
  L=(K+1)/2
  IF (IRI(K)-IRID(K)) 852,854,852
854 DO 856 M=JX1,JX2
856 SPECT(M,IRIK)=SPECT(M,IRIK)-SPECT(M,IRIK1)*BETA(K+1)
  BETA(K)=B(L,1)
  BETA(K+1)=BETA(K)*BETA(K+1)
  GO TO 860
852 DO 858 M=JX1,JX2
858 SPECT(M,IRIK1)=SPECT(M,IRIK1)-SPECT(M,IRIK)*BETA(K)
  BETA(K+1)=B(L,1)
  BETA(K)=BETA(K+1)*BETA(K)
860 CONTINUE

C CALCULATE THE DEVIATIONS FOR RELATED SPECTRA
C
C
  ISUB = 1
  DO 870 K=1,JNRI1,2
  IF (BETA(K)-BETA(K+1)) 868,868,872
868 BETR(K)=(R/DOF)*ABS(A(ISUB,ISUB))
871 BETR(K)=SQRT(BETR(K))
  BETR(K+1)=BETR(K) * (BETA(K+1)/BETA(K))
  GO TO 869
872 BETR(K+1)=(R/DOF)*ABS(A(ISUB,ISUB))
  BETR(K+1)=SQRT(BETR(K+1))
  BETR(K)=BETR(K+1)* (BETA(K)/BETA(K+1))
869 ISUB = ISUB + 1
870 CONTINUE

C
DO 873 K=1,JNRI
873 WRITE (6,875) ID(1,K),ID(2,K),BETA(K),BETR(K)
875 FORMAT (20H0 RELATED INT.,3X,I4,I4,5X,F12.8,6X,F10.8)

C WRITE OUT INDEX FOR ALL OTHER STANDARDS USED IN FIT
C
C
877 CONTINUE
  JFSK=JFS(K)
  RDOF=(R/DOF)*ABS(A(K,K))
  RDOF=SQRT(RDOF)
880 WRITE (6,882) ID(1,JFSK),ID(2,JFSK),B(K,1),RDOF
876 CONTINUE

```

```

882 FORMAT (18H0          STANDARD  ,5X,I4,I4,5X,F12.8,6X,F10.8)
      GO TO 883
885 DO 887 K=1,JSFTD
      JFSK=JFS(K)
      RDOF=(R/DOF)*ABS(A(K,K))
      RDOF=SQRT(RDOF)
887 WRITE (6,890)ID(1,JFSK),ID(2,JFSK),B(K,1),RDOF
890 FORMAT (18H0          STANDARD  ,5X,I4,I4,6X,F11.2,6X,F10.8)
883 WRITE (6,881)R
881 FORMAT(39H0          CHI-SQUARED          =          ,E14.8)
      WRITE (6,884)IDOF
884 FORMAT(37H0          DEGREES OF FREEDOM          =          ,I3)
      QOFN = R/DOF
      WRITE (6,886)QOFN
886 FORMAT(34H0          QUALITY OF FIT NUMBER / =,F10.3)
C
      WRITE (6,888)
888 FORMAT(1H0)
      IF(JWT-1) 891,906,891
891 WRITE (6,892)
892 FORMAT(80H0          WEIGHTED FIT - QUALITY OF FIT NUMBER SHO
      ULD BE APPROXIMATELY 1.0)
      IF(QOFN-25.0) 894,894,893
893 WRITE (6,895)
895 FORMAT(63H0          QUALITY OF FIT NUMBER INDICATES A VERY P
      LOOR FIT.)
      GO TO 907
894 IF(QOFN-5.0) 897,897,896
896 WRITE (6,898)
898 FORMAT(58H0          QUALITY OF FIT NUMBER INDICATES A POOR F
      IT.)
897 IF(QOFN-1.2) 902,907,907
900 WRITE (6,901)
901 FORMAT(58H0          QUALITY OF FIT NUMBER INDICATES A GOOD F
      IT.)
      GO TO 907
902 IF(QOFN-0.7) 899,899,900
899 IF(QOFN-0.1) 903,907,907
903 WRITE (6,904)
904 FORMAT(42H0          SIGMA VALUES ARE TOO LARGE.)
      GO TO 907
906 WRITE (6,909)
909 FORMAT (91H0          UNWEIGHTED FIT - CHI SQUARED AND QUALIT
      Y OF FIT NUMBER HAVE NO SIGNIFICANCE.)
C
      TEST FOR NEGATIVE INTENSITIES AND OBTAIN IDENTITY
      NUMBERS FOR NEGATIVE OR ZERO INTENSITIES
C
907 IF(JOPT1) 950,950,908
908 L=JINDX
      DO 920 I=1,JSFTD
      IF (B(I,1)) 922,922,920
922 XICB(I)=B(I,1)
      JFST(I)=JFS(I)
      JFS(I)=0
      L=L+1
920 CONTINUE
      IF (L-JINDX) 926,950,926

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```

926 L=L-1
      JINDX=L
      JSFTD=JSFTD-JINDX
      KFLAG=0
      IF(JNRI) 927,944,927
927 JTAB= JNRI
      DO 930 K=1,L
      DO 929 J=1,JNRI
      IF (JFST(K)-IRI(J)) 929,928,929
928 KFLAG=KFLAG-1
      IRI(J)=0
929 CONTINUE
930 CONTINUE
      IF(KFLAG) 932,941,932
932 JNRI=JNRI-2
      KFLAG=KFLAG-1
      IF (KFLAG) 932,933,932
933 DO 938 K=1,JTAB.2
      IF (IRI(K)) 935,936,935
935 IF (IRI(K+1)) 938,936,938
936 IRI(K)=0
      IRI(K+1)=0
938 CONTINUE
      M=1
      DO 940 J=1,JTAB
      IF (IRI(J)) 942,940,942
942 IRI(M)=IRI(J)
      IRID(M)=IRID(J)
      FIXRT(M)=FIXRT(J)
      BETA(M)=BETA(J)
      M=M+1
940 CONTINUE
941 CALL PAGE(IPAGE)
      WRITE (6,946)
946 FORMAT(58H0          PROBLEM RECYCLE ELIMINATES NEGATIVE INTENSITY SPEC
      ITRA)
      MARX=1
      GO TO 540
944 CALL PAGE(IPAGE)
      WRITE (6,946)
      GO TO 583
950 CALL PRINT
      GO TO 970
905 WRITE (6,910)
910 FORMAT(45H0MATRIX IS SINGULAR, NO SOLUTION IS POSSIBLE.)
960 FORMAT(15H0          ,11A6)
970 RETURN
      END

```

```

C      DUTPUT SUBROUTINE FOR NUMBERING PAGES
C
      SUBROUTINE PAGE(IPAGE)
      IPAGE=IPAGE+1
      WRITE (6,1)IPAGE
1  FORMAT(100H1:
1  FITTING PROGRAM
      RETURN
      END

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7040 LINEAR LEAST SQUARES SPECTRUM
      PAGE ,12)

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      SUBROUTINE PRINT
0  DIMENSION SPECT(400,26),ID(2,26),TITLE(11),ISPLTS(2,26),
1  IPPLTS(2,26),ID1(2,10),FIXINT(10),ID2(2,10),FIXRT(10),
2  INCLO(20),SIGMA(400),BGINT(6),JFS(26),JNIS(26),IF1(10),
3  IRI(10),IRID(10),BETA(10),BETR(10),SIGMAS(400),XICB(20),
4  JFST(20),RSDL(20),A(40,20),B(40,20),C(40,20),DATA(400)
0  COMMON SPECT,ID,TITLE,ISPLTS,IPPLTS,ID1,FIXINT,ID2,FIXRT,
1  INCLO,SIGMA,BGINT,JFS,JNIS,IF1,IRI,IRID,BETA,BETR,SIGMAS,
2  XICB,JFST,RSDL,A,B,C,DATA,JSFTD,IFS,JN,JNFI,JNRI,JX1,JX2,
3  JSUB,JWT,JNCLO,JOPT1,JOPT2,JNST,IPAGE
      CALL PAGE(IPAGE)
C
      WRITE (6,114)(TITLE(I),I=1,11)
      WRITE (6,4)
4  FORMAT(109H0CHAN. Y SIGMA Y-BKG
1  YCALC. SIGMA Y-BKG RESIDUAL R/SG.Y-BKG)
C
      ILOW=ISPLTS(1,1)
      IHIGH=ISPLTS(2,1)
      ITEST = 51
      DO 50 K=ILOW,IHIGH
      IF (K-ITEST) 1,46,1
46  CALL PAGE(IPAGE)
      ITEST = ITEST + 50
      WRITE (6,4)
1  IF (K-JX1) 5,2,5
2  WRITE (6,3)
3  FORMAT (46H FIT OF DATA BEGINS WITH THE NEXT CHANNEL)
5  IF (K-(JX2+1)) 9,6,9
6  WRITE (6,7)
7  FORMAT (50H FIT OF DATA ENDS WITH THE PRECEEDING CHANNEL)
9  IF (JNCLO) 10,15,10
10 DO 14 M=1,JNCLO
      IF (INCLO(M)-K) 14,11,14
11 WRITE (6,12)
12 FORMAT (48H THE NEXT CHANNEL WAS OMITTED FROM THE FIT)
14 CONTINUE
15 YI=DATA(K)
      SIGYI=SQRT(YI)
      IF (JWT) 16,18,16
16 YISTR=SIGMAS(K)
      SYISTR=ABS(SQRT(SIGMA(K)))
      GO TO 20
18 YISTR=SIGMA(K)
      SYISTR=ABS(SQRT(SIGMAS(K)))
C
      CALCULATE YBAR
C
20 YBAR=0.0
      IF (JNRI) 21,28,21
21 DO 22 L=1,JNRI
      IRIK=IRI(L)
22 YBAR=YBAR+SPECT(K,IRIK)*BETA(L)
      IF ((JNRI/2)-JSFTD) 24,32,24
24 DO 25 I=1,JSFTD
      DO 26 M=1,JNRI
      IF (IRI(M)-JFS(I)) 26,25,26

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```

26 CONTINUE
   JFSK=JFS(I)
   YBAR=YBAR+SPECT(K,JFSK)*B(I,1)
25 CONTINUE
   GO TO 32
28 DO 30 I=1,JSFTD
   JFSI=JFS(I)
   YBAR=YBAR+SPECT(K,JFSI)*B(I,1)
30 CONTINUE
32 IF (JNFI) 33,35,33
33 DO 34 J=1,JNFI
   IFIK=IFI(J)
34 YBAR=YBAR+SPECT(K,IFIK)*FIXINT(J)
35 RES=YISTR-YBAR
   IF(SYISTR) 36,38,36
36 QUAN=RES/SYISTR
C
37 WRITE (6,39)K,YI,SIGYI,YISTR,YBAR,SYISTR,RES,QUAN
39 FORMAT(2X,I3,5X,F11.2,5X,F9.3,4X,F11.2,4X,F11.2,4X,F9.3,4X,F13.4,
14X,F9.3)
   GO TO 50
38 WRITE (6,40)K,YI,SIGYI,YISTR,YBAR,SYISTR,RES
40 FORMAT(2X,I3,5X,F11.2,5X,F9.3,4X,F11.2,4X,F11.2,4X,F9.3,4X,F13.4,
14X,5HBLANK)
50 CONTINUE
   IF(IHIGH-JX2) 43,47,43
47 WRITE (6,7)
43 IF(JUPT2-1) 42,51,51
42 WRITE (6,45)
45 FORMAT(46H0 OPTION FOR RESIDUALS PRINTOUT NOT SPECIFIED//
1 32H0 END OF PROBLEM)
   RETURN

```

C
C
C

```

PRINT OUT THE RESIDUALS OF THE FIT.
51 CALL PAGE(IPAGE)
   WRITE (6,114)(TITLE(I),I=1,11)
   WRITE (6,52)
52 FORMAT(52H0 RESIDUALS OF THE FIT IN ORDER OF RESULT LISTING//
166H CHAN. Y-BKG. YCALC. ALL RESIDUALS OF THE
IF(I)
   ITEST = 51
   DO 100 K=ILOW,IHIGH
   IF(K-ITEST) 56,115,55
115 CALL PAGE(IPAGE)
   ITEST = ITEST + 50
   WRITE (6,52)
56 IF(JWT) 53,54,53
53 YISTR=SIGMA(K)
   GO TO 55
54 YISTR=SIGMA(K)
55 YBAR=0.0
   IF(JNRI) 61,68,61
61 DO 62 L=1,JNRI
   IRIK=IRI(L)
62 YBAR=YBAR+SPECT(K,IRIK)*BETA(L)
   IF ((JNRI/2)-JSFTD) 64,72,64

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```

64 DO 65 I=1,JSFTD
   DO 66 M=1,JNRI
   IF(IRI(M)-JFS(I)) 66,65,66
66 CONTINUE
   JFSK=JFS(I)
   YBAR=YBAR+SPECT(K,JFSK)*B(I,1)
65 CONTINUE
   GO TO 72
68 DO 70 J=1,JSFTD
   JFSK=JFS(J)
   YBAR=YBAR+SPECT(K,JFSK)*B(J,1)
72 IF (JNFI) 73,77,73
73 DO 74 J=1,JNFI
   IFIK=IFI(J)
74 YBAR=YBAR+SPECT(K,IFIK)*FIXINT(J)
77 DEC=0.0
   DO 76 M=1,20
76 RSOL(M)=0.0
   M=0
   IF (JNFI) 75,80,75
75 DO 78 M=1,JNFI
   IFIK=IFI(M)
   DEC=DEC+SPECT(K,IFIK)*FIXINT(M)
78 RSOL(M)=YISTR-DEC
   M=JNFI
80 IF (JNRI) 75,85,79
79 DO 81 I=1,JNRI
   IRIK=IRI(I)
   DEC=DEC+SPECT(K,IRIK)*BETA(I)
   MI=M+I
81 RSOL(MI)=YISTR-DEC
   M=M+JNRI
   IF ((JNRI/2)-JSFTD) 82,90,82
82 JNRI21=(JNRI/2)+1
   ISUB = M - (JNRI/2)
   DO 84 L=JNRI21,JSFTD
   JFSK=JFS(L)
   DEC=DEC+SPECT(K,JFSK)*B(L,1)
   ISUBL=ISUB+L
84 RSOL(ISUBL)=YISTR-DEC
   M=M+JSFTD-(JNRI/2)
   GO TO 90
85 IF (JSFTD) 86,90,86
86 DO 88 J=1,JSFTD
   JFSK=JFS(J)
   DEC=DEC+SPECT(K,JFSK)*B(J,1)
   MJ=M+J
88 RSOL(MJ)=YISTR-DEC
   M=M+JSFTD
90 WRITE (6,92)K,YISTR,YBAR,(RSOL(L),L=1,7)
92 FORMAT(3X,I3,6X,9F12.2)
   IF(M-7) 100,100,94
94 WRITE (6,96):RSOL(L),L=8,14)
96 FORMAT(36H ,7F12.2)
   IF(M-14) 100,100,98
98 WRITE (6,99):RSOL(L),L=15,21)
99 FORMAT(36H ,7F12.2)

```


	CLA*	5,4		059MAINS	TIX	BL5,4,1	116MAINS
	STO	N	VALUE OF N	060MAINS	CLA	J	117MAINS
	CLA	6,4		061MAINS	SUB	=1	118MAINS
	STO	DET	ADDRESS OF DET	062MAINS	TZE	BL6	119MAINS
	CLA	7,4		063MAINS	STO	J	120MAINS
	STO	IFS	ADDRESS OF IFS	064MAINS	CLA	INS4	121MAINS
•				065MAINS	ADD	CON1	122MAINS
•	UNPACK THE MATRIX			066MAINS	STO	INS4	123MAINS
•				067MAINS	CLA	INS5	124MAINS
	CLA	M		068MAINS	ADD	CON1	125MAINS
	STO	J		069MAINS	STO	INS5	126MAINS
	CLA	A		070MAINS	STA	INS6	127MAINS
	ADD	M		071MAINS	TRA	BL4	128MAINS
	STA	INS1		072MAINS			129MAINS
	ADD	M		073MAINS	• MAIND	TRA	130MAINS
	STA	INS2		074MAINS		CLA	131MAINS
	STA	INS3		075MAINS		STO	132MAINS
BL1	AXT	0,1		076MAINS		SXA	133MAINS
	AXT	0,2		077MAINS		SXA	134MAINS
	LXA	M,4		078MAINS		SXA	135MAINS
BL2	TXI	**1,2,1		079MAINS		LAC	136MAINS
INS2	STZ	**2	***A+2*M	080MAINS		CLA	137MAINS
	TXI	**1,1,1		081MAINS		STO	138MAINS
	TXI	**1,2,1		082MAINS		CLA*	139MAINS
INS1	CLA	**1	***A+M	083MAINS		STO	140MAINS
INS3	STO	**2	***A+2*M	084MAINS		CLA	141MAINS
	TIX	BL2,4,1		085MAINS		STO	142MAINS
	CLA	J		086MAINS		CLA*	143MAINS
	SUB	=1		087MAINS		STO	144MAINS
	TZE	BL3		088MAINS		CLA	145MAINS
	STO	J		089MAINS		STO	146MAINS
	CLA	INS1		090MAINS		CLA	147MAINS
	ADD	CON1		091MAINS		STO	148MAINS
	STO	INS1		092MAINS			149MAINS
	CLA	INS2		093MAINS	•	INITIALIZATION	150MAINS
	ADD	CON1		094MAINS	•		151MAINS
	STO	INS2		095MAINS	•		152MAINS
	STA	INS3		096MAINS	BL6	LXA	153MAINS
	TRA	BL1		097MAINS		AXT	154MAINS
BL3	CLA	N		098MAINS	LOOP	TXI	155MAINS
	TZE	BL6		099MAINS		STZ	156MAINS
	STO	J		100MAINS		STZ	157MAINS
	CLA	B		101MAINS		TIX	158MAINS
	ADD	M		102MAINS		LAC	159MAINS
	STA	INS4		103MAINS		CON1,2	160MAINS
	ADD	M		104MAINS		SXD	161MAINS
	STA	INS5		105MAINS		SXD	162MAINS
	STA	INS6		106MAINS		SXD	163MAINS
BL4	AXT	0,1		107MAINS		SXD	164MAINS
	AXT	0,2		108MAINS		CLA	165MAINS
	LXA	M,4		109MAINS		STA	166MAINS
BL5	TXI	**1,2,1		110MAINS		STA	167MAINS
INS5	STZ	**2	***B+2*M	111MAINS		SUB	168MAINS
	TXI	**1,1,1		112MAINS		STA	169MAINS
	TXI	**1,2,1		113MAINS		SUR	170MAINS
INS4	CLA	**1	***B+M	114MAINS		STA	171MAINS
INS6	STO	**2	***B+2*M	115MAINS		STA	172MAINS

STA	INA6	173MAINS	STO*	DET	230MAINS	
STA	INA7	174MAINS	CLA	=1	231MAINS	
STA	INA8	175MAINS	STO*	IFS	232MAINS	
STA	INA9	176MAINS	STO	K	233MAINS	
STA	INA10	177MAINS	BL7	STZ	PIVOT	234MAINS
STA	INA11+1	178MAINS	CLA	=1	235MAINS	
STA	INA12+1	179MAINS	STO	J	236MAINS	
STA	INA13	180MAINS	BL8	LAC	J,1	237MAINS
STA	INA14+1	181MAINS	CLA	JCOL-1,1	238MAINS	
STA	BL27	182MAINS	TNZ	BL11	239MAINS	
STA	INA15	183MAINS	CLA	J	240MAINS	
STA	INA16	184MAINS	SUB	=1	241MAINS	
STA	INA17	185MAINS	LRS	35	242MAINS	
STA	INA18	186MAINS	MPY	CON1	243MAINS	
STA	INA19	187MAINS	LLS	35	244MAINS	
STA	INA20	188MAINS	PAC	,4	245MAINS	
STA	INA21	189MAINS	CLA	=1	246MAINS	
ADD	=1	190MAINS	STO	I	247MAINS	
STA	INA5+1	191MAINS	BL9	LAC	I,2	248MAINS
STA	INA6+1	192MAINS	TXI	**1,4,-2	249MAINS	
STA	INA7+1	193MAINS	CLA	IROW-1,2	250MAINS	
STA	INA8+1	194MAINS	TNZ	BL10	251MAINS	
STA	INA10+1	195MAINS	INA4	CLA	** ,4	252MAINS
STA	INA13+1	196MAINS	SSP			253MAINS
STA	BL27+1	197MAINS	CAS	PIVOT		254MAINS
STA	INA15+1	198MAINS	TRA	**3		255MAINS
STA	INA16+1	199MAINS	TRA	**2		256MAINS
STA	INA17+1	200MAINS	TRA	BL10		257MAINS
STA	INA18+1	201MAINS	STO	PIVOT		258MAINS
STA	INA19+1	202MAINS	CLA	J		259MAINS
STA	INA20+1	203MAINS	STO	JP		260MAINS
STA	INA21+1	204MAINS	CLA	I		261MAINS
CLA	B	205MAINS	STO	IP		262MAINS
STA	INB1	206MAINS	BL10	CLA	I	263MAINS
STA	INB2	207MAINS	CAS	M		264MAINS
SUB	=1	208MAINS	TRA	BL11		265MAINS
STA	INB3	209MAINS	TRA	BL11		266MAINS
SUB	=1	210MAINS	ADD	=1		267MAINS
STA	BL20	211MAINS	STO	I		268MAINS
STA	INB4	212MAINS	TRA	BL9		269MAINS
STA	INB5+1	213MAINS	BL11	CLA	J	270MAINS
STA	INB6	214MAINS	CAS	M		271MAINS
STA	BL28	215MAINS	TRA	BL12		272MAINS
STA	INB7	216MAINS	TRA	BL12		273MAINS
STA	INB8	217MAINS	ADD	=1		274MAINS
STA	INB9	218MAINS	STO	J		275MAINS
ADD	=1	219MAINS	TRA	BL8		276MAINS
STA	INB4+1	220MAINS	.			277MAINS
STA	INB6+1	221MAINS	.	TEST TO SEE IF MATRIX IS SINGULAR		278MAINS
STA	BL28+1	222MAINS	.			279MAINS
STA	INB7+1	223MAINS	BL12	CLA	JP	280MAINS
STA	INB8+1	224MAINS	SUB	=1		281MAINS
STA	INB9+1	225MAINS	LRS	35		282MAINS
.		226MAINS	MPY	CON1		283MAINS
.	FIND THE PIVOT ELEMENT	227MAINS	LLS	35		284MAINS
		228MAINS	STA	TEMP		285MAINS
	CLA =1.0	229MAINS	ADD	IP		286MAINS

INA5	ADD	IP		287MAINS	INA10	DSTO	**,1	==A-2	344MAINS
	PAC	,4		288MAINS		LAC	TEMP,2		345MAINS
	DCLA	**,4	==A-2	289MAINS		CLA	J		346MAINS
	DSTO	PIVOT		290MAINS		SUB	=1		347MAINS
	LDQ	PIVOT		291MAINS		LRS	35		348MAINS
	FMP	DET		292MAINS		MPY	CON1		349MAINS
	STO	DET		293MAINS		LLS	35		350MAINS
	CLA	PIVOT		294MAINS		PAC	,4		351MAINS
	TNZ	+3		295MAINS		CLA	=1		352MAINS
	STZ	IFS		296MAINS		STO	I		353MAINS
	TRA	BL41		297MAINS	BL16	TXI	**1,2,-2		354MAINS
				298MAINS		TXI	**1,4,-2		355MAINS
				299MAINS		CLA	I		356MAINS
				300MAINS		SUB	IP		357MAINS
				301MAINS		TZE	BL17		358MAINS
				302MAINS		DCLA	ALPHA		359MAINS
				303MAINS	INA11	OFMP	**,2	==A-2	360MAINS
				304MAINS	INA12	DFAU	**,4	==A-2	361MAINS
				305MAINS	INA13	DSTO	**,4	==A-2	362MAINS
				306MAINS	BL17	CLA	I		363MAINS
				307MAINS		CAS	M		364MAINS
				308MAINS		TRA	BL18		365MAINS
				309MAINS		TRA	BL18		366MAINS
				310MAINS		ADD	=1		367MAINS
				311MAINS		STO	I		368MAINS
				312MAINS		TRA	BL16		369MAINS
				313MAINS	BL18	CLA	J		370MAINS
				314MAINS		CAS	M		371MAINS
				315MAINS		TRA	BL19		372MAINS
				316MAINS		TRA	BL19		373MAINS
				317MAINS		ADD	=1		374MAINS
				318MAINS		STO	J		375MAINS
				319MAINS	INS7	TXI	BL15,1,**	== -MMAX	376MAINS
				320MAINS					377MAINS
				321MAINS					378MAINS
				322MAINS					379MAINS
				323MAINS					380MAINS
				324MAINS	BL19	CLA	N		381MAINS
				325MAINS		TZE	BL24		382MAINS
				326MAINS		CLA	IP		383MAINS
				327MAINS		ADD	IP		384MAINS
				328MAINS		PAC	,1		385MAINS
				329MAINS		CLA	=1		386MAINS
				330MAINS		STO	J		387MAINS
				331MAINS	BL20	CLA	**,1	==B-2	388MAINS
				332MAINS		TZE	BL23		389MAINS
				333MAINS		STO	ALPHA		390MAINS
				334MAINS	INB3	LDQ	**,1	==B-1	391MAINS
				335MAINS		STQ	ALPHA+1		392MAINS
				336MAINS		DFDP	PIVOT		393MAINS
				337MAINS	INB4	DSTO	**,1	==B-2	394MAINS
				338MAINS		LAC	TEMP,2		395MAINS
				339MAINS		CLA	J		396MAINS
				340MAINS		SUB	=1		397MAINS
				341MAINS		LRS	35		398MAINS
				342MAINS		MPY	CON1		399MAINS
				343MAINS		LLS	35		400MAINS
						PAC	,4		

INA5	ADD	IP		287MAINS	INA10	DSTO	**,1	==A-2	344MAINS
	PAC	,4		288MAINS		LAC	TEMP,2		345MAINS
	DCLA	**,4	==A-2	289MAINS		CLA	J		346MAINS
	DSTO	PIVOT		290MAINS		SUB	=1		347MAINS
	LDQ	PIVOT		291MAINS		LRS	35		348MAINS
	FMP	DET		292MAINS		MPY	CON1		349MAINS
	STO	DET		293MAINS		LLS	35		350MAINS
	CLA	PIVOT		294MAINS		PAC	,4		351MAINS
	TNZ	+3		295MAINS		CLA	=1		352MAINS
	STZ	IFS		296MAINS		STO	I		353MAINS
	TRA	BL41		297MAINS	BL16	TXI	**1,2,-2		354MAINS
				298MAINS		TXI	**1,4,-2		355MAINS
				299MAINS		CLA	I		356MAINS
				300MAINS		SUB	IP		357MAINS
				301MAINS		TZE	BL17		358MAINS
				302MAINS		DCLA	ALPHA		359MAINS
				303MAINS	INA11	OFMP	**,2	==A-2	360MAINS
				304MAINS	INA12	DFAU	**,4	==A-2	361MAINS
				305MAINS	INA13	DSTO	**,4	==A-2	362MAINS
				306MAINS	BL17	CLA	I		363MAINS
				307MAINS		CAS	M		364MAINS
				308MAINS		TRA	BL18		365MAINS
				309MAINS		TRA	BL18		366MAINS
				310MAINS		ADD	=1		367MAINS
				311MAINS		STO	I		368MAINS
				312MAINS		TRA	BL16		369MAINS
				313MAINS	BL18	CLA	J		370MAINS
				314MAINS		CAS	M		371MAINS
				315MAINS		TRA	BL19		372MAINS
				316MAINS		TRA	BL19		373MAINS
				317MAINS		ADD	=1		374MAINS
				318MAINS		STO	J		375MAINS
				319MAINS	INS7	TXI	BL15,1,**	== -MMAX	376MAINS
				320MAINS					377MAINS
				321MAINS					378MAINS
				322MAINS					379MAINS
				323MAINS					380MAINS
				324MAINS	BL19	CLA	N		381MAINS
				325MAINS		TZE	BL24		382MAINS
				326MAINS		CLA	IP		383MAINS
				327MAINS		ADD	IP		384MAINS
				328MAINS		PAC	,1		385MAINS
				329MAINS		CLA	=1		386MAINS
				330MAINS		STO	J		387MAINS
				331MAINS	BL20	CLA	**,1	==B-2	388MAINS
				332MAINS		TZE	BL23		389MAINS
				333MAINS		STO	ALPHA		390MAINS
				334MAINS	INB3	LDQ	**,1	==B-1	391MAINS
				335MAINS		STQ	ALPHA+1		392MAINS
				336MAINS		DFDP	PIVOT		393MAINS
				337MAINS	INB4	DSTO	**,1	==B-2	394MAINS
				338MAINS		LAC	TEMP,2		395MAINS
				339MAINS		CLA	J		396MAINS
				340MAINS		SUB	=1		397MAINS
				341MAINS		LRS	35		398MAINS
				342MAINS		MPY	CON1		399MAINS
				343MAINS		LLS	35		400MAINS
						PAC	,4		

INA5	ADD	IP		287MAINS	INA10	DSTO	**,1	==A-2	344MAINS
	PAC	,4		288MAINS		LAC	TEMP,2		345MAINS
	DCLA	**,4	==A-2	289MAINS		CLA	J		346MAINS
	DSTO	PIVOT		290MAINS		SUB	=1		347MAINS
	LDQ	PIVOT		291MAINS		LRS	35		348MAINS
	FMP	DET		292MAINS		MPY	CON1		349MAINS
	STO	DET		293MAINS		LLS	35		350MAINS
	CLA	PIVOT		294MAINS		PAC	,4		351MAINS
	TNZ	+3		295MAINS		CLA	=1		352MAINS
	STZ	IFS		296MAINS		STO	I		353MAINS
	TRA	BL41		297MAINS	BL16	TXI	**1,2,-2		354MAINS
				298MAINS		TXI	**1,4,-2		355MAINS
				299MAINS		CLA	I		356MAINS
				300MAINS		SUB	IP		357MAINS
				301MAINS		TZE	BL17		358MAINS
				302MAINS		DCLA	ALPHA		359MAINS
				303MAINS	INA11	OFMP	**,2	==A-2	360MAINS
				304MAINS	INA12	DFAU	**,4	==A-2	361MAINS
				305MAINS	INA13	DSTO	**,4	==A-2	362MAINS
				306MAINS	BL17	CLA	I		363MAINS
				307MAINS		CAS	M		364MAINS
				308MAINS		TRA	BL18		365MAINS
				309MAINS		TRA	BL18		366MAINS
				310MAINS		ADD	=1		367MAINS
				311MAINS		STO	I		368MAINS
				312MAINS		TRA	BL16		369MAINS
				313MAINS	BL18	CLA	J		370MAINS
				314MAINS		CAS	M		371MAINS
				315MAINS		TRA	BL19		372MAINS
				316MAINS		TRA	BL19		373MAINS
				317MAINS		ADD	=1		374MAINS
				318MAINS		STO	J		375MAINS
				319MAINS	INS7	TXI	BL15,1,**	== -MMAX	376MAINS
				320MAINS					377MAINS
				321MAINS					378MAINS
				322MAINS					379MAINS
				323MAINS					380MAINS
				324MAINS	BL19	CLA	N		381MAINS
				325MAINS		TZE	BL24		382MAINS
				326MAINS		CLA	IP		383MAINS
				327MAINS		ADD	IP		384MAINS
				328MAINS		PAC	,1		385MAINS
				329MAINS		CLA	=1		386MAINS
				330MAINS		STO	J		387MAINS
				331MAINS	BL20	CLA	**,1	==B-2	388MAINS

BL21 CLA =1
 STO I
 TXI **1,2,-2
 TXI **1,4,-2
 CLA I
 SUB IP
 TZE BL22
 DCLA ALPHA
 INA14 DFMP **2
 INR5 DFAD **4
 INR6 DSTO **4
 BL22 CLA I
 CAS M
 TRA BL23
 TRA BL23
 ADD =1
 STO I
 TRA BL21
 BL23 CLA J
 CAS N
 TRA BL24
 TRA BL24
 ADD =1
 STU J
 INS8 TXI BL20.1,**
 BL24 CLA K
 CAS M
 TRA BL25
 TRA BL25
 ADD =1
 STU K
 TRA BL7
 *
 *
 *
 ROW PERMUTATIONS
 BL25 CLA =1
 STO K
 BL26 LAC K,1
 CLA IROW-1,1
 STO I
 CAS K
 TRA **2
 TRA BL30
 CLS DET
 STO DET
 LXA M,4
 CLA K
 ADD K
 PAC ,1
 CLA I
 ADD I
 PAC ,2
 BL27 DCLA **2
 DSTO TEMP1
 INA15 DCLA **1
 INA16 DSTO **2
 DCLA TEMP1

**=A-2
 **=B-2
 **=B-2
 **=-MMAX

401MAINS
 402MAINS
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INA17 DSTO **1
 INS9 TXI **1,1,**
 INS10 TXI **1,2,**
 TIX BL27,4,1
 CLA N
 TZE BL29
 PAX ,4
 CLA K
 ADD K
 PAC ,1
 CLA I
 ADD I
 PAC ,2
 BL28 DCLA **2
 DSTO TEMP1
 INR7 DCLA **1
 INR8 DSTO **2
 DCLA TEMP1
 INR9 DSTO **1
 INS11 TXI **1,1,**
 INS12 TXI **1,2,**
 TIX BL28,4,1
 BL29 LAC K,1
 LAC I,2
 CLA IROW-1,2
 STO IROW-1,1
 CLA I
 STO IROW-1,2
 TRA BL26
 BL30 CLA K
 CAS M
 TRA BL31
 TRA BL31
 ADD =1
 STO K
 TRA BL26
 *
 *
 *
 COLUMN PERMUTATIONS
 BL31 CLA =1
 STO K
 BL32 LAC K,1
 CLA JCOL-1,1
 STO J
 CAS K
 TRA **2
 TRA BL34
 SUB =1
 LRS 35
 MPY CON1
 LLS 35
 PAC ,1
 CLA K
 SUB =1
 LRS 35
 MPY CON1
 LLS 35

**=A-2
 **=-MMAX
 **=-MMAX
 **=B-2
 **=B-2
 **=B-2
 **=B-2
 **=-MMAX
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	PAC	,2	
	LXA	M,4	
BL33	TXI	**1,1,-2	
	TXI	**1,2,-2	
INA18	DCLA	**,1	***A-2
	DSTO	TEMP1	
INA19	DCLA	**,2	***A-2
INA20	DSTO	**,1	***A-2
	DCLA	TEMP1	
INA21	DSTO	**,2	***A-2
	TIX	BL33,4,1	
	LAC	J,1	
	LAC	K,2	
	CLA	JCOL-1,1	
	STO	JCOL-1,2	
	CLA	J	
	STO	JCOL-1,1	
	TRA	BL32	
BL34	CLA	K	
	CAS	M	
	TRA	BL35	
	TRA	BL35	
	ADD	=1	
	STO	K	
	TRA	BL32	
BL35	CLA	CHK	
	TNZ	BL41	
•			
•	PACK THE MATRICES		
•			
	CLA	=1	
	STO	J	
BL36	CLA	M	
	SUB	=1	
	PAX	,4	
	CLA	J	
	SUB	=1	
	LRS	35	
	MPY	CON1	
	LLS	35	
	PAC	,1	
	PAC	,2	
BL37	TXI	**1,1,-2	
	TXI	**1,2,-1	
INA1	CLA	**,1	***A
INA2	STO	**,2	***A
	TIX	BL37,4,1	
	CLA	J	
	CAS	M	
	TRA	BL38	
	TRA	BL38	
	ADD	=1	
	STO	J	
	TRA	BL36	
BL38	CLA	N	
	TZE	BL41	
	CLA	=1	

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	STO	J	
BL39	CLA	M	
	SUB	=1	
	PAX	,4	
	CLA	J	
	SUB	=1	
	LRS	35	
	MPY	CON1	
	LLS	35	
	PAC	,1	
	PAC	,2	
BL40	TXI	**1,1,-2	
	TXI	**1,2,-1	
INB1	CLA	**,1	***B
INB2	STO	**,2	***B
	TIX	BL40,4,1	
	CLA	J	
	CAS	N	
	TRA	BL41	
	TRA	BL41	
	ADD	=1	
	STO	J	
	TRA	BL39	
•			
•	RESET INDEX REGISTERS AND RETURN		
•			
BL41	LXA	IND1,1	
	LXA	IND2,2	
	LXA	IND4,4	
	CLA	CHK	
	TZE	MAINS	
	TRA	MAIND	
•			
•	RESERVED AREAS		
•			
A	BSS	1	
ALPHA	BSS	2	
B	BSS	1	
CHK	BSS	1	
DET	BSS	1	
I	BSS	1	
IFS	BSS	1	
IND1	BSS	1	
IND2	BSS	1	
IND4	BSS	1	
IP	BSS	1	
IROM	BSS	MMA/2	
J	BSS	1	
JCOL	BSS	MMA/2	
JP	BSS	1	
K	BSS	1	
M	BSS	1	
N	BSS	1	
ONE	DEC	1.0,	
PIVOT	BSS	2	
TEMP	BSS	1	
TEMP1	BSS	2	

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CON1 PZE MMAX 629MAINS
MMAX EQU 40 630M
END 631MAINS

* IBCMAP DPSUB DECK
* DOUBLE PRECISION SUBROUTINES FOR THE 7040 D SPEAS, L GANNON 9-63 0010PSUB
* MODIFICATION OF THE 7090 FORTRAN II SUBROUTINES FOR USE WITH 7040 MAP0020PSUB

* MS MOST SIGNIFICANT 0040PSUB
* LS LEAST SIGNIFICANT 0050PSUB
* ACH PSEUDO ACCUMULATOR MS 4) 1 FORTRAN II 0060PSUB
* ACL PSEUDO ACCUMULATOR LS 4)-1 0070PSUB
* ACH MQ MS 4)-2 0080PSUB
* ACL MQ LS 4)-3 0090PSUB

* Z= Y OP X YMS AND YLS MUST BE IN THE AC AND MQ, X IS
* SPECIFIED BY THE OP CODE, ZMS AND ZLS WILL BE
* IN THE AC AND MQ 0100PSUB

ENTRY DFAUS 0110PSUB
ENTRY DFSBS 0120PSUB
ENTRY DFMP 0130PSUB
ENTRY DFDP 0140PSUB

* DFAD ROUTINE 0150PSUB
DFADS PZE ** 0160PSUB
TSL SETADD 0170PSUB
CLA ACH MOST SIG. AC 0180PSUB
FAD XMS MOST SIG. VARIABLE 0190PSUB
STO ACH SAVE MOST SIG. SUM 0200PSUB
STQ ERASE3 LEAST SIG. PART OF SUM TO AC 0210PSUB
CLA ERASE3 0220PSUB
UFA ACL 0230PSUB
UFA XLS ADD LEAST SIG. PART OF VARIABLE 0240PSUB
FAD ACH ADD MOST SIG. SUM 0250PSUB
TRA DFAUS RETURN TO CALLING PROGRAM 0260PSUB

* DFSB ROUTINE 0270PSUB
DFSBS PZE ** 0280PSUB
TSL SETADD 0290PSUB
CLA ACH MOST SIG. AC 0300PSUB
FSB XMS MOST SIG. PART OF VARIABLE 0310PSUB
STO ACH SAVE MOST SIG. DIFFERENCE 0320PSUB
STQ ERASE3 LEAST SIG. DIFFERENCE TO AC 0330PSUB
CLA ERASE3 0340PSUB
UFA ACL PLUS LEAST SIG. AC 0350PSUB
UFS XLS LESS LEAST SIG. PART OF VARIABLE 0360PSUB
FAD ACH PLUS DIFFERENCE OF MOST SIG. PARTS 0370PSUB
TRA DFSBS RETURN TO CALLING PROGRAM 0380PSUB

* DFMP ROUTINE 0390PSUB
DFMPS PZE ** 0400PSUB
TSL SETADD 0410PSUB
LDQ ACH MOST SIG. AC 0420PSUB
FMP XMS MOST SIG. PART OF VARIABLE 0430PSUB
STO ERASE1 MOST SIG. PART OF PRODUCT 0440PSUB
STQ ERASE2 LEAST SIG. PART OF PRODUCT 0450PSUB
LDQ ACH MOST SIG. AC 0460PSUB
FMP XLS LEAST SIG. PART OF VARIABLE 0470PSUB

UFA ERASE2 PLUS LEAST SIG. PART OF FIRST PRODUCT 0540PSUB
STO ERASE2 SAVE 0550PSUB
LDQ XMS MOST SIG. PART OF VARIABLE 0560PSUB
FMP ACL LEAST SIG. AC 0570PSUB
UFA ERASE2 PLUS PREVIOUS PRODUCT OF LEAST PARTS 0580PSUB
FAD ERASE1 PLUS PRODUCT OF MOST PARTS 0590PSUB
TRA DFMP RETURN TO CALLING PROGRAM 0600PSUB

* UFDOP ROUTINE 0610PSUB
DFDPS PZE ** 0620PSUB
TSL SETADD 0630PSUB
CLA ACH MOST SIG. AC 0640PSUB
FDP XMS / MOST SIG. PART OF VARIABLE 0650PSUB
STQ ERASE1 SAVE MOST SIG. QUOTIENT 0660PSUB
UFA ACL REMAINDER PLUS LEAST SIG. PART OF VARIABLE 0670PSUB
FDP XMS / MOST SIG. PART OF VARIABLE 0680PSUB
STQ ERASE2 SAVE MOST SIG. PART 0690PSUB
CLS XLS 0700PSUB
FCP XMS $(A+B)/(C+D) = ((A+B)/C) * (1-D/C)$ 0710PSUB
FMP ERASE1 0720PSUB
UFA ERASE2 0730PSUB
FAD ERASE1 0740PSUB
TRA DFDP RETURN TO CALLING PROGRAM 0750PSUB

* SUBROUTINE TO SET THE RETURN ADDRESS AND THE ADDRESSES OF XMS AND
* XLS WHICH ARE USED INDIRECTLY IN THE ARITHMETIC SUBROUTINES 0760PSUB
* AND STORE THE AC AND MQ IN ACH AND ACL. 0770PSUB

* XMS ADDRESS OF ADDRESS OF MOST SIGNIFICANT PART OF VARIABLE 0780PSUB
* XLS ADDRESS OF ADDRESS OF LEAST SIGNIFICANT PART OF VARIABLE 0790PSUB

SETADD PZE ** 0800PSUB
SXA XA,4 0810PSUB
STO ACH 0820PSUB
LAC SETADD,4 0830PSUB
CLA -2,4 0840PSUB
STO XMS 0850PSUB
ADD =1 0860PSUB
STO XLS 0870PSUB
CLA -2,4 0880PSUB
ADD =1 0890PSUB
STO -2,4 0900PSUB
XA AXI ** 0910PSUB
TRA SETADD 0920PSUB

* XMS PZE ADDRESS OF MS 0930PSUB
XLS PZE ADDRESS OF LS 0940PSUB
ACH BSS 1 0950PSUB
ACL BSS 1 0960PSUB
ERASE1 PZE 1 0970PSUB
ERASE2 PZE 0980PSUB
ERASE3 PZE 0990PSUB
END 1000PSUB

1000PSUB
1010PSUB
1020PSUB
1030PSUB
1040PSUB
1050PSUB
1060PSUB
1070PSUB

```

C      SUBROUTINE GSHIFT(ISPUL,IPPLL,IPPUL,TRUE,AS,AL,BL,RATIO)
C      GAIN SHIFT SUBROUTINE
C      G.A.CAZIER PHILLIPS PETROLEUM CO.  NOVEMBER 1962
C
0 DIMENSION SPECT(400,26),ID(2,25),TITLE(11),ISPLTS(2,26),
1   IPPLTS(2,26),ID1(2,10),FIXINT(10),ID2(2,10),FIXRT(10),
2   INCLO(20),SIGMA(400),BGINT(6),JFS(26),JNIS(26),IFI(10),
3   IRI(10),IRED(10),BETA(10),BETP(10),SIGMAS(400),XICB(20),
4   JFST(20),RSDL(20),A(40,20),B(40,20),C(40,20),DATA(400)
0 COMMON SPECT,ID,TITLE,ISPLTS,IPPLTS,ID1,FIXINT,ID2,FIXRT,
1   INCLO,SIGMA,BGINT,JFS,JNIS,IFI,IRI,IRID,BETA,BETR,SIGMAS,
2   XICB,JFST,RSDL,A,B,C,DATA,JFSTO,IFS,JN,JNFI,JNRI,X1,X2,
3   JSUB,JWT,JNCLO,JOPT1,JOPT2,JNST,TPAGE
C
C      DIMENSION C2(400)
C      INITIALIZATION
C
306 IF(RATIO)307,306,307
   W = 100.0*DATA(IPPLL)**2
   DO 308 J=1,3
   DO 308 I=1,3
308   A(J,I)=0.0
   DO 500 I=1,3
500   B(I,1)=0.0
   XN=0.0
C
C      SUBTRACT STRAIGHT LINE AL+BL*CHANNEL NUMBER
C
410 IF(AL+BL)350,410,350
415 DO 415 I=1,ISPUL
   C2(I)=DATA(I)
   GO TO 309
350 DO 353 J=IPPLL,IPPUL
   X1=J
353   C2(J)=DATA(J)-AL-BL*X1
C
C      FORM SOLUTION MATRIX
C
309 DO 310 K=IPPLL,IPPUL
   XN2=XN*XN
   XN3=XN2*XN
   XN4=XN3*XN
   P=C2(K)*C2(K)/W
   ZN=ALOG(C2(K))
   A(1,1)=A(1,1)+P*XN4
   A(1,2)=A(1,2)+P*XN3
   A(1,3)=A(1,3)+P*XN2
   A(2,3)=A(2,3)+P*XN
   A(3,3)=A(3,3)+P
   B(1,1)=B(1,1)+XN2*P*ZN
   B(2,1)=B(2,1)+XN*P*ZN
   B(3,1)=B(3,1)+P*ZN
310   XN=XN+1.0
   A(2,1)=A(1,2)
   A(3,1)=A(1,3)
   A(2,2)=A(1,3)

```

```

A(3,2)=A(2,3)
C
C      CALCULATE THE POSITION OF THE PHOTO PEAK
C
   DET=C.0
   CALL MAINS(A,E,B,1,DET,IFS)
C
329 PPLL=IPPLL
   XO=(-B(2,1)/(2.0*B(1,1)))+PPLL
   RATIO=TRUE/(XC-AS)
307 X=0.0
   I1=0
   SPUP=ISPUL
   ISPULM=SPUP*RATIO+0.5
C
C      TEST DATA FOR ZERO COUNTS IN CHANNELS 1,2,3
C
   IF(DATA(1)) 312,313,312
313 IF(DATA(2)) 314,315,314
315 IF(DATA(3)) 315,318,316
C
314 DATA(1)=DATA(2)
   GO TO 312
316 DATA(1)=DATA(3)
   DATA(2)=DATA(3)
   GO TO 312
318 DATA(1)=DATA(4)
   DATA(2)=DATA(4)
   DATA(3)=DATA(4)
C
C      FIT 3 POINTS OF DATA WITH PARABOLA AND EVALUATE
C
312 X=X+1.0
   I1=I1+1
317 XP=(X/RATIO)+AS
   IF(XP-1.1600,600,603
603 IF(XP-2.1601,319,319
600 C2(I1)=DATA(I1)/RATIO
   GO TO 312
601 X1=1.0
   X2=2.0
   X3=3.0
   Y1=DATA(1)
   Y2=DATA(2)
   Y3=DATA(3)
   GO TO 604
319 IX2=XP+0.5
   IF(IX2-ISPUL)320,323,323
320 IX1=IX2-1
   IX3=IX2+1
   Y1=DATA(IX1)
   Y2=DATA(IX2)
   Y3=DATA(IX3)
602 X1=IX1
   X2=IX2
   X3=IX3
604 AA=(Y3-2.0*Y2+Y1)/2.0

```

```

      BB=1-Y3*(X2+X1)+2.0*Y2*(X1+X3)-Y1*(X3+X2))/2.0
      CC=((X1*X2*Y3)-2.0*(X1*X3*Y2)+(X2*X3*Y1))/2.0
323  C2(I1)=(AA*XP*XP+BB*X2+CC)/RATIO
      IF(ISPULM-I1)322,322,312
322  DO 324  I=1,400
324  DATA(I)=C.0
331  DO 330  I=1,ISPULM
330  DATA(I)=C2(I)
      ISPUL=ISPULM
      RETURN
      END

```


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