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A COMPUTER CODE TO ANALYZE ALPHA SPECTRA.(U)

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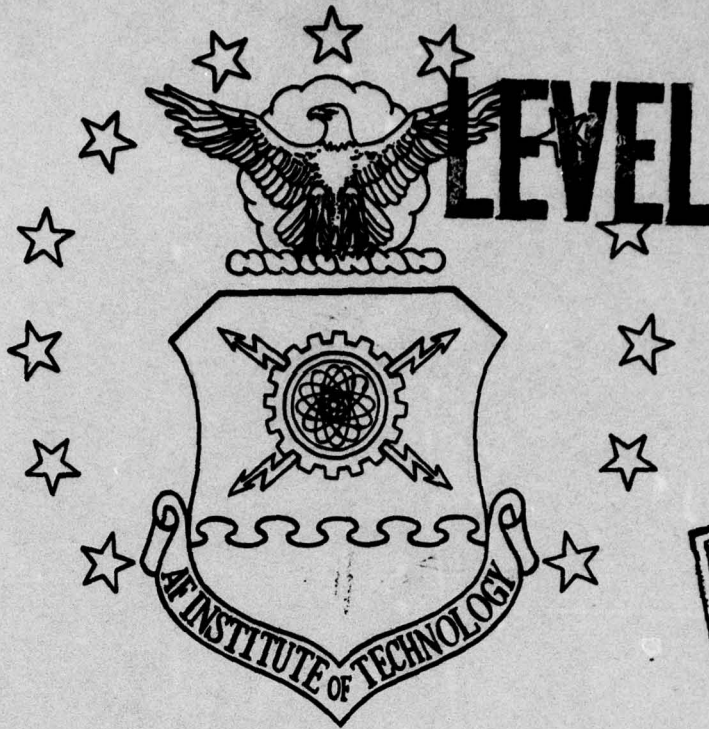
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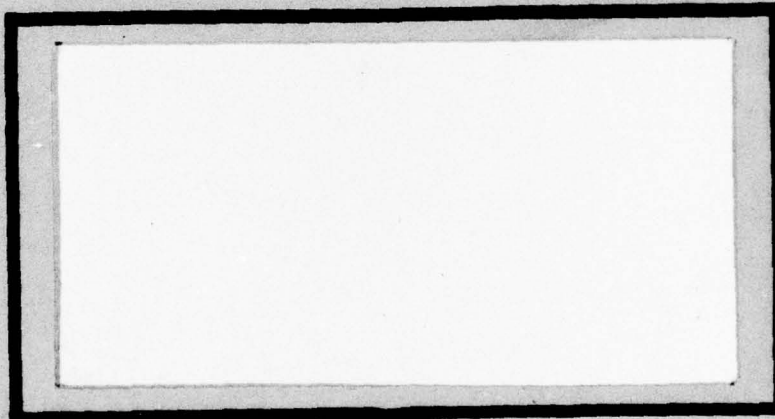
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A COMPUTER CODE TO ANALYZE

ALPHA SPECTRA

THESIS

Presented to the Faculty of the School of Engineering

Air Force Institute of Technology

Air University

in Partial Fulfillment of the

Requirements for the Degree of

Master of Science

By

Richard S. Hartley
2nd Lt USAF

Graduate Nuclear Engineering

March 1978

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Preface

This thesis is concerned with the development of a computer code to analyze alpha particle spectra. The reference peak used in the program, obtained from a Po^{210} source, was expressed as a table of values specifying the peak shape channel by channel. The results of the analysis were not within the limits desired but this is thought to be a result of different source thicknesses used.

I would like to extend my sincere gratitude to Dr. George John and Dr. Richard Hagee, my thesis advisors, and to Phil Poirier from whom the original program AUTOFIT was obtained. I would also like to thank Dr. Harold Kirby who enlightened me as to the depth of the problem which was to be undertaken, and Capt Jerome Clifford of the McClellan Laboratory for his interest in the project.

Finally, I would like to thank my wife Cathy, who typed this thesis and whose affection and understanding saw me through this project.

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Abstract

An existing computer code, written to analyze pulse-height spectra from charged particles measured with a mass spectrograph, was modified to analyze pulse-height spectra detected by semiconductor detectors. The program fits the spectra with a reference peak which is expressed as a table of values specifying the peak shape, channel by channel. The modification involved increasing the size of the reference peak to 2048 channels to allow analysis of pulse-height spectra from alpha particles with energies between 4 and 6 MeV. The results of the analysis were strongly dependent upon the reference peak chosen; hence, reference peak selection became the main emphasis of this report. The three reference peaks used were obtained from (1) an empirical function, (2) a single alpha peak obtained from Po^{210} , and (3) an entire spectrum of an isotope to be analyzed. It was desired that the error resulting in determining the area be within three standard deviations of the actual area. The error resulting in each analysis was greater than the prescribed value and was suspected to have occurred because of miscalculation of the reference peak.

A COMPUTER CODE TO ANALYZE ALPHA SPECTRA

I. Introduction

This report presents the results of an investigation of methods for the analysis of pulse-height spectra produced by alpha particles detected by semiconductor detectors. Several goals explored activities of radionuclides, resolution of spectra, the effects of parameters such as source thickness and width of pulse-height interval in obtaining the pulse-height spectra, and various types of algorithms to analyze pulse-height spectra. Major emphasis was placed on obtaining a peak shape representative of a single alpha peak and using this as a reference peak along with existing algorithms to fit alpha spectra.

Background

The general technique of pulse-height analysis consists of determining the area under each peak in the pulse-height spectrum. The area is frequently determined by obtaining an analytical expression which will reproduce the peak shape. The expression is fit to the data by the method of least squares; then numerically integrated to obtain the area. The area represents the total number of particles, with a certain energy, detected by the equipment.

The method of pulse-height analysis has been applied to gamma-ray spectra for quite some time. In gamma-ray spectra, the photopeaks are approximated by Gaussian functions, which can be numerically integrated without difficulty to provide

precise determination of the areas under the photopeaks.

Alpha particles unlike gamma-rays lose energy in small decrements as they collide with the atoms in the detector. As a result of the possibility of small energy losses, the peaks in the pulse-height spectrum are no longer characterized by a pure Gaussian function, but rather by a Gaussian shaped leading edge and an exponential shaped trailing edge. It is difficult to obtain an analytical expression for the resulting peak shape.

Currently, a crude alpha pulse-height analysis technique is being used to analyze alpha spectra obtained from sources, such as Pu^{239} and Pu^{240} . The transition energies of the alpha particles emitted by these isotopes differ by only a few keV; therefore, semiconductor detectors are not able to resolve the peaks resulting from each isotope. However, the contribution from each isotope can be determined by using the sum of the counts from both isotopes along with the known relative amounts of each isotope obtained by mass spectrometry. The limiting factor in this procedure is the determination of the absolute sum of the counts from both isotopes. A summation region approach is currently being used to determine the sum of the counts. This method consists of determining the area under the peak by summing the counts per channel for all channels within a specified region containing the peak. A serious drawback in this method results from information lost in the tails of the peaks. This occurs because of the necessity to specify a region into which the peak must fall. The regions chosen are mutually exclusive; hence, counts found in the long tail extending beyond

the specified region are lost. Greater precision could be obtained if the alpha spectra could be analyzed using a peak shape which would closely approximate the actual alpha peak shape.

Problem Statement

The object of this thesis was to modify an existing computer code and to obtain a peak shape representative of a single alpha peak. This peak shape was then used as a reference peak by the program to analyze the alpha spectra.

Scope

The study was restricted to the use of an existing computer code which was modified to allow analysis of alpha spectra. A reference peak representative of the peaks to be analyzed was required by the program to perform the analysis; hence, a large amount of effort was devoted to obtain a representative alpha peak.

General Approach

The program used in this study was obtained from a program called AUTOFIT, written by J. R. Comfort of Argonne National Laboratory. The major modification was to increase the allowed number of channels in the reference peak from 40 channels to 2048 channels. After modification, the program was renamed ALPHAFIT and was tested to determine its peak fitting capability.

An analytical function was used to generate emulated pulse-height spectra. For simplicity, a Gaussian pulse-height distribution was used. Studies were made of the capabilities of

the computer program to resolve two peaks whose relative amplitudes and positions were varied. Other variables studied were the effects of resolution and magnitude of pulse-height interval used to generate the simulated spectra. Two series of tests were performed. Statistical fluctuations of the individual points in the simulated spectra were included in the second series of tests, but not in the first series of tests.

Several methods were used to obtain a reference peak which would be representative of the alpha peaks to be analyzed. The first method, developed by P. De Regge (Ref 2:271-272), allowed a single alpha peak to be extracted from a complex alpha spectrum such as that obtained from Am^{241} .

The second method involved using a single alpha peak obtained from Po^{210} directly as a reference peak.

The last method was based on using an entire spectrum as a reference peak. Since the types of isotopes in the spectra are known, a reference peak composed of an entire spectrum of each isotope in the spectra can be used as a reference peak for that isotope. The resulting analysis should be more precise and less time-consuming than using single alpha peaks.

II. Theory

Before becoming involved in the techniques used to determine the area under the peaks in a pulse-height spectrum, it is important to know the cause and meaning of the pulse-height distributions. The information presented in this section describes the source of alpha particles and the way they interact with the detector to produce the pulse-height distributions. A method on how to relate the area under the pulse-height spectrum to the activity of the source is described followed by a description of the algorithm used by the program to minimize the error between the reference peak and the actual spectrum.

Alpha Decay Process

The motivation behind the development of a computer code to analyze alpha spectra was the need to analyze alpha spectra produced by mixtures of low-activity sources, such as plutonium, americium, and curium. However, during the development of the program, it was necessary to use sources of sufficient activity to reduce counting times and to increase counting statistics. The two main sources used in the developmental stage were Am²⁴¹ and Po²¹⁰. These isotopes decay by alpha particle emission either to the ground states or the excited states of their daughter nuclei. Figure 1 shows the simplified alpha decay scheme, describing the major branchings (Ref 4:435,403).

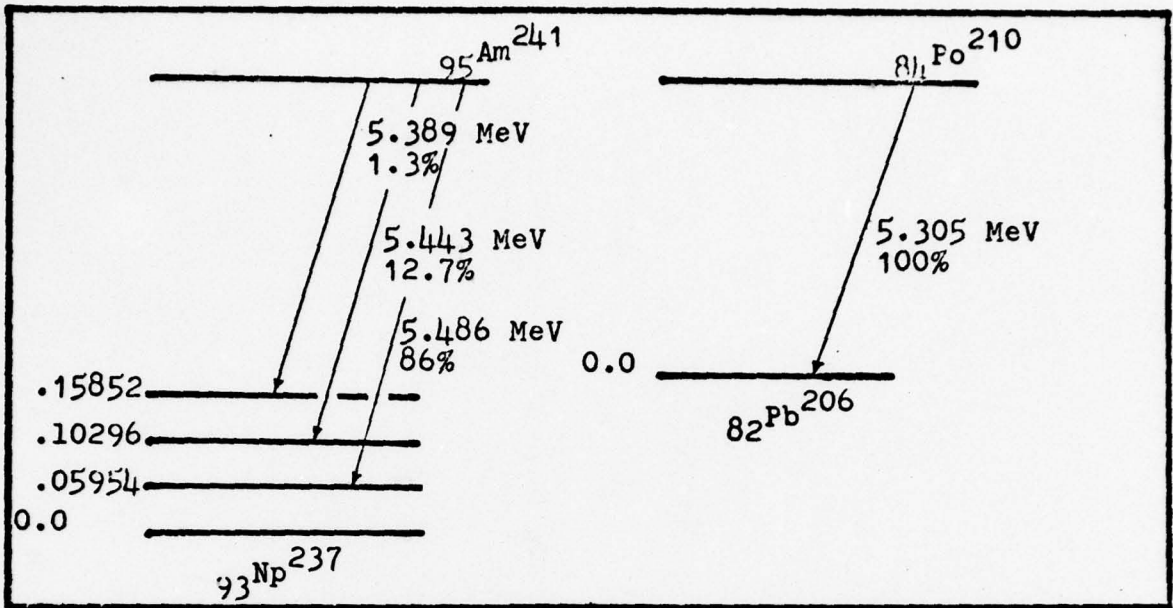


Figure 1. Decay Schemes for Am^{241} and Po^{210}

Alpha Particle Interaction

When alpha particles pass through matter, they lose energy by excitation and ionization of the atoms of that matter. The mechanism responsible for this energy loss is the interaction of the Coulomb fields of the particle with those of the bound electrons in the material. Deflection of the incoming alpha particles is negligible because of the large mass of the alpha particle relative to the mass of the electrons.

As an alpha particle passes through a medium, the energy dE transferred to that medium by ionization and excitation

along a differential path length dx is given by the following theoretical expression (Ref 5:3-4):

$$-dE/dx = 4\pi e^4 z^2 NB/mv^2 \quad (1)$$

where B is defined as the atomic stopping number and is given by

$$B = Z[\ln(2mv^2/I) - \ln(1-\beta^2) - \beta^2] \quad (2)$$

with

e = electronic charge

m = electron rest mass

E = kinetic energy of primary particle

ze = charge of primary particle

v = velocity of primary particle

N = number of absorber atoms per cm^3

Z = atomic number of absorber

β = v/c , where c = velocity of light in a vacuum

I = geometric-mean ionization and excitation potential of absorbing atoms; cannot be calculated accurately and generally regarded as a constant for each element. The value of I must be experimentally determined for each element.

In the nonrelativistic energy range, the rate of energy loss $-dE/dx$ depends on the velocity of the alpha particle through the $1/v^2$ term in Eq(1). The increase in the rate of energy loss with decrease in velocity is to be expected. At

lower velocity the alpha particle spends more time in the vicinity of bound absorber electrons, thereby increasing the probability of ionization and excitation.

In the relativistic energy range, the rate of energy loss $-dE/dx$ passes through a minimum which is followed by a slow increase with increasing particle energy.

The ranges of alpha particles, which are initially monoenergetic, are not precisely the same. This variation, or straggling, is due to the statistical nature of the energy-loss process. The energy losses which bring the alpha particles to rest consist of a large number of individual energy-transfer events of varying magnitudes. Most of the energy transfers are relatively small. The statistical nature of the energy-loss process allows variations in the number of events occurring per unit path length and variations in the amount of energy transferred per event. Few events involve large amounts of energy transfer.

The absorption of alpha particles is usually studied experimentally by measuring the number of ion pairs produced per unit path length of travel. This quantity is commonly referred to as the specific ionization. The rate of energy loss is related to the specific ionization through a quantity w , which is the ratio of the energy lost by a charged particle to the total ionization produced by that charged particle. Values of w depend upon the material and the state of the material with which interaction occurs, and the type and the energy of the incident particle.

Alpha Pulse Height Distributions

Alpha particles incident on solid state detectors deposit energy within the charge-depletion region of the detectors. The energy deposited by the alpha particles produces a number of charge carriers (electron-hole pairs) proportional to the energy deposited. These free charge carriers which are swept from the depletion region produce a pulse height which is proportional to the number of electron-hole pairs collected, and therefore proportional to the energy deposited by the incident radiation. The pulse height out of the detector can be expressed by the following equation:

$$ph = [(E_{dep}/w) \times e \times \gamma] \times 1/C \quad (\text{volts}) \quad (3)$$

with

E_{dep} = energy deposited by the alpha particle (eV)

w = average energy required for the production of an electron-hole pair (eV/e-h pair)

e = electron charge (coulombs)

γ = charge collection efficiency.
This is essentially 1 in detectors made of high quality single crystals

$N = E_{dep}/w$ = number of electron-hole pairs produced

$q = Ne\gamma$ = total charge collected (coulombs)

C = capacitance of the detector (picofarads)

Eq (3) can be rewritten as

$$ph = q/C \quad (\text{volts}) \quad (4)$$

The pulse-height at the output of the linear amplifier is given by

$$PH = q \times G \quad (\text{volts}) \quad (5)$$

with

q = total charge collected
(coulombs)

G = gain of linear amplifier
(volts/coulomb)

A multichannel analyzer is used to count the number of times pulses with amplitudes between h and $h + \Delta h$ occur during the acquisition time. This information is displayed on an oscilloscope with the pulse-height intervals plotted on the abscissa and the number of times each pulse-height is observed on the ordinate. Since the energy-loss process is statistical in nature, the resulting pulse-heights will form a pulse-height distribution. The energy of the alpha particles are associated with the location of the maximum in the pulse-height distribution. The distribution of pulse-heights does not reflect a distribution of energy lost by the alpha particles because each particle loses an energy E_0 in the detector. The tailing effect on the low energy side of the pulse-height distribution occurs when the energy of the alpha particles is degraded by passage through material in the source and the dead layer of the detector.

The length of the path and thus the loss in energy by each alpha particle depends on the angle at which it is emitted from the source and the extent to which it deviates from normal incidence when it passes through the dead layer of the detector. The effects of various path lengths of alpha particles through gold can be seen in Figure 2.

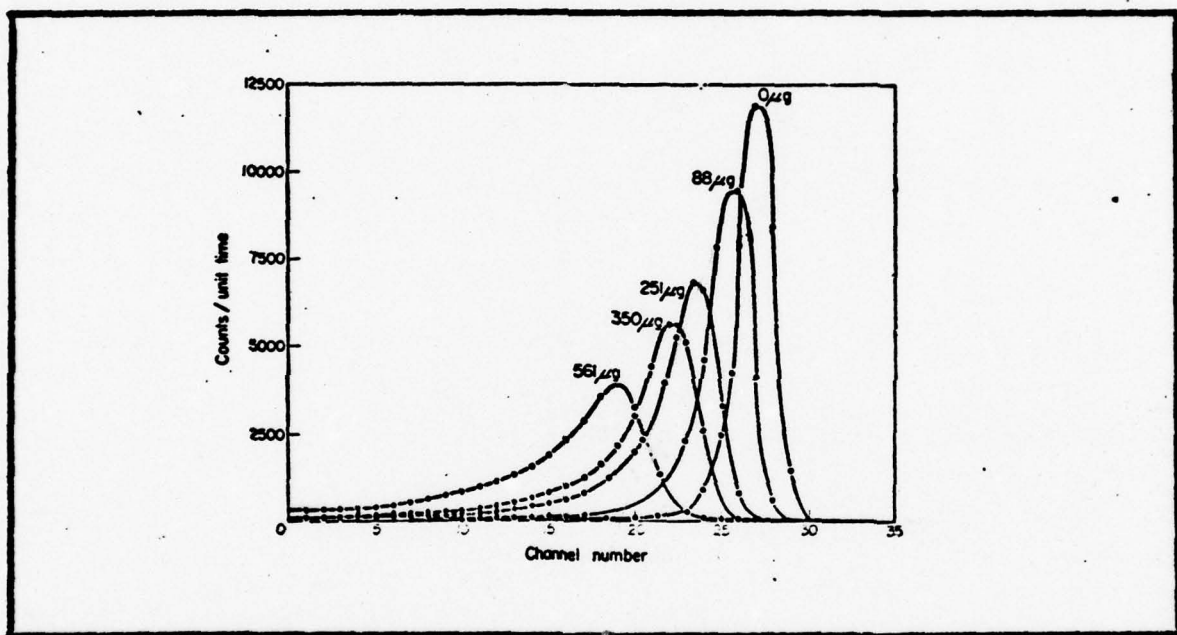


Figure 2. The α -particle Energy Distribution for a Thin Source of Pu^{239} After Transmission Through Various Thicknesses of Gold (Ref 6:108)

Electronic noise in the detection system will further increase the spread of the peak in the pulse-height spectrum. Electronic noise can be determined by measuring the spread in the pulse-height spectrum from a pulser signal which is equal to the average pulse-height produced at the input to the

preamplifier by the source. The peak spreading caused by electronic noise can be neglected in spectrum analysis if the same equipment is used to obtain both the reference peak and the data to be analyzed.

Relating Observed Counts To Activity

The pulse-height spectra obtained from alpha particles emitted by isotopes of the actinide series are expected to be a composite of peaks described above. In order to analyze these alpha spectra, it is necessary to determine the area under each peak in the spectra. After the area has been determined, it is necessary to determine the activity of the contributing isotopes. The area, which is the total number of counts observed for each isotope, can be related to the activity of the sample by the following equation:

$$N_t/t_c = A \times G \times f_{ss} \times f_w \times \delta \times f_t \times f_\alpha \quad (6)$$

with

N_t = total number of counts = the total area for each isotope

t_c = counting time (sec)

A = activity of source in nuclear transformations per second (ntps)

G = solid angle subtended by the sensitive region of the detector relative to the source

f_{ss} = scatter of radiation from surroundings

- f_w = absorption by air, detector window,
and dead layer
 δ = intrinsic efficiency of detector =
fraction of particles which enter
sensitive volume and produce a pulse,
assuming no dead time (#cnts/# α 's)
 f_t = correction for dead time
 f_α = number of alpha particles observed for
each nuclear transformation (# α 's/nt)

If it is assumed that equipment is not changed, scattering does not occur, and dead time does not exist, Eq (6) can be simplified and can be solved for the activity as follows:

$$A = (N_t/t_c) \times (1/f_\alpha) \times (1/G) \times (1/\delta) \quad (7)$$

Therefore, if the area of each peak in the spectrum can be calculated, then the activity of an unknown sample giving rise to those peaks can be determined.

Program ALPHAFIT

Program AUTOFIT was written to analyze charged particle spectra from a mass spectrograph. The modifications on AUTOFIT included (1) increasing the size of the reference peak from 40 channels to 2048 channels, (2) disposing of the peak search routine and Q-value options, and (3) decreasing the number of peaks to be analyzed from 200 peaks to 20 peaks. The peak fitting algorithms were not modified. After the above modifications were performed, the name of the program was changed to ALPHAFIT to avoid confusion. A detailed description of the peak analysis is listed below.

Detailed Peak Analysis. A complex spectrum can be represented by an array [E] which is formed from the sum of a set of resolved components Z(x). Each element of the array can be expressed as

$$E_i = \sum_{l=1}^L a_l Z_l(x_1) \quad (8)$$

where $Z_i(x_1)$ designates the number of counts in the i th channel of an unnormalized reference peak located at an abscissa x_1 , and a_l is a normalization factor. The sum extends over L individual components in the complex spectrum. The quantity $Z_i(x_1)$ is defined as zero if the reference peak located at x_1 does not extend to the i th channel. The quantities x_1 and a_l are varied until the array [E] is closely matched to the array of ordinates [Y] of the data. This is quantitatively accomplished by forming a chi-squared function

$$F = \sum_{i=1}^N (Y_i - E_i)^2 / (\delta Y_i)^2 \quad (9)$$

summed over all the channels of the data. The function F is then minimized with respect to a_l and x_1 . During minimization, the weights δY_i are taken to be $\sqrt{Y_i + 10}$, where Y_i is the ordinate of the i th data point. Since Poisson Statistics apply in counting experiments, this weighting factor is approximately equal to the square root of the variance. The addition of 10 to Y_i slightly increases the relative weighting of the data near the tops of the peaks and prevents division by zero.

The chi-squared function represents the ratio of the observed spread between the data and the reference peak to the expected spread between the data and the reference peak. By minimizing the chi-squared function, the best approximation to the real data is obtained.

Program ALPHAFIT separates the minimization of F with respect to the a_1 's and the x_1 's. If the x_1 's are known from the initial estimates of peak positions, the a_1 's can be obtained by setting the partial derivative of F with respect to a_1 equal to zero. The set of linear equations, which need to be solved in order to find the correct value of a_1 and which will allow minimization of F , is set up in Subroutine FCN. Standard matrix-inversion techniques are then used to solve these equations.

The position of the peaks are established by a variable metric minimization procedure (Ref 7:ANL-5990) coded in a set of subroutines. As the x_1 's are varied by Subroutine SHIFT, the function F is recalculated (each time with a best set of a_1 's) and inspected. If the change in F between successive complete iterations is less than a convergence criterion, the procedure is terminated. A final best set of a_1 's is calculated, and the results are transmitted to the calling program.

III. Experimental Equipment and Procedures

Introduction

In order to test Program ALPHAFIT, it was necessary to obtain selected alpha spectra with certain parameters fixed. For this reason experiments were performed on site with existing alpha sources such as Am²⁴¹, Po²¹⁰, and Pu²⁴⁰.

Equipment

The alpha spectroscopy was performed using a semiconductor detector in an evacuated chamber to maximize the resolution capabilities of the system.

Vacuum Chamber. The vacuum chamber was a two-piece, cylindrical steel canister. The top of the canister was fastened to a wood support which held the chamber assembly approximately one foot above the table top. Three openings were located in the top of the canister, two of which were an inlet and an outlet for the vacuum pump. The remaining opening allowed the direct connection of the preamplifier to the detector by two BNC connectors. The detector was mounted to the top of the canister and was facing downward toward the moveable source platform. The bottom portion of the canister was removeable to allow the changing of sources and was held in place by the vacuum created by the roughing pump.

Detectors. A high resolution detector with an active area of 25 mm² was used for data acquisition. The small surface of this detector required a necessary increase in the counting

times and required the reduction of the source to detector distance. The resolution obtained by this detector was 18 keV FWHM for the 5.486 MeV peak of Am^{241} with a source to detector distance of 1 cm. The resolution was not appreciably affected by variations in source to detector distances between 1 to 3 cm; however, the counting times for the sources used were much too long for distances above 1 cm.

Amplifiers. An ORTEC, Model 142-B, preamplifier was used in conjunction with a linear amplifier and a biased amplifier to obtain the desired alpha spectra. The linear amplifier was a Tennelec, Model TC203 BLR, and the biased amplifier used was a Tennelec, Model TC250A.

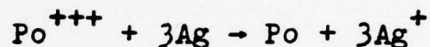
Experimental

Throughout the entire set of experiments, the maximum amount of separation between the peaks of the spectra was desired. This required using a biased amplifier which would cut out signals of low energy and expand the remaining signals to allow the maximum peak spread possible.

Energy Calibration. All energy calibrations were performed using the 5.486 MeV and the 5.443 MeV peaks of Am^{241} . The energy calibration obtained from Am^{241} was used when sources, such as Po^{210} (which has only one peak) and Pu^{240} (which had low activity), were used. It was assumed that the energy calibration obtained from Am^{241} could be used with other sources as long as the linear amplifier and the biased amplifier remained at the same settings.

Sources and Source Preparation. During the course of this study, six different sources were used. Three of the sources had been prepared at an earlier date. These sources were Am²⁴¹ with an activity of 0.1 μ Ci and two plutonium samples labeled Pu²⁴⁰ - 1 and Pu²⁴⁰ - 2 with activities of 2.583×10^5 α 's/min \pm 1.5% and 2.598×10^4 α 's/min \pm 2%, respectively.

Two polonium sources were made during the course of this study. The first polonium source, labeled Po²¹⁰ - 1, was made by the electrochemical displacement of Po²¹⁰ onto a silver disk from a RaDEF solution. The plating occurred because of the following reaction:



This disposition occurs without the application of external current when the RaDEF is dissolved in nitric acid (Ref 6:100). The activity of this polonium source was roughly approximated to be of the order of 0.03 μ Ci.

The second polonium source was prepared using a method described by H. W. Kirby (Ref 3:2043-2047). A half inch platinum square was rinsed in water; then fired to a red heat for ten to twenty seconds. After cooling, the square was sprayed with Krylon with the center of the square masked by a brass rod approximately 7 mm in diameter. The RaDEF solution which was in 0.8N HNO₃ was dried under a heat lamp; then redissolved with 1.5N HCL. The solution was placed in the center of the platinum

square which was then placed on a hot plate until the solution was completely evaporated. Then, 3N acetic acid was added to the center of the square and allowed to dry. The source was rinsed with water and then acetone to remove the Krylon. The activity was calculated to be approximately 1 μCi .

IV. Data Reduction

Three series of tests were performed on Program ALPHAFIT to determine its peak fitting capability.

Test Series I involved spectra composed of two Gaussian shaped peaks with statistical fluctuations which were generated to emulate spectra obtained by experimental methods. The purpose of this series of tests was to determine the error involved in determining the areas under the peaks when parameters such as peak amplitude, peak separation, and magnitudes of pulse-height intervals were varied.

Test Series II involved actual experimental spectra. The emphasis in this series of tests was to extract a single alpha peak shape from a complex alpha spectra by a method developed by P. De Regge (Ref 2:269-280).

Test Series III involved experimental spectra and emphasis was again placed on obtaining a single alpha peak shape. However, in this test series, the single alpha peak was obtained from Po^{210} , a single alpha emitter.

Test Series I

In this test series, a Gaussian pulse-height spectrum with statistical fluctuations was used to generate emulated pulse-height spectra. Studies were made of the capabilities of the computer program to resolve two peaks whose relative positions and amplitudes were varied along with variation in the magnitude of the pulse-height interval used to generate the simulated

spectra. The error involved in each study was reported in terms of relative percent error in peak area (RPE_A).

$$RPE_A = \left| (\text{computed area} - \text{actual area}) / \text{actual area} \right| \times 100 \quad (10)$$

If it is assumed that the statistical fluctuations in counts are described by a Poisson distribution, then the standard deviation in the number of counts is equal to the square root of the average total count or the square root of the area under the peak. In this report the criterion that the area computed should be within three standard deviations of the actual area was used in order for the results of the analysis to be valid. The satisfaction of this criterion would allow the user to state, with 99.7% confidence, that the limiting factor in the analysis is not the program but the counting statistics. This criterion can be expressed in terms of relative percent error in peak area due to statistical fluctuations ($RPE_{\sqrt{A}}$).

$$RPE_{\sqrt{A}} = (3\sqrt{\text{actual area}} / \text{actual area}) \times 100 \quad (11)$$

The results of the tests described above are plotted in Figures 4 and 5. In Figure 4 the relative percent error in peak area is plotted versus the separation of the peaks in units of full width at half maximum, whereas in Figure 5 the relative percent error in peak area is plotted versus the magnitude of the pulse-height interval in units of σ /channel where σ is the standard deviation of the Gaussian distribution. In each figure the error resulting in the determination of Peak 2 is being

plotted, Peak 2 (P2) being to the left of Peak 1 (P1) in the pulse-height spectrum. The two heavy dashed lines running horizontally across each graph signifies the relative percent error in peak area for one and three standard deviations. It is assumed that the results shown in Figures 4 and 5 are applicable to other complex alpha spectra obtained by experimental methods. The user must make certain that the spectrum to be analyzed has a peak separation and pulse-height interval which will allow the areas of the peaks to be determined within three standard deviations. This will not guarantee that the areas of the peaks in the experimental spectrum will be determined within three standard deviations, but affords the best possible chance of it occurring.

The program appears to operate more efficiently as the peak separation is decreased and as the pulse-height interval is increased. This unrealistic result which occurs for peaks of unequal amplitude is suspected to result from the minimization algorithm used by the program (see page 15). The exact cause was not investigated in this report; therefore, the results plotted in Figures 4 and 5 will be used.

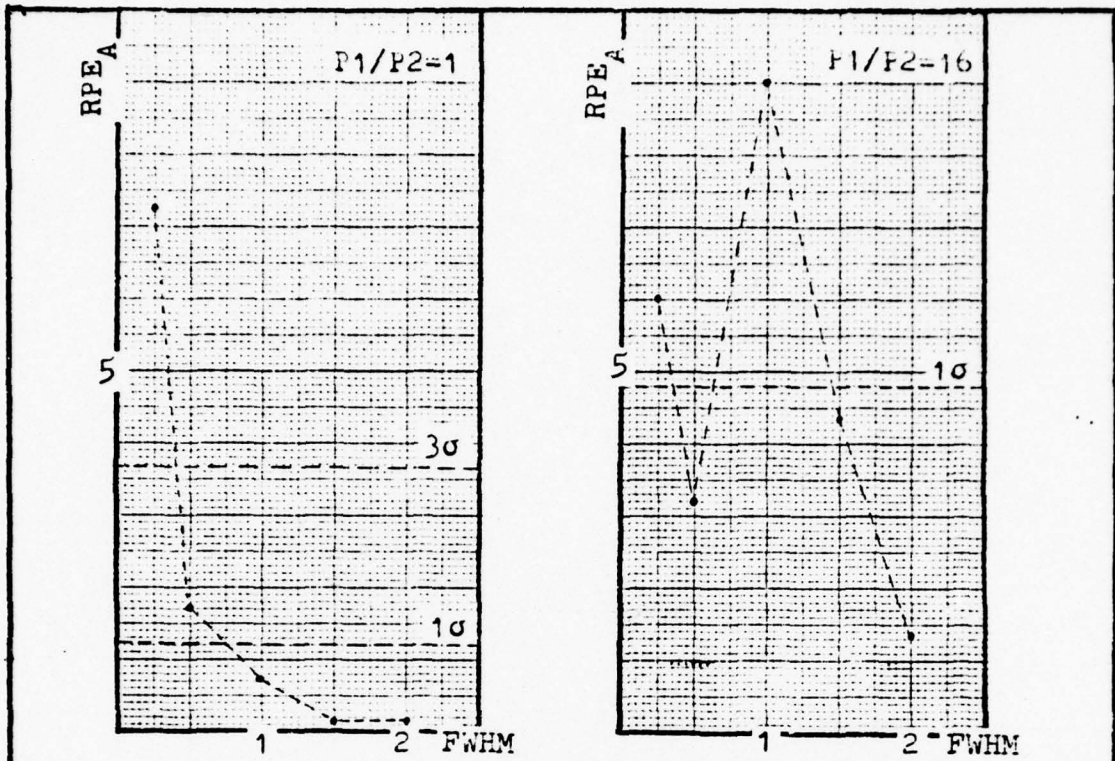


Figure 4. RPE_A vs. Separation in FWHM

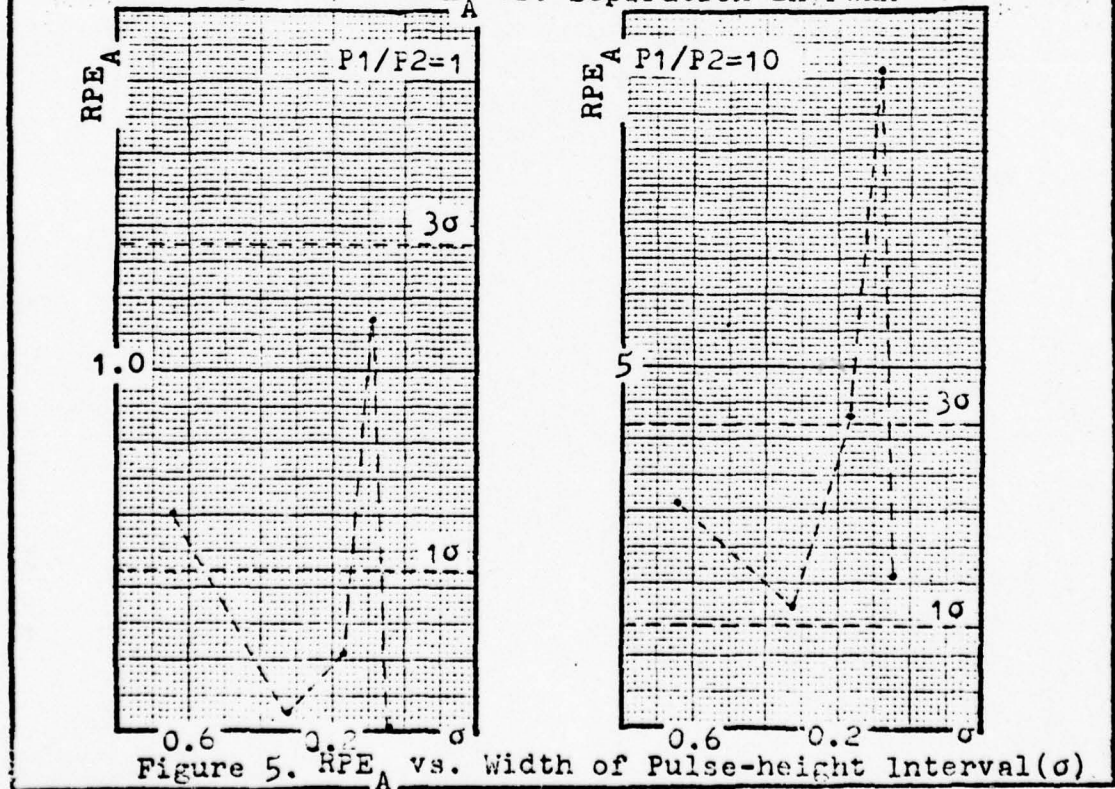


Figure 5. RPE_A vs. Width of Pulse-height Interval (σ)

Test Series II

After Program ALPHAFIT's peak fitting capability was determined using peaks of known areas, analysis of actual alpha spectra began.

The first alpha spectra were obtained from Am^{241} . The peaks resulting from Am^{241} had a separation greater than 1 FWHM. If it is valid to apply the results obtained in the limit of precision test on the ideal peaks to actual alpha spectra, the area under the peaks should be able to be calculated within three standard deviations if the correct reference peak is used. The problem which resulted was how to obtain the proper reference peak. All available sources of sufficient activities emitted at least three different energy alpha particles. Each alpha particle creates a peak with a long exponential tail. When more than one peak exists in the spectrum, confusion exists as to exactly how much each peak contributes to the tail.

Since it was impossible to obtain a reference peak directly from the Am^{241} , a method developed by P. De Regge was applied (Ref 2:269-280). De Regge based his empirical relation on observations made on a single alpha peak. It was suspected that the single alpha peak was obtained from Po^{210} . The empirical relation was derived from an alpha peak plotted in 2048 channels on semilog paper (schematically shown in Figure 6). The low energy side of the peak was divided into three regions. The first region ranges from 0 to 3 MeV below the peak energy and can be represented by a constant flat line (a-b).

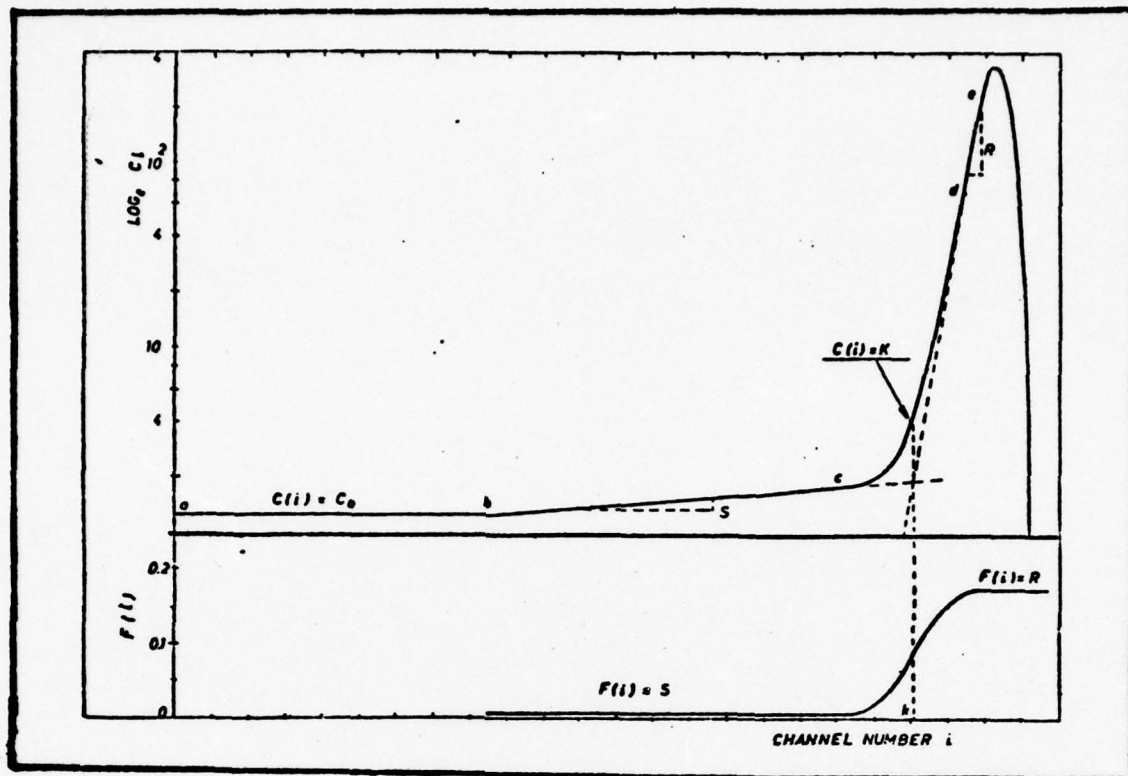


Figure 6. Schematic of De Regge's Alpha Peak

The second region can be best represented by a straight line (b-c) with a slope S. The third region can best be represented by a straight line (d-e) with a slope R, which is much greater than slope S. Considering the spectrum to the left of the peak value, the following equation was proposed:

$$C_{i+1} = C_i e^{F(i)} \quad (12)$$

where

C_i = content of channel i

$F(i)$ = a function of the channel number i

S for the region (b-c)

R for the region (d-e)

The transition region (c-d) between the two straight line sections can be represented by

$$C(i) = e^{\int F(i) di} \quad (13)$$

where the function $F(i)$ is best fit by a hyperbolic tangent function of the form

$$F(i) = (R+S/2) + [(R-S/2)\tanh\alpha(i-k)] \quad (14)$$

where α is a coefficient to accommodate various transitions from the tail to the peak regions. Negative as well as positive values are required for the argument of the hyperbolic tangent; therefore, the origin of the i -axis is shifted by an amount k to coincide with the bending point of the hyperbolic tangent. Integration of Eq(14) and substitution into Eq(13) yields

$$C(i) = 2^{1/z} K [e^{zR(i-k)} + e^{zS(i-k)}]^{1/z} \quad (15)$$

with K being the constant of integration and

$$z = 2\alpha/(R-S)$$

The tail region (b-c) is characterized by channel numbers $i \ll k$. The channel contents in this region yield a straight line with slope S on a semilog plot.

$$\ln C(i) = \ln K - 1/z \ln 2 + S(i-k) \quad (16)$$

The straight line with slope R , fitting the logarithm of the channel contents in the region (d-e), is given by

$$\ln C(i) = \ln K - 1/z \ln 2 + R(i-k) \quad (17)$$

The intersection point of these straight lines is located at channel number k .

Eq(15) is fit to the data by obtaining C_0 , the tail height between a and b , and determining the slope R from a least squares fit of Eq(17) to the logarithm of the contents of the channels between d and e . The slope S was found to be constant in several spectra and had a value of 0.004. The point b where the tail region changes from a constant value to a gently increasing curve was chosen as channel number $(k-700)$ according to observations made on several alpha spectra. Substitution of the above into Eq(16) yields

$$\ln C_0 = \ln K - 1/z \ln 2 - 2.8 \quad (18)$$

which, when substituted into Eq(17), yields

$$\ln C(i) = \ln C_0 + 2.8 + R(i-k) \quad (19)$$

which allows the calculation of the location of point k on the abscissa. The value of z is determined only by the ratio α/R since the value of S is much smaller than R . The ratio α/R is expected to be independent of the resolution and of the shape of the alpha peaks, because both α and R increase with better resolution. Values for $2\alpha/R$ have been found to be nearly constant and equal to 0.59 for typical resolutions between 20 and 80 keV.

The value of K is calculated by replacing $C(i)$ in Eq(15) with the real contents of a few undisturbed channels near the

top of the peak and by solving the equation for K. The mean value of K is then substituted back into Eq(15) to calculate the channel contents in the region (b-e). The high energy edge of the peak is assumed undisturbed and is simply integrated.

An attempt was made to apply the method described above to obtain a reference peak from an Am^{241} spectrum. This was done to determine whether the method developed by De Regge was applicable to alpha spectra other than Po^{210} . However, unlike De Regge, only 512 channels were used to store the spectrum. This was done to allow for easier manipulation of data. The Am^{241} spectrum was obtained in 512 channels with the aid of a biased amplifier which eliminated the low energy end of the spectrum and expanded the remaining spectrum. This allowed the prominent alpha peaks to be well separated but at the cost of losing the constant part of the tail (Region (a-b), Figure 6). It was impossible to determine the value of k using the method De Regge described above; therefore, a simpler method was devised.

An assumption was made from the outset that the addition of a biased amplifier would not change the values of the constants obtained by De Regge. A simplified method was then developed using this assumption and using the fact that the point k is located at the intersection of the lines drawn from (b-c) and (e-d) (see Figure 6). The line (e-d) and slope R were easily obtained by applying the method of least squares to the contents of a few channels near the top of the 5.486 MeV

peak of the Am^{241} spectrum. However, line (b-c) was not so easily obtained, and a few more assumptions had to be made.

The assumptions made in obtaining line (b-c) were

- a) each tail could be approximated by an exponential,
- b) the slope of each tail is the same,
- c) the total tail is composed of a linear combination of the contribution from each peak,
- d) each peak contributed an amount to the tail proportional to the area under its peak, and
- e) the tail contributions above the 5.486 MeV peak are negligible.

The total tail resulting from the three main alpha peaks can be represented by

$$N_i = C_1 e^{-S(x_{p1} - x_i)} + C_2 e^{-S(x_{p2} - x_i)} + C_3 e^{-S(x_{p3} - x_i)} \quad (20)$$

with

N_i = counts in the total tail in channel i

S = slope of tail as was defined by De Regge

x_{p1} , x_{p2} , x_{p3} = channel number of peak 1, peak 2, peak 3, respectively

C_1 , C_2 , C_3 = relative abundance of peak 1, peak 2, peak 3, respectively

x_i = channel number of interest

Peak 1 = 5.486 MeV peak of Am^{241}

Peak 2 = 5.443 MeV peak of Am^{241}

Peak 3 = 5.389 MeV peak of Am^{241}

The slope S was calculated by using a least squares fit on the tail of the Am^{241} spectrum. The peak locations were known and the constants C_1 and C_2 could be written in terms of C_3 . The constant C_3 could be calculated after substituting a known value for N_i , along with the corresponding channel number, into Eq(20). With C_3 known, the tail resulting only from the 5.486 MeV peak could be calculated. The point k was visually obtained by extending the line formed by this tail until it intersected line (d-e).

Having obtained the slopes S and R and the value of the point k , the next step was to determine the value of the integration constant K in Eq(15). The value of K was calculated by substituting a few values of $C(i)$ in Eq(15) with the real content of a few undisturbed channels near the top of the 5.486 MeV peak. The mean value of K was substituted back into Eq(15) to determine the intermediate channel contents between the tail and the top of the peak.

The values resulting from Eq(15) were checked against one important criterion. Since the actual data was being used to determine a reference peak shape, it would be necessary to require that the contents in every channel calculated by Eq(15) be less than or equal to the contents in the corresponding channel of the real spectrum. If the calculated peak violated this criterion, the peak would be considered invalid. Several different Am^{241} alpha spectra were analyzed using a reference peak obtained from Eq(15). The results of one such analysis are listed in Table I. The results from this analysis are not

directly comparable to those obtained by De Regge because his results represent an average of 13 separate measurements. Only a few of the many analyzes performed using the simplified method were able to satisfy the above criterion and so this method was not used.

Table I

Am^{241} Analyzed Using Reference Peak Obtained by
Eq(15) and Simplified De Regge Method

	<u>Alpha I</u>	<u>Alpha II</u>	<u>Alpha III</u>
Peak energy	5.486 MeV	5.443 MeV	5.389 MeV
Peak area	240799	37749	5187
Branching factor *	86.0%	12.7%	1.3%
Computed branching factor	84.4%	13.2%	1.8%
De Regge's computed branching factor	81.8%	14.5%	3.7%

*(From Ref 4:435)

Test Series III

This series of tests involved using the ability of Program ALPHAFIT to accept as reference peak as a table of values specifying the peak shape channel by channel. The tests series evolved around the single alpha emitter, Po^{210} . There were several desired objectives in using Po^{210} . These objectives included reproducing De Regge's work, with hopes of obtaining new constants, which would allow more reliable reproduction of the reference peak in different spectra and evaluating the change

of the resulting peak shape with source thickness. However, before any of these steps were begun, a series of tests were performed in which an actual Po^{210} spectrum was used as a reference peak. The empirical expression, developed by De Regge, was an approximation to a single alpha peak such as obtained from Po^{210} . The best fit that could be obtained would result when the mathematical expression exactly described the single alpha peak. De Regge states that alpha peaks have the same shape independent of their energy when thin sources are used (Ref 2:271). If this assumption is viable, then the limit of precision of the procedure developed by De Regge can be quickly determined by using the single alpha peak (such as obtained from Po^{210}) as the reference peak in the analysis. The results of this analysis are listed in Table II. Using Po^{210} directly as a reference peak did not seem to give better results than those obtained by De Regge's method. The larger error in branching ratios could have resulted from the effects of varying source thicknesses. The resulting error could mean that the sources are of different thicknesses and do not qualify as a thin source; hence, the sources are not expected to be fit using Po^{210} . The variations in source thicknesses are clearly evident in the analysis of $\text{Po}^{210} - 2$ using $\text{Po}^{210} - 1$ as a reference peak. The residual is very large and is due to a different source thickness and a different level of source contamination. A much improved analysis is expected to result when the sources are nearly the same thickness.

Table II
Isotopes Analyzed Using $Po^{210} - 1$ Directly
as the Reference Peak

$Po^{210} - 1$	<u>Alpha I</u>			
Energy (MeV)	5.305			
Computed Peak Area =	302894			
Actual Peak Area =	<u>302946</u>			
Residual =	52		$RPE_A = 0.02\%$	
$3\sqrt{A}$ =	1651		$RPE_{\sqrt{A}} = 0.55\%$	
Am^{241}	<u>Alpha I</u>	<u>Alpha II</u>	<u>Alpha III</u>	
Energy (MeV)	5.486	5.443	5.389	
Computed Peak Area	811711	80328	1178	
Branching Factor	86%	12.7%	1.3%	
Computed Branching Factor	90.9%	8.9%	0.13%	
Computed Total Area =	893217			
Actual Total Area =	<u>898127</u>			
Residual =	-4910		$RPE_A = 0.55\%$	
$3\sqrt{A}$ =	2843		$RPE_{\sqrt{A}} = 0.32\%$	
$Pu^{240} - 1$	<u>Alpha I</u>	<u>Alpha II</u>	<u>Alpha III</u>	<u>Alpha IV</u>
Energy (MeV)	5.499	5.456	5.168	5.123
Computed Peak Area	21939	8928	702697	493291
Branching Factor	0.1224%	0.0476%	74.75%	23.6%
Computed Branching Factor	1.8%	0.73%	57.3%	40.2%

Table II (cont.)

Pu²⁴⁰ - 1 (cont.)

Computed Total Area = 1229505

Actual Total Area = 1226633

Residual = 2872

RPE_A = 0.23% $3\sqrt{A}$ = 3323RPE _{\sqrt{A}} = 0.27%Pu²⁴⁰ - 2Alpha IAlpha IIAlpha IIIAlpha IV

Energy (MeV)

5.499

5.456

5.168

5.123

Computed Peak Area

2501

514

90664

30760

Branching Factor

0.1224%

0.0476%

74.75%

23.6%

Computed Branching Factor

2%

0.41%

72.9%

24.7%

Computed Total Area = 127271

Actual Total Area = 125341

Residual = 1930

RPE_A = 1.54% $3\sqrt{A}$ = 1062RPE _{\sqrt{A}} = 0.85%Po²¹⁰ - 2Alpha I

Energy (MeV)

5.305

Computed Peak Area = 8745688

Actual Peak Area = 8761782

Residual = -16094

RPE_A = 0.18% $3\sqrt{A}$ = 8880RPE _{\sqrt{A}} = 0.10%

Table II (cont.)

Composite Spectrum ($\text{Po}^{210} - 2$, Am^{241} , $\text{Pu}^{240} - 2$)				
Am^{241}	<u>Alpha I</u>	<u>Alpha II</u>	<u>Alpha III</u>	
Energy (MeV)	5.486	5.433	5.389	
Computed Peak Area	853899	80306	946	
Branching Factor	86%	12.7%	1.3%	
Computed Branching Factor	91.3%	8.6%	0.1%	
Computed Total Area	=	935151		
Actual Total Area	=	<u>898127</u>		
Residual	=	37024	$\text{RPE}_A = 4.12\%$	
$3\sqrt{A}$	=	2843	$\text{RPE}_{\sqrt{A}} = 0.32\%$	

Composite Spectrum (cont.)				
$\text{Pu}^{240} - 2$	<u>Alpha I</u>	<u>Alpha II</u>	<u>Alpha III</u>	<u>Alpha IV</u>
Energy (MeV)	5.499	5.456	5.168	5.123
Computed Peak Area	0	0	60259	15170
Branching Factor	0.1224%	0.0476%	74.75%	23.6%
Computed Branching Factor	0%	0%	79.9%	20.1%
Computed Total Area	=	75429		
Actual Total Area	=	<u>125341</u>		
Residual	=	-49912	$\text{RPE}_A = 39.82\%$	
$3\sqrt{A}$	=	1062	$\text{RPE}_{\sqrt{A}} = 0.85\%$	

Table II (cont.)

 Composite Spectrum (cont.)

Po²¹⁰ - 2 Alpha I

Energy (MeV) 5.305

Computed Peak Area = 1499604

Actual Peak Area = 1810354

Residual = -310750

RPE_A = 17.17%

3√A = 4036

RPE_{√A} = 1.30%

The last set of tests in Test Series III involved using an entire spectrum of an isotope as a reference peak. The composite spectrum to be analyzed is known to contain certain isotopes ($\text{Pu}^{240} - 2$, $\text{Po}^{210} - 2$, Am^{241}). Several experiments were performed in which the spectrum from each isotope was obtained. The three spectra were then added together to simulate a composite spectrum containing the three isotopes. During the analysis, the spectrum from each isotope was used as the reference peak for that isotope. The results of this analysis are listed in Table III.

Table III

Composite Spectrum Analyzed Using Respective Spectrum
from each Isotope as the Reference Peak

Composite Spectrum ($\text{Po}^{210} - 2$, Am^{241} , $\text{Pu}^{240} - 2$)				
	<u>Computed Area</u>	<u>Actual Area</u>	<u>Residual</u>	<u>$3\sqrt{A}$</u>
Am^{241}	2712695	898127	1814568	2843
$\text{Pu}^{240} - 2$	2578378	125341	2453037	1062
$\text{Po}^{210} - 2$	1995679	1810354	185325	4036

The residuals resulting from this analysis are well above the desired limit. This error is suspected to have resulted from not utilizing the program's full capability. The analysis was performed as follows:

- a) Spectrum to be analyzed read into program
- b) Reference peak (entire spectrum of one isotope) read into program
- c) Reference peak fit to the data and results printed out
- d) Program cleared
- e) Spectrum to be analyzed read back into program
- f) Next reference peak read into program
- g) Reference peak fit to the data and results printed out
- h) etc.

A better analysis would result if after the spectrum to be analyzed has been read into the program all three reference peaks were read into the program simultaneously. The program, working up to its full potential, could then vary the relative positions and amplitudes of the reference peaks to obtain the best fit possible.

V. Conclusions and Recommendations

Throughout this thesis, reference was made to the "proper reference peak". The "proper reference peak" is one which best represents the parent population. The "proper reference peak" was used in Test Series I. The spectra in these tests were the parent populations, statistically varied to simulate actual experimental spectra. However, this was done with the qualification that both the reference peak and the spectra were from the same type of source, having the same thickness and backing material.

The ability of Program ALPHAFIT to fit unknown alpha spectra depends upon the ability of the user to find the "proper reference peak". In order to find the "proper reference peak", one needs to study a single undisturbed alpha peak. This was done in the past using Po^{210} (Ref 2:269-280). Even after using the single alpha peak, De Regge had to try to find some empirical function which would allow him to approximate part of the peak. This approach gives good results, but errors result due to the assumptions made by De Regge. Most of the error arose from the empirical function used to represent the peak. Some error could have arisen from the assumption that a complex alpha spectrum is composed of individual alpha peaks which do not interfere with each other, but only add linearly to one another. With the aid of Program ALPHAFIT, the approximations used in trying to find an analytical function to describe the alpha peak are circumvented. Instead, the single alpha peak

from Po^{210} can be directly used by the program to analyze complex alpha spectrum. However, the assumption that complex spectra can be linearly composed of single alpha peaks must still be used. If this is true and if it can be assumed for the moment that for sufficiently thin sources (Ref 2:269-280) the alpha peaks will look the same, then ALPHAFIT should give the most precise results obtainable assuming the Po^{210} alpha peak is obtained by the same detector.

The last series of tests performed were based on the use of an entire spectrum as a reference peak. This would allow circumvention of both approximations made by De Regge. No empirical function would be needed, nor would there be a need for the assumption of linear addition of single alpha peaks. This should allow the most precise analysis possible. The fact that large errors resulted in the first attempt to apply this method should not hinder its further development. Perhaps a spectrum stripping approach would be advisable in this case.

The application of either method requires known samples of high activity to obtain good statistics in the tail region. If the same isotope is to be used to obtain this high activity source, it will require either more area or a thicker source. This is expected to reduce the effectiveness of the reference peak, because the peak shape will change. The change in peak shape should be relatively unchanged if thin sources are used (Ref 3:2043-2047). The exact error incurred would require further tests using varying source thicknesses.

At this time, there appear to be three different methods

which would allow a possible solution to the alpha fitting problem:

- I. Reproduce De Regge's work to determine the change in peak shape with source thickness.
- II. Investigate further the possibility of using a single alpha emitter such as Po^{210} as a reference peak.
- III. Investigate further the possibility of using each respective spectrum in the composite spectrum as a reference peak.

It would be advantageous to include a correction factor for source thickness in each of these methods. This could be accomplished with a library of reference peaks for sources of various thicknesses. An example of such a library could be taken from data such as is found in Figure 2. Knowing a few parameters, such as the shape of the high energy edge of the peak or the full width at half maximum, would allow the user to enter the library and pick the appropriate reference peak. If a sufficient number of reference peaks are catalogued, linear interpolation could be assumed between reference peaks. This would provide an unlimited number of possible reference peaks for a variety of source thicknesses.

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APPENDIX A

Program ALPHAFIT

Main Program. The main program controls the reading of the input cards, initializes variables, checks for error conditions, and prepares the data for analysis.

All of the data is read in the main program except for the spectrum data set, which is obtained from Subroutine SPCTRM. A subroutine, named ARYODR, is called to rearrange background points and peak positions into ascending order of abscissas.

As the data is prepared for analysis, the main program establishes the logic for selecting a reference peak, estimating peak positions, and removing background. Two subroutines, named BGRND and REFPEK, are called for establishing the background and the reference peak shape, respectively. Afterwards, a new spectrum with background subtracted is computed with the requirement that none of the computed ordinates be less than zero.

Before analysis of the peaks begins, a final check is made to determine whether the estimated peak locations are in the range of the spectrum. Peaks outside the range are deleted from further processing.

Subroutine RESLTS. Subroutine RESLTS is then called to process the data. Subroutine RESLTS transmits the spectrum to a subroutine, called PREPAR, which establishes the initial error matrix, the weights for the data points, and the convergence

criterion. On returning from Subroutine PREPAR, the normalized fitted peaks are summed to obtain the areas. A printout of the channel number, the raw data, the background, the normalized individual peaks (with background included), and the composite spectrum of the fitted peaks can be obtained by the user upon request.

A final summary page lists the information characterizing the spectrum and tabulates:

- a) peak position (channel number),
- b) error in peak position (channels),
- c) number of counts in the peak,
- d) statistical error in the number of counts computed by the program during analysis procedures,
- e) sum of the background underneath the peak, and
- f) estimated error in the number of counts (this is the square root of the sum of the counts and the background).

Subroutine REFPEK. The one characteristic that made this program look promising was the ability to input any peak shape. This reference peak is not obtained from an analytical function but is expressed as a table of values specifying the peak shape, channel by channel, with linear interpolation assumed between channels.

The reference peak is read into the computer in the main program, and then evaluated by Subroutine REFPEK. This subroutine uses parameters, such as peak width and shape, to

characterize the reference peak. The parameters used are the total width in channels and the distances DELTA1 and DELTA2 shown schematically in Figure 3.

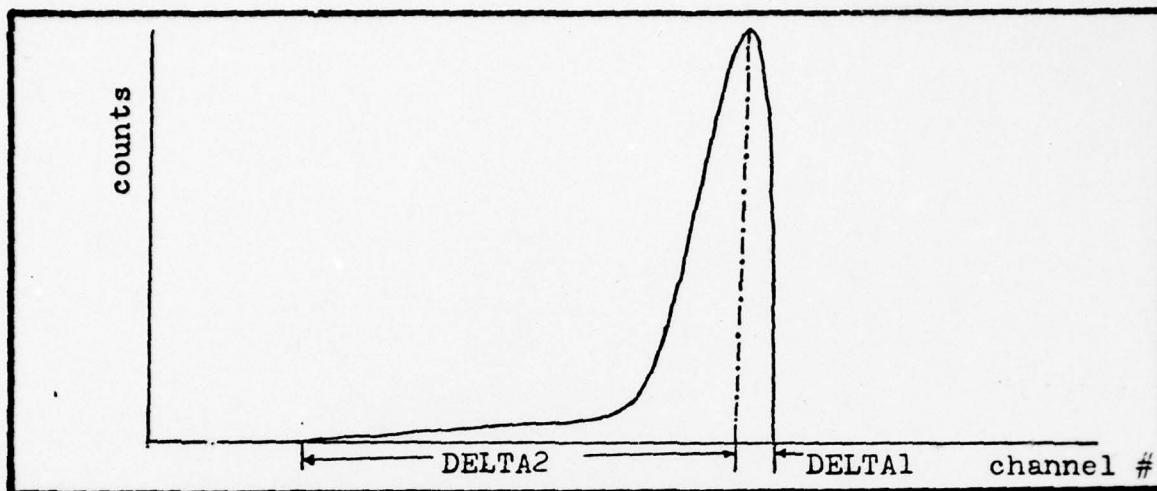


Figure 3. Reference Peak Shape

Subroutine BGRND. Three options are available for removing backgrounds from the spectrum. One option is completely automatic; the other two require information from the user.

Background option I allows the user to specify coordinates of a set of background points throughout the spectrum. Subroutine BGRND then calculates a continuous line that passes through all of these points. The regions between the points are calculated using Lagrange's three-point interpolation formula. Three successive points are used to calculate a curve between the first two points. The first point is then dropped, and the next three successive points are used to calculate the next section. This results in a final curve which is a patchwork of parabolas. The computed background line is continuous,

but its derivative may be discontinuous at each background point. The background is never allowed to be less than zero.

With background option II, the spectrum can be divided into sections with a constant background value in each section. The limits of the sections and the background value of those sections are supplied by the user. This option is useful when the user desires to have a constant background for the entire spectrum.

Background option III, the automatic background option, requires that the estimated locations of the peaks be supplied. Subroutine BGRND examines the regions between such peaks and excludes the channels that contain the tails of the peaks. If such a region is longer than ten channels, it is divided into subregions of about ten channels each. The abscissa of a background point is taken to be the midpoint of the abscissas of the subregion, and the ordinate of a background point is taken to be the average of the ordinates of the data points in the subregion. Since most physical spectra have backgrounds that decrease as the channel number increases, a constraint is imposed on the background points. The ordinate of each new background point $Y_{b,i}$ is compared with the ordinate of the last background point $Y_{b,i-1}$. If the new background point exceeds the value $Y_{b,i-1} + 2\sqrt{Y_{b,i-1}}$, the point is rejected. After at most fifty background points have been selected, a subroutine, named LSQPOL, applies the method of least squares to compute a polynomial of order less than four through the background points.

APPENDIX B

INPUT CARDS FOR PROGRAM ALPHAFIT

<u>Column</u>	<u>Variable</u>	<u>Value</u>	<u>Usage</u>
<u>CARD 1.</u> Title Card			
	TITLE (1), I = 1, 8		
	FORMAT (8A10)		
1-80	TITLE =		Any alphanumeric string.
NOTE:	If columns 1-4 are blank, the program terminates. The program also terminates on an end-of-file card.		
<u>CARD 2a.</u> Option Control Card			
	NBACK, NPKRD, NREF, NSSW1, NSSW2, MAXREF		
	FORMAT (I4, 4I2, I4)		
1-4	NBACK =	0	Background determined automatically by program.
	=	+n	Background option I. The X and Y coordinates for n background points will be read in; program calculates a curve passing through all points.
	=	-n	Background option II. n background intervals will be read in (background is a constant between the limits of each interval).
NOTE 1:	$n \leq 50$.		If $n > 50$, the program will truncate it to 50.
NOTE 2:	$n \geq 3$ for background option I (positive sign). But also see Note 2 for card 3.		
5-6	NPKRD \geq	+1	Initial peak positions to be read, as values of channel number.

7-8	NREF	=	0	Reference peak to be selected from spectrum. (This option is generally not recommended.)
		=	-1	Reference peak values to be read from separate cards.
10	NSSW1	=	0	Suppress printed output from variable-metric-minimization routines. (Standard!)
		=	1	Print the v.m.m. calculations.
12	NSSW2	=	0	Suppress printed output of raw data, resolved peaks, and composite spectra.
		=	1	Print the above.
13-16	MAXREF	=		The maximum number of channels in the reference peak.

CARD 2b. Option Control Card

KEPREF, KEPDAT
 FORMAT (I1, 3x, I1)

1	KEPREF	=	0	New reference peak used for each spectrum analyzed.
		=	1	Allows the reference peak to be kept for next analysis.
5	KEPDAT	=	0	New data spectrum to be analyzed.
		=	1	Allows the data spectrum to be kept for next analysis.

CARD 3. Background Data Cards (Not used for NBACK = 0.)

DB(I), BACK(I), I = 1, NBACK
 FORMAT (16F5.0)

1-5	DB(I)	=		For NBACK > 0 (option I):
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11-15, etc.

DB(I) is the channel number at which a background value is to be specified.

For NBACK < 0 (option II):

DB(I) is the channel number at the lower end of the Ith interval for which a background value is to be specified. DB(1) is supplied by the program and may be left blank.

6-10 BACK(I) = The value of the background for the Ith background position (NBACK > 0), or for the Ith background interval (NBACK < 0).

NOTE 1: The pairs DB(I), BACK(I) may be given in any order. The program will rearrange them in increasing order of DB(I).

NOTE 2: For NBACK > 0, the program requires backgrounds for the first and last channels of data. If not given explicitly, the program will use BACK (1) for the first channel, and BACK (NBACK) for the last channel. These program-supplied values may be counted for meeting the minimum requirement of 3 background points.

CARD 4a. Reference Peak Values Card (Use only for NREF < -1.)

N

FORMAT (I4)

1 N = The number of channels in the reference peak.

DUMCHN, (STOREF(J+K), K = 1, 10)

FORMAT (F6.0/10(F6.0, 2x))

1-6 DUMCHN = Every tenth channel number of the reference peak. These values are not needed in the reference peak and so are not stored. This allows cards punched from MCA to be read without conversion.

CARD 6. Peak Position Cards (Use with NPKRD > +1.)

PEKPOS(I), IFIXPK(I)

FORMAT (F9.4, I1)

- | | | | | |
|-----|-----------|---|------------|---|
| 1-9 | PEKPOS(I) | = | | The estimated third-height location of the <u>I</u> th peak to be considered by the program, specified in channel number. |
| 10 | IFIXPK(I) | = | 0 or blank | The program will adjust PEKPOS(I) for the best fit to the data. (Standard option.) |
| | | > | 1 | PEKPOS(I) will be held fixed by the program. |

NOTE: The cards may be in any order. The program will rearrange them into ascending order of PEKPOS(I).

CARD 7. Peak Position Termination Card

PEKPOS(I) < -1.0 This will terminate peak locations and the program will process a new set of data, beginning with Card 1.

APPENDIX C

RECOMMENDATIONS FOR INPUT

The following suggestions are intended to aid the user in setting up the input card decks to ALPHAFIT.

Backgrounds

The automatic background option is sometimes capable of providing a reasonable estimate of the background, but it can also produce very unrealistic results. The use of the automatic option is not recommended if high-quality results are desired. Background option I (NBACK > 0) gives the user the maximum control over the background curve. If enough points are specified, the background can be tailored to any specification.

With background option II (NBACK = -1) constant backgrounds can be entered into the program. Option I can also be used with NBACK = +1 if DB(1) specifies any abscissa in the middle of the spectrum and BACK(1) specifies the background value.

Peak Selection

The option that requests the program to hold positions of peaks fixed while obtaining their areas is not generally recommended. It is useful if the program has troubles in separating closely-spaced peaks whose positions are known in advance. However, the positions of peaks are almost never known a priori. Even if their energy values are precisely known, experimental uncertainties and insufficient yields may make their positions in a spectrum poorly known.

Printout Options

The input $NSWW1 = 1$ produces messages from the variable-metric-minimization package. This is useful for error tracing or debugging. Otherwise, set $NSSW1 = 0$.

The input $NSSW2 = 1$ produces a printout of the channel numbers, raw data, and individual peaks fit to the raw data. It is sometimes useful if the user wishes to make minor corrections to the final results from ALPHAFIT by manually summing the counts in a peak.

APPENDIX D

INTERPRETING THE OUTPUT

Special Messages

Most of the printed output is self-explanatory. In addition to the error messages indicating improper data (listed in the descriptions of the utility subroutines), a few other messages can be produced under special conditions.

nn Peaks Deleted. Some of the peak positions that were read in are not in the range of abscissa values.

Epsilon Too Small--Cannot Converge For Peaks At xxx, yyy. Twenty-five complete iterations have been made by the variable-metric package in an attempt to minimize the function F for the peaks located at the positions listed. Convergence was not achieved and the results of the last iteration are returned to the calling programs. Normally, these are sufficiently accurate. However, this message is sometimes produced if the spectrum is very complex and either too many or too few peaks are specified. One should revise the estimates of the peak positions and rerun the program.

Results of the Peak-Fitting Analysis

The final printed summary of results should be examined for signs that the calculated fits to the data may not be reliable. If necessary, the input deck can be revised and another pass made.

Errors. One can roughly estimate the errors expected for

the final positions and areas of the peaks and compare these with the calculated errors. Large discrepancies require attention. The expected error in the area (NUMB. COUNTS) A is \sqrt{A} . The expected error in the peak position is roughly $FWHM/(2.5\sqrt{A})$, where FWHM is the full-width at half maximum of the peak.

Normally, the positions and areas of the peaks will be determined much more precisely than the listed errors would indicate. A large discrepancy between estimated and listed error is thus only a sign that the program experienced difficulties in the analysis, not that the answers are necessarily unreliable.

Negative Peaks. The program sometimes produces peaks with negative areas. This is usually a sign that ALPHAFIT has been asked to place too many peaks in a small region. Some should be eliminated and the data should be reanalyzed. If the user intends to have all the peaks he requested, a revised set of estimated peak positions can sometimes eliminate negative peaks.

Peaks with Zero Areas and Errors. The printout may show that some peaks have areas and errors which are exactly zero. This results from a spurious condition. During the variable-metric analysis, these peaks have been moved outside the range of the spectrum in the work area (not outside the total spectrum) and therefore have zero amplitudes. The errors are arbitrarily set to zero. The cause is usually the same as for negative peaks and should be treated accordingly.

Appendix E:
Program ALPHAFIT Listing

```
PROGRAM ALPHET (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT, PUNCH,  
1 TAPE7=PUNCH, TAPE8)  
PROGRAM ALPHET WAS OBTAINED FROM PROGRAM AUTOFIT WRITTEN BY  
J.P. COMFORT OF ARGONNE NATIONAL LABORATORY  
THIS PROGRAM ALLOWS THE FOLLOWING:  
A MAXIMUM OF 2112 CHANNELS FOR A REFERENCE PEAK  
A MAXIMUM OF 2112 CHANNELS FOR A SPECTRUM  
A MAXIMUM OF 50 CHANNELS FOR A BACKGROUND INPUT  
COMMON /A00/ VM1(732), NSSW1, NSSW2  
COMMON /A02/ DIMENS(161), STORV1(2100), RAWX(2100), ITIME, NNX  
COMMON /A03/ TITLE(20), PEKPOS(20), IFIXPK(20), BETA, GSTATE,  
1 GSSVAL, NT, NCALO, IGS, LO  
COMMON /A04/ INTREF(20,10), STOREF(2100), DELTA1, DELTA2, DELTA3,  
1 STOIPP, REEMAX, ID1, ID2, IDT, NB, NF, NREF  
COMMON /A05/ BACK2(2100), OR(50), BACK(50), NJ, NBACK, NPKRD  
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNDI, TODAY, FREQ, OFTEN,  
1 NOFTEN, NCHAIN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2  
COMMON /OPTM/ KEFREF, KEFDAT  
DIMENSION REFSID(2100)  
EQUIVALENCE (IBLNK, BLNK, OBLNK)  
DATA (OBLNK=34 )  
...START CALCOMP AND GET DATE...  
IERR = 0  
CALL DATE(TODAY)  
GO TO 50  
...TERMINATE PROGRAM...  
45 WRITE(5,101)  
101 FORMAT(3X,184 ENDPLOT EXECUTED)  
STOP  
...READ AND WRITE TITLE CARD. EXIT ON E.O.F...  
50 READ(5,10) (TITLE(I),I=1,8)  
IF (EOF(5)) 45,49  
49 IF (TITLE(1).EQ.OBLNK) GO TO 45  
WRITE(5,30) (TITLE(I),I=1,8), TODAY  
...INPUT OF DATA...  
READ(5,12) NBACK, NPKRD, NREF, NSSW1, NSSW2, MAXREF  
KEFREF IS AN OPTION TO ALLOW THE USER TO KEEP THE SAME REFERENCE  
PEAK FOR ALL ANALYSIS  
KEFREF.GT.0 ALLOWS THE USE OF THE SAME REFERENCE PEAK FOR ENTIRE  
ANALYSIS  
KEFREF.EQ.0 REQUIRES A NEW REFERENCE PEAK WITH EACH SPECTRUM  
ANALYZED  
KEFDAT IS AN OPTION TO ALLOW THE SAME DATA SET TO BE USED FOR ALL  
ANALYSIS.  
KEFDAT.GT.0 ALLOWS THE SAME DATA SET TO BE USED FOR THE ANALYSIS.  
KEFDAT.EQ.0 REQUIRES A NEW DATA SET FOR EACH ANALYSIS.  
READ*, KEFREF, KEFDAT  
MAXP2 = MAXREF + 2  
IF (NREF.GT.20) NREF = 11  
WRITE(5,32) NBACK, NPKRD, NREF, NSSW1, NSSW2, MAXREF  
PRINT*, " KEFREF = ", KEFREF, " KEFDAT = ", KEFDAT
```

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      IF (NRACK) 70,110,80
70  NJ = -NRACK
      NRACK = 2
      GO TO 90
80  NJ = NRACK
      NRACK = 1
90  IF (NJ.GT.50) NJ = 50
      READ(5,14) (DB(I),PACK(I),I=1,NJ)
      IF (NJ.GT.1) CALL ARYODR(DB,PACK,NJ,2)
      ...INITIALIZATION...
100 LO = 0
      STOTPR = 0.0
      DO 105 I=1,20
105  IFTYPK(I) = 0
      DO 110 I=1,MAXREF
110  STORF(I) = 0.0
      ...MORE DATA INPUT...
      IF (NREF) 120,130,150
120  IF (KEPREF.GT.0) GO TO 778
      READ*,N
      IF (N.GT.MAXREF) N = MAXREF
      DO 777 I=1,N,10
      J = I-1
      READ 111,DUMCHN,(STORF(J+K),K=1,10)
111  FORMAT(F6.0/10(F6.0,2X))
777  CONTINUE
      NSTOP = N
      DO 77 I = 1,N
      REFSO(I) = STORF(I)
77  CONTINUE
      GO TO 1100
778  DO 79 I = 1,NSTOP
      STORF(I) = REFSO(I)
99  CONTINUE
1000 CONTINUE
      GO TO 150
130 READ(5,18) STOTPR,DELTA1,DELTA2,DELTA3
150 CONTINUE
      ...GET A STANDARD SPECTRUM DATA SET...
      IF (KEPSTAT.GT.0) GO TO 170
170 CALL SPOTRM
175 IF (IFER.GT.0) GO TO 45
      WRITE(5,34) NCHAN
      DELTA3 = 0.0
      ...READ PEAK POSITIONS, DISTANCE
200 DO 220 I=1,21
210 READ(5,24) PEKPOS(I),IFTYPK(I)
      IF (PEKPOS(I).LE.-1.) GO TO 230
220 CONTINUE
      NT = 20
      GO TO 240

```

```

231 NT = T - 1
241 IF (NT.GT.1) CALL AFXCOR(PEKPOS,IFIXPK,NT,0)
331 DO 351 I=1,NCHANN
351 RAWX(I) = COUNTS(I)
    ...CALC. BACKGROUND, SELECT REFERENCE PEAK AND PICK PEAKS...
    MNX = 0
    IF ((NPACK.EQ.0).AND.(NPKRD.EQ.0)) GO TO 440
    IF (NPACK.EQ.0) GO TO 370
    IF (DB(1).LT.DIST(1)) DB(1) = DIST(1)
    IF (DB(NJ).GT.DIST(NCHANN)) DB(NJ) = DIST(NCHANN)
370 CALL BGRND
    MNX = MNX + 1
    DO 420 I=1,NCHANN
    IF (RAWX(I) .GT. 420,420,410)
410 RAWX(I)=RAWX(I)-BACK2(I)
    IF(RAWX(I).LT.0.0) RAWX(I) = 0.0
420 CONTINUE
440 CALL REFPEK
    IF (NPKRD.NE.0) GO TO 500
460 DO 470 I=1,NT
470 PEKPOS(I) = PEKPOS(I) + DELTA3
    IF (MNX) 370,370,520
500 WRITE(6,38)
    GO TO 530
520 WRITE(6,40)
    ... MAKE SURE THAT ALL PEAKS ARE IN THE RANGE OF THE SPECTRUM
530 M = 0
    DO 550 I=1,NT
    IF ((PEKPOS(I)-DELTA2-2.*CFEN).LT.DIST(1)) GO TO 550
    IF ((PEKPOS(I)+DELTA1+2.*CFEN).GT.DIST(NCHANN)) GO TO 550
    M = M + 1
    PEKPOS(M) = PEKPOS(I)
    IFIXPK(M) = IFIXPK(I)
550 CONTINUE
    IF (M.GE.NT) GO TO 580
    T = NT - M
    WRITE(6,44) I
580 NT = M
    WRITE(6,42) (PEKPOS(I),I=1,NT)
    DO 600 I=1,NCHANN
600 STORV1(I) = BACK2(I)
    CALL RESULTS
    GO TO 50
11 FORMAT(3A10)
12 FORMAT( I4,4I2,I4 )
14 FORMAT(15F5.0)
15 FORMAT(15,15F5.0)
13 FORMAT(4F10.5)
24 FORMAT(F9.4,I1,F10.5)
30 FORMAT(1H1,1X,5A10,10X,A10)
32 FORMAT(10H0
    4XBHNPACK = I4,4XBHNPKRD = I2,4X7HNREF = I2
    1,4X7H
    4XBHNSW1 = I2,4XBHNSW2 = I2,4X9H1AXPEF = I4)

```

```
3. FORMAT(11H0 NCHAN = I3,FY7H )
33 FORMAT(35H0 INITIAL GUESSES OF PEAK POSITIONS)
43 FORMAT(40H0 CALCULATED ESTIMATES OF PEAK POSITONS)
42 FORMAT(11F12.7)
4. FORMAT(140,I4.14H PEAKS (LETED)
END
SUBROUTINE RESULTS
DIMENSION ENT(3), WORD(21)
DIMENSION PEKPR(200), PKBACK(210), XSECTS(200), XSECFR(200),
1 DELT(200), EX(200)
COMMON /A00/ V44(502), IHOLD(20), NSSW1, NSSW2
COMMON /A11/ STOPT(2102,20), S(2102), IZSTRT(21), IZSTOP(20), RUM(9538)
COMMON /A12/ SIGMA(20), ERR7(20), PERSTO(21), STOPHH(20),
1 XINTIS(20), INDEX(20), INITAL(20), IFINAL(20), STORV1(2100),
2 PAWX(2100), ITMES, NNY
COMMON /A23/ TITLE(20), PEKPOS(21), IFIXPK(20), BETA, GSTATE,
1 GROVAL, NT, NCALC, IGS, LQ
COMMON /A34/ INTERF(20,10), STOREF(2100), DELTA1, DELTA2, DELTA3,
1 STOIPP, REEMAX, ID1, ID2, IDT, ND, NE, NPEF
COMMON /A45/ BACK2(2100), BB(50), BACK(50), NJ, NBACK, NPKRD
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
1 NOFTEN, NCHAN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
DATA (FMT=8H(1X)F10.4,, 7H3F10.2,, 1H , 5H10.2, 5H/40X,, 3H 9F10.2))
DATA (WORD = 8H 9, 8H 10X, 8, 8H 21X, 7,
1 8H 30X, 6, 8H 40X, 5, 8H 50X, 4, 8H 60X, 3, 8H 70X, 2,
2 8H 80X, 1, 8H 9, 8H 10X, 8, 8H 20X, 7, 8H 30X, 6,
3 8H 40X, 5, 8H 50X, 4, 8H 60X, 3, 8H 70X, 2, 8H 80X, 1,
4 8H 9, 8H 10X, 8)
DATA (YSS=INT), (IBLNK=1H )
...INITIALIZATION...
J0 = 0
J0R = 0
NNY = 1
NT2 = 1
NTT = 1
NT1 = NT
...STORE INFORMATION AND GET READY TO CALL PREPAR...
60 DO 70 I=1,NT
J = NNY + I - 1
IHOLD(I) = IFIXPK(J)
70 PERSTO(I) = PEKPOS(J)
90 DELTA1 = DELTA1/OFTEN
DELTA2 = DELTA2/OFTEN
CALL PREPAR
DO 140 I=1,NT
J = NNX + I - 1
140 IFIXPK(J) = IHOLD(I)
NNY = NNX + NT
IF (NSSW2.GT.0) WRITE(6,9042)
9042 FORMAT(10H0 DISTANCE,2X8HPAW DATA,2X10HBACKGROUND,2X9HCOMPOSITE,4X
116HRESOLVED SPECTRA)
```

```

... CALCULATE AREAS AND ERRORS FOR THIS GROUP...
    GO 31 I=1,NT
    YINTIS(I) = 0.
    GO 3005 J=1,MAXP2
3005 XINTIS(I) = XINTIS(I) + STORZ(J,I)
    JQ=IQ+1
    PERSTO (JQ)=PERSTO (I)
    PERERR (JQ)=SIGMA(I)
    PERACK(JQ) = 0.0
    XSECTS(JQ)=XINTIS(I)
    91 XSECTER(JQ) = XSECTS(JQ)+ERRZ(I)
    ...ADD BACKGROUNDS AND PRINT THE RESOLVED AND COMPOSITE SPECTRA
    JPP = 0
    007300 I=1,ITIMES
    MOP = JPP + 1
    JPP=MOP+INDEX(I)-1
    MZ7=INITAL (I)
    MMX=IFINAL(I)
    IF (MSSW2.EQ.0) GO TO 1570
    IF(MZ7-MIT) 2011,2011,2012
2010 MZ7 = MZ7 - 1
    GO 2012 L = MIT, MZ7
2012 WRITE(6,FMT) DIST(L),COUNTS(L),BACK2(L)
2011 WRITE(6,9982) (PERSTO (JP),JP=MOP,JPP)
9082 FORMAT(40X,9F11.2)
1530 GO 2010 J=MZ7,MMX
    K1 = 0
    K2 = 0
    M = J - MZ7 + 1
    STORV1(J) = BACK2(J)
    GO 1310 JP = MOP, JPP
    J2 = JP
    IF ((M.GE.IZSTRT(JP)).AND.(M.LE.IZSTOP(JP))) GO TO 1320
1310 K1 = K1 + 1
    IF (MSSW2.EQ.0) GO TO 3010
    WRITE(6,FMT) DIST(J),COUNTS(J),BACK2(J)
    GO TO 3010
1320 GO 1330 JP = JP, JPP
    IF ((M.LT.IZSTRT(JP)).OR.(M.GT.IZSTOP(JP))) GO TO 1340
    JR = JPP + JP
    PERACK(J2) = PERACK(J2) + BACK2(J)
1325 K2 = K2 + 1
    IIT = M - IZSTRT(JP) + 1
    STORV1(J) = STORV1(J) + STORZ(IIT,JP)
    STORZ(IIT,JP) = STORZ(IIT,JP) + BACK2(J)
1330 S(K2) = STORZ(IIT,JP)
1340 FMT(3) = WORD(K1 + 1)
    IF (MSSW2.EQ.0) GO TO 3010
3009 WRITE(6,FMT) (DIST(J),COUNTS(J),BACK2(J),STORV1(J),(S(K),K=1,K2))
3010 CONTINUE
    MIT = MMX + 1

```

```

330) CONTINUE
    J02 = J02 + NT
    92 IF (NSEN2.EQ.0) GO TO 3401
    007.12 I=MTI, NCHANN
3400 WRITE(6,FMT) DIST(I),COUNTS(I),BACK2(I)
    ...PRINT HEADINGS...
3401 WRITE(6,35) (TITLE(I),I=1,8),TODAY
    WRITE(6,200)
    550 DO 360 I=1,J0
    IPF = IRLNK
    IF (IFIXPK(I).GT.0) IPF = ISF
    APTA = XSECTS(I)+PKBACK(I)
    STYERR = 0.
    IF (AREA.GT.0.) STYERR = SORT(AREA)
    WRITE(6,212) PEKPOS(I),ISF,PEKERR(I),XSECTS(I),XSECE(I),
    1 PKBACK(I),STYERR
560 WRITE(7,215) PEKPOS(I),XSECTS(I),PKBACK(I),PEKERR(I),XSECE(I)
130 WRITE(7,230)
    RETURN
    85 FORMAT (14I,1X,2A10,10X,110)
20) FORMAT (/5X4HPEAK,2FX7H,19X5HNUMS.,35X4HEST./4X8HPOSITION,6X7H
    1,6X5H,5X5HERROR,7X6HCOUNTS,12X5HERROR,13X10HBACKGROUND
    2,6X5HERROR/)
201 FORMAT(3XF9.7,1XA1,3XF8.4,4XF8.4,4XF6.2,5XF9.2,3(4XF9.2))
202 FORMAT(F9.4,1X,2F10.4,2F10.2,F8.2,F8.1,3XA6,F5.1)
221 FORMAT(3XF9.3,1XA1,3XF8.4,15XF6.2,5XF9.2,3(4XF9.2))
222 FORMAT(F9.4,1XF10.4,10X,2F10.2,F8.2,F8.1,3XA6,F5.1)
212 FORMAT(3XF9.3,1XA1,2XF6.2,5XF12.2,3(4XF11.2))
215 FORMAT(F9.4,21X,2F10.2,F8.2,F8.1,3XA6,F5.1)
230 FORMAT(2H-1)
    END
SUBROUTINE SPOTRM
...READS THE SPECTRUM CARDS AND SETS THE DISTANCE AND COUNT ARRAYS
DIMENSION YSAV(10)
COMMON/ DATA/X(2100),Y(2100),RUNDI0,TODAY,FREQ,DELX,NOFTEN,
    1 N,TI,IJ,ISPECT,IEMT,IERR,MAXREF,MAXP2
COMMON /OPTM/ KERRER,KERRAT
..... INITIALIZE COUNTS ARRAY TO ZERO
DO 100 I=1,2100
100 Y(I)=0.0
    N=1
    DELX = 1.0
    .... READ IN THE FIRST TEN VALUES OF SPECTRUM .....
130 READ(5,6) 01,(Y(I),I=1,10)
    ... LOAD IN NEXT TEN VALUES OF SPECTRUM INTO YSAV .....
135 READ(5,6) 0,(YSAV(I),I=1,10)
    IF(EOF(5)) 250,75
    75 CONTINUE
    ... TEST FOR SPECTRUM TERMINATION CARD .....
23) IF(YSAV(1).LE.-1) GO TO 250
    ... TEST FOR ILLEGAL ORDER OF CHANNELS ...

```

```

IF(N.LT.01) GO TO 230
.... COMPUTE THE PROPER ARRAY LOCATION FOR THE LAST READ .....
M1=(0-01)/DFLY + 1.1
M2=M1 + 9
IF(N.LT.M2) M=M2
IF(N.GT.2100) GO TO 235
... STORE DATA LOADED IN YSAV INTO NEXT TEN SLOTS OF Y ....
DO 220 I=M1,M2
J=I-M1+1
220 Y(I)=YSAV(J)
GO TO 135
.... ERROR MESSAGES ....
230 WRITE(6,1)0,01
GO TO 245
235 WRITE(6,2) N
245 T=1
GO TO 300
.... SET THE DISTANCE VALUES ....
250 Y(1)=01
DO 250 I=2,N
250 Y(I)=01 + FLOAT(I-1)*DELX
300 RETURN
310 FORMAT(F5.0,257.0,FX53.0)
1 FORMAT(6H0 D = ,F9.3,16H LESS THAN 01 = ,F9.3)
2 FORMAT(11H0 NOMAIN = ,F5,16H GREATER THAN 2100)
6 FORMAT(F5.0/10(F5.0,2X))
END
SUBROUTINE ARYORD(A,P,N,L)
ORDERS THE ARRAY A, AND MAKES SAME ORDERING TO B IF L=2.
INTEGER B
DIMENSION A(1),B(1)
NP = N - 1
DO 50 I=1,NP
K = I + 1
DO 50 J = K,N
IF (A(I)-A(J)) 50,50,20
20 IF (L-1) 40,40,70
30 ISAV = B(I)
B(I) = B(J)
B(J) = ISAV
40 SAVE = A(I)
A(I) = A(J)
A(J) = SAVE
50 CONTINUE
RETURN
END
SUBROUTINE REFPEK
DETERMINES THE PARAMETERS OF THE REFERENCE PEAK
COMMON /A02/ DIMANC(101), STORM1(2100), RAUX(2100), ITINES, NNX
COMMON /A03/ SKIP(66),LC
COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
1 STOIPP, REFMAX, ID1, ID2, IDI, NR, NE, NREF

```

```

COMMON /AJEF/ BACK2(2100), BB(50), BACC(50), NU, NBACC, NBKRO
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
1  NOSTEN, NCHANN, NI, IU, ISPECT, IFMT, IERR, MAXREF, MAXP2
COMMON /OPTN/ KERRF, KERRAT
IF (LO) 10,31,10
10 IF (NREF) 300,210,300
30 IF (NREF) 100,210,30
< SELECT REFSHAPE FROM INTERNAL DATA
80 DO20 I=1,20
90 STOREF(I) = INTREF(I,NREF)
  FIND LOWER EDGE OF PEAK
100 DO10 I=1,MAXREF
  IF(STOREF(I)) 110,110,120
110 CONTINUE
120 IMIN = I
  IF (I.GT.1) IMIN = I - 1
  FIND UPPER EDGE OF PEAK
  T = MAXREF
130 IF (STOREF(I)) 140,140,150
140 I=T-1
  GO TO 130
150 IMAX = I
  IF(I.LT.MAXREF) IMAX = I+1
  FIND TOP OF PEAK
  REFMAX=0.0
  DO 170 I=IMIN,IMAX
  IF (REFMAX-STOREF(I)) 160,170,170
160 REFMAX = STOREF(I)
  ITOP=I
170 CONTINUE
  FIND THIRD HEIGHT
  REPTH0 = REFMAX/3.
  DO 180 I=ITOP,IMAX
  IF (STOREF(I)-REPTH0) 190,180,180
180 CONTINUE
190 RT=T
  OFFSET = (REPTH0-STOREF(I))/(STOREF(I-1)-STOREF(I))
  RTHPOS=RT-OFFSET
  IF (OFTEN.EQ.1.0) RTHPOS = FLOAT(ITOP)
  DELTA1 = (FLOAT(IMAX)-RTHPOS)*OFTEN
  DELTA2 = (RTHPOS-FLOAT(IMIN))*OFTEN
  DELTA3 = (RTHPOS-FLOAT(ITOP))*OFTEN
  RTHPOS = (RTHPOS-1.0)*OFTEN
  STORF = 0.0
200 ID1=(DELTA2+DELTA1)/OFTEN + 1.1
  ID2=(DELTA1+DELTA3)/OFTEN + 0.1
  ID3=(DELTA2-DELTA3)/OFTEN +.1
  NE = NCHANN - ID1
  NR = ID2 + 1
  IF (NREF) 220,210,230
  SELECT REFSHAPE FROM RAW SPECTRUM

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210 KU = (STOIPP-DIST(1))/OFTEN + 0.1
    IJ = KU - IJ
    IMIN = 1
    IMAX = IMIN + IJ - 1
    STORE = OFTEN*FLOAT(IJ) + DIST(1)
    RTHPOS = STOIPP + DELTA3
    DO 220 IR=1,IJ
220 STOREF(IR)=RAMP(IJ+IR)
230 IF (LO) 240,241,300
240 DO 250 I=IMIN,IMAX
250 STOREF(I-IMIN+1) = STOREF(I)
    IF (MNK) 400,400,300
300 WRITE(6,310) DELTA1, DELTA2, DELTA3
310 FORMAT(11H0 DELTA1 = ,F9.0,8X0HDELTA2 = ,F9.0,8X0HDELTA3 = ,F9.0)
    IF (KEPRFF.GT.0) GO TO 342
    IF (KEPRDT.GT.0) GO TO 342
    WRITE(6,320)
320 FORMAT(15H0 REFERENCE PEAK/11H CHANNEL #,10X7H COUNTS)
    DO 340 I=1,IJ
    WRITE(6,330) STORE,STOREF(I)
330 FORMAT(1XF9.4,10XF10.2)
340 STORE = STORE + OFTEN
342 CONTINUE
    WRITE(6,350) RTHPOS
350 FORMAT(32H REFERENCE PEAK THIRD HEIGHT = ,F9.4)
400 RETURN
END
SUBROUTINE RSRHD
...CALCULATES THE BACKGROUNDS...
COMMON /A02/ DE(I2), RHG2(B2), W(50), X(10), A(10,10), DUMMY(4099)
COMMON /A03/ TITLE(20),PEAK(20),BLNK(23),NPEAK,NCALC,IGS,LO
COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
1 STOIPP, REFMX, IO1, IO2, IJ, NR, NE, NREF
COMMON /A05/ BACK2(2100), DR(50), BACK(50), NJ, NBACK, NPKRD
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FRE1, OFTEN,
1 OFTEN, NCHAN, SKIP(5),MAXREF,MAXP2
    DO = DIST(1)
    IF (NBACK-1) 10,700,000
    ...AUTOMATIC BACKGROUND SELECTION...
10 NP = NPEAK + 1
    IJ = 0
    NJ = 0
    PH2(NJ) = 1.F10
    DO 200 JJ=1,NP
    IJ = IJ + 1
    IF(IJ-NP) 20,80,400
20 LOOPK = (PEAK(IJ)-DELTA3-DO)/OFTEN + 1.1
    IF(IJ-1) 40,40,50
40 NDEL = LOOPK - IO2 - 1
    NJ = 0
    GO TO 100

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60 NDPL = IFIX((PEAK(IJ)-PEAK(IJ-1))/OFTEN + 0.1) - IOT
   MA = LOOPK - IOT - NDPL - 1
   GO TO 100
80 LOOPK = (PEAK(IJ)-DELTA(3-00))/OFTEN + 1.1
   NDPL = NCHAN - LOOPK - IOT
   MA = LOOPK + IOT
100 IF(NDPL-10) 110,120,120
120 JBACK = FLOAT(NDPL)/10.0 + 0.2
   JP = NDPL/JBACK
   SHIFT = FLOAT(JP)/2.
   DO 130 I=1,JBACK
   NJ = NJ + 1
   B = 0.2
   DO 140 IP=1,JP
140 R = B + Y(MA+IP)
   RH02(NJ) = R/FLOAT(JP)
   RACK(NJ) = RH02(NJ)
   CHECK = RH02(NJ-1) + 2.*SQRT(RH02(NJ-1)+1.)
   IF (RH02(NJ)-CHECK) 150,150,150
150 NJ = NJ - 1
   GO TO 170
160 DF(NJ) = DIST(MA+1) + OFTEN*SHIFT
   DR(NJ) = DE(NJ)
   ...TEST FOR LIMIT OF 50 POINTS AND TAKE APPROPRIATE ACTION...
170 IF (NJ-40) 180,175,400
175 IF (IJ.GE.NP) GO TO 400
   IJ = NP
   GO TO 80
180 MA = MA + JP
200 CONTINUE
400 IF (NJ-5) 410,420,420
410 M = NJ - 1
   GO TO 430
420 M = 4
470 N = NJ
500 MM = M + 1
   DO 510 I=1,N
510 W(I) = 1.0
   CALL LSOPOL(M,M,I)
   DO 540 I=1,NCHAN
   RACK2(I) = X(I)
   DO 520 IP=1,M
520 RACK2(I) = RACK2(I) + X(IP+1)*DIST(I)**IP
   IF(RACK2(I)) 530,540,540
530 RACK2(I) = 0.0
540 CONTINUE
   GO TO 400
   ...INTERPOLATE THE BACKGROUND THROUGH THE POINTS READ IN...
700 J01=0
   J02=0
   IF(DR(1)-DIST(1)) 710,710,705

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```

705 J01=1
DE(1) = DIST(1)
PH02(1)=BACK(1)
710 IF(NJ(NJ)-DIST(NCHANN)) 715,750,750
715 J02=1
DE(NJ+J01+1) = DIST(NCHANN)
PH02(NJ+J01+1)=BACK(NJ)
750 DO 755 I=1,NJ
DE(I+J01)=DR(I)
755 PH02(I+J01)=BACK(I)
N=I+J01+J02
IF (N.LT.3) GO TO 900
J=2
DO 760 I=1,NCHANN
DIY = DIST(I)
770 IF(DIY-DE(J+1)) 760,775,775
775 J=J+1
IF (J.GE.N) J= J - 1
780 DE1=(DE(J-1)-DE(J))*(DE(J-1)-DE(J+1))
DE12=(DE(J)-DE(J-1))*(DE(J)-DE(J+1))
DE13=(DE(J+1)-DE(J-1))*(DE(J+1)-DE(J))
BACK2(I)=(DIY-DE(J))*(DIY-DE(J+1))/DE11*RH02(J-1)
1 + (DIY-DE(J-1))*(DIY-DE(J+1))/DE12*PH02(J)
2 + (DIY-DE(J-1))*(DIY-DE(J))/DE13*PH02(J+1)
IF(BACK2(I).LT.0.0) BACK2(I)=0.0
790 CONTINUE
800 WRITE(6,610) (DE(I),PH02(I),I=1,N)
810 FORMAT(25H60POINTS USED BY BACKGROUND/(2F12.3))
GO TO 1000
...CALCULATE THE BACKGROUND INTERVALS...
900 IJ = 2
DR(1) = DIST(1)
IF (NJ.EQ.1) DR(2) = DIST(NCHANN) + OFTEN
DO 920 I=1,NCHANN
IF (DIST(I).GE.DR(IJ)) IJ = IJ + 1
IF (IJ.EQ.NJ) DR(NJ+1) = DIST(NCHANN) + OFTEN
920 BACK2(I) = BACK(IJ-1)
WRITE(6,930)
930 FORMAT(13H0 DISTANCE,17X11H BACKGROUND)
DO 940 I=1,NJ
DIY = DR(I+1) - OFTEN
940 WRITE(6,950) (DIY,DIY,DIY,DIY)
950 FORMAT(F9.3,14-,F9.3,14XF6.2)
1000 RETURN
END
SUBROUTINE LSPPOL(MSUR,MSUD)
LEAST SQUARE POLYNOMIAL FIT
COMMON /SP2/ X(52), Y(52), W(50), B(10), A(10,10), XPOWER(50),
1  Q(144) (4049)
N=MSUB
M=MSUB

```

```

M1=M+1
M2=1+M+1
M31=M3-1
M41=M31+M

```

FORMATION AND INVERSION OF SYSTEM OF NORMAL EQUATIONS

```

DO 100 K2=M1,M41
XPPOWER(K2)=0.0
100 CONTINUE
DO 200 K1=1,N
TERM=X(K1)
DO 200 K2=M1,M31
XPPOWER(K2)=TERM+XPPOWER(K2)
TERM=X(K1)*TERM
200 CONTINUE
DO 300 I=1,M
DO 300 J=1,M
K2=I+J+M-1
A(I,J)=XPPOWER(K2)
300 CONTINUE
DO 400 K=1,M
TERM=W(K)*Y(K)
DO 400 K2=M2,M41
XPPOWER(K2)=TERM+XPPOWER(K2)
TERM=X(K)*TERM
400 CONTINUE
DO 500 I=1,M
K2=I+M31
B(I)=XPPOWER(K2)
500 CONTINUE
CALL MATINV(A,M,2,1,DETERM,10)
700 CONTINUE
RETURN
END

```

SUBROUTINE PREPAR

...CONVERTS DATA TO CHANNEL NUMBERS AND PREPARES IT FOR THE VARIABLE-METRIC PACKAGE...

REAL LRF

```

COMMON /A00/ H4(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
1 GR(20),FR,GS,SL,SL,FR,CSP,TQ,ZZZ,Q,AA,GST,FQ,GTP,FR,GTI,GSR,
2 DELTA,EE,LT,IS,IT,L,IHOLD(20),NSSW1,NSSW2
COMMON /A01/7(2100,20),SS(2102),IZSTRT(20),IZSTOP(20),P(2102),
1 Y(2100),W(2100),E(2100),O(20,20),A(20),G(20),ERR(20),DEL,
2 PFO,F,FRIST,LPS(22),LP(22),IRS,IPR,IPSE,IIC,ITC,IOFF
COMMON /A02/ SIGMA(20),ERRZ(20),PEPSTO(21),STORW4(20),
1 YINTIS(20),INDEX(20),INITAL(20),IFINAL(20),STORV1(2100),
2 DANY(2100),ITIMES,NMY
COMMON /A03/ QUANY(63),NR,NCALC,IGS,LQ
COMMON /A04/ INTREF(20,10),STORPE(2100),DELTA1,DELTA2,DELTA3,
1 STOIPR,DEEMAX,IO1,IO2,IOI,NR,NE,NREF
COMMON /DATA/ DIST(2100),COUNTS(2100),RUNID,TODAY,FREQ,OFTEN.

```

```

1  CKIP(7),MAXPFF,MAXP2
   DEL = 3.1
   Q0 = QIST(1)
   ...CONVERT ALL UNITS TO CHANNEL NUMBER...
   DO 1060 I=1,NF
   PERSTO(I)=(PERSTO(7)-Q0)/OFTEN + 1.0
1060 STOREH(I) = 1.0
   PERSTO (NF+1)=5110.0
   DELT1 = AINT(DELTA1+DELTA2+0.1)
   IFF=(2.0+DELTA2)
   IFFE=((2.0+DELTA2)-FLOAT(IPR))*10.0
   DO 1061 I = 1,MAXP2
1061 R(I)=0.0
   DO 1065 I=1,ITF
1065 R(I+1) = STOREF(I)
   IFF = IFF + 1
   T10=1
   ITTMEG=0
   IIT = 1
   IIT = (NUMBER OF PEAKS ALREADY ANALYZED) + 1
2000 IOFF = IIT - 1
   ...DIVIDE GROUP OF PEAKS INTO NON-OVERLAPPING SUBGROUPS...
   MS=0
   LT=0
   IF(IIT-NF)2001,2001,3000
   I10SS = (FIRST CHANNEL NUMBER OF FIRST PEAK IN SUBGROUP) - 1
2001 I10SS = PERSTO(IIT) - DELTA2 + 0.1
   IF(I10SS.GT.1) I10SS = I10SS - 1
   DO 2015 JJ=1,20
   LT=LT+1
   IF(PERSTO (IIT+JJ)-PERSTO (IIT+JJ-1)- DEL3) 2015,2015,2020
2015 CONTINUE
2020 YXX = PERSTO(IIT)
   ITC = TOTAL NUMBER OF CHANNELS IN THE SUBGROUP
   ITC = PERSTO(LT+IOFF) - YXX + DELTA1 + DELTA2 + 3.1
   ...SETUP INITIAL MATRIX, DATA, WEIGHTS, AND PARAMETERS...
   DO 2025 I=1,LT
   DO 2025 J=1,LT
2025 WH(I,J)=0.0
   DELTA=1.0
   DO 2030 I=1,LT
   IM = IOFF + I
   PER(I) = PERSTO(IM) - YXX + DELTA2 + 2.
   WH(I,I)=STOREH (IM)**2
   IF (IHOLD(IM)) 2026,2026,2027
2027 WH(I,I) = 0.0
   GO TO 2030
2028 DELTA = DELTA+WH(I,I)
2030 CONTINUE
   DO 2035 I=T10,ITC
   JJ = I + I10SS - 1
   X(I)=RAWX(JJ)

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2035 W(T)=1./SQRT(X(T)+10.0)
      FF = FLOAT(ITC-LT)*0.05
      CALL DAVION
      ITTIMES=ITTIMES+1
      INDFX = NUMBER OF PEAKS IN SUBGROUP
      INITAL = STARTING CHANNEL NUMBER IN SUBGROUP
      IFINAL = FINAL CHANNEL NUMBER FOR SUBGROUP
      INDFX(ITTIMES)=LT
      INITAL(ITTIMES) = I10SS
      IFINAL(ITTIMES) = I10SS + ITC - 1
      Q3 = ITC - LT
      ...CALC. ERRORS IN POSITIONS AND COMPUTE NORMALIZED INDIV. PEAKS
      DO 2042 I=1,LT
      IM = I0FF + I
      PERSTO (IM)=(PER(I)+XXY-DELTA2-3.0)*OFTEN + 00
      STORHH(IM)=HH(I,I)
      SIGMA(IM)=SQRT (ABS ((2.0*STORHH (IM)+FREST)/Q3))*OFTEN
      IF(I(I)) 2115,2110,2115
2110 ERR(I)=0.0
      GO TO 2120
2115 ERR(I)=ERR(I)/A(I)
2120 DO 2040 J=1,MAY22
2040 Z(J,IM) = Z(J,IM)*A(I)
2042 CONTINUE
      IF (IT.GE.25) WRITE(6,1001) (PERSTO(I),I=1,LT)
      IIT = IIT + LT
      GO TO 2030
3000 RETURN
1001 FORMAT(5140 EPSILON TOO SMALL - CANNOT CONVERGE FOR PEAKS AT ,5F10
1.2/(10F10.2))
      END
      SUBROUTINE ORDER
      COMMON /A00/ HH(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
1 GR(20),F,GS,EL,SL,FR,GR,T),Z,C,A,GSS,F0,GTP,FR,GTT,GSS,
2 DELTA,F,N,MS,IT,L,IHOLD(20),NGSW1,NSSW2
      JC = N - 1
      DO 100 I=1,JC
      K = I + 1
      DO 100 J=K,N
      IF (PER(I)-PER(J)) 100,100,60
60 SAVE = PER(I)
      PER(I) = PER(J)
      PER(J) = SAVE
      SAVE = HH(I,I)
      HH(I,I) = HH(J,J)
      HH(J,J) = SAVE
      ISAV = IHOLD(I)
      IHOLD(I) = IHOLD(J)
      IHOLD(J) = ISAV
100 CONTINUE
      RETURN
      END

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SUBROUTINE FOM(LLTT,GR,FC,PER,M1)
...SETS UP THE LINEAR EQUATIONS AND OBTAINS RELATIVE PEAK HEIGHTS.
REAL LPE
DIMENSION FFR(20),GR(20)
COMMON/001/7(2100,20),SS(2102),IZSTRT(20),TZSTOP(20),R(2102),
1 Y(2100),W(2100),T(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2 REP, F, FREST, LPE(20),LP(20),IRS,IPP,IPRE,I10,ITC,I0FF
COMMON /DATA/ DIST(2100), COUNTS(2100), PUMID, TODAY, FREQ, OFTEN,
1 WOFTEN, NCHANN, II, IU, ISPECT, IFMT, IERR,MAXREF,MAXP2
LT=LLTT
IF(M1.EQ.1) FREST = 1.0E10
4006 DO 31 L=1,LT
LP(L) = PER(L)
LPE(L) = (PER(L)-FLOAT(LP(L)))*10.0
91 CALL SHIFT(L)
205 IF (M1-3) 222,210,222
DUMMY CALL TO FUN TO FORM THE ARRAY E
210 CALL FUN(LT)
DO 220 I=I10,ITC
220 W(I) = 1.0/SQRT(ABS(E(I))+10.)
222 DO 210 M=1,LT
MM = M + I0FF
DO 210 L=1,M
LL = L + I0FF
C(M,L) = 0.0
DO 200 I=I10,ITC
IF ((I.LT.IZSTRT(LL)).OR.(I.GT.IZSTOP(LL))) GO TO 210
IF ((I.LT.IZSTRT(MM)).OR.(I.GT.IZSTOP(MM))) GO TO 210
IL = I - IZSTRT(LL) + 1
IM = I - IZSTRT(MM) + 1
C(M,L) = C(M,L) + W(I)*W(I)*Z(IL,LL)*Z(IM,MM)
200 CONTINUE
210 C(L,M) = C(M,L)
DO 201 M=1,LT
MM = M + I0FF
A(I) = 0.0
DO 201 I=I10,ITC
IF ((I.LT.IZSTRT(MM)).OR.(I.GT.IZSTOP(MM))) GO TO 201
IM = I - IZSTRT(MM) + 1
A(I) = A(I) + W(I)*W(I)*Y(I)*Z(IM,MM)
201 CONTINUE
CALL MATINV(C,LT,A,1,DETERM,2)
CALL DERIVP(LT,PER)
DO 1600 L=1,LT
1600 GR(L) = G(L)
CALL FUN(LT)
IF(M1-3) 206,1011,206
1011 F7 = F/(ITC-I10-LT)
DO 1005 L=1,LT
REP = F7*C(L,L)
1005 FFR(L) = SQRT(ABS(REP))

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285 F9 = F
IF (F9.LI.FREST) FREST = F9
RETURN
END
SUBROUTINE DERIV (LLTT, PFR)
...CALCULATES DERIVATIVES OF FUNCTION F(FUN) WITH CHANGE
IN POSITION
REAL LPF
DIMENSION PFR(20)
COMMON/AD1/7(2100,20),SS(2100),I7STRT(20),I7STOP(20),R(2100),
1 X(2100),W(2100),T(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2 PFR, F, FREST, LRF(22), LP(22), IPS, IPR, IPCE, IIC, ITC, IOFF
COMMON /DATA/ DIST(2100), COUNTS(2100), PUMIN, TODAY, FREQ, OFTEN,
1 MOFTEN, NCHAN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
LT=LLTT
DO 35 L=1,LT
LL = L + IOFF
DO 34 I=1,MAXP2
94 SS(I) = Z(I,LL)
ISAV1 = I7STRT(LL)
ISAV2 = I7STOP(LL)
LOP=LP(L)
LOP2=LPF(L)
Y=PFR(L)+DEL
LP(21) = Y
LPF(21) = (Y-FLOAT(LP(21)))*10.0
Y=PFR(L)-DEL
LP(22) = Y
LPF(22) = (Y-FLOAT(LP(22)))*10.0
LP(L)=LP(21)
LPF(L)=LPF(21)
CALL SHIFT(L)
CALL FUN(LT)
F=F
LP(L)=LP(22)
LPF(L)=LPF(22)
CALL SHIFT(L)
CALL FUN(LT)
G(L) = (F9-F) / (2.)*DEL
DO 35 I=1,MAXP2
95 Z(I,LL) = SS(I)
I7STRT(LL) = ISAV1
I7STOP(LL) = ISAV2
LP(L)=LOP
95 LOP2(L)=LOP2
RETURN
END
SUBROUTINE SHIFT (LP)
...CONTROLS INTERPOLATION OF FREQ. PEAK FOR SHIFTING FRACTIONS
OF CHANNELS

```

```

REAL LRF
COMMON/AC1/7(2100,20),SS(2102),IZSTRT(20),TZSTOP(20),R(2100),
1 X(2100),W(2100),F(2100),G(20,20),A(20),G(20),ERR(20),DEL,
2 IPR, F, FREQ, LRF(20), LP(20), IPR, IPP, IPRE, IIC, ITC, IOFF
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
1 NOFTEN, NCHAIN, II, IU, ISPECT, IFMT, IERR, MAXPEF, MAXP2
L=L1
LL = L + IOFF
DO 100 J=1,MAXP2
C1=LP(L)
C2=LRF(L)
U=C1+C2/10.0
R8=IPR
R9=IPRE
100 Z(J,LL) = 0.0
R1=R8+R9/10.0
IF (R1-U) 300,13,0
SUBROUTINE SHIFTL L LESS THAN R
9 J=1
IZSTRT(LL) = 1
IF (IPRE-LRF(L)) 10,11,12
10 F = 10+IPRE-LRF(L)
T = IPR-LP(L)
GO TO 14
11 F=0.0
GO TO 13
12 F = IPRE-LRF(L)
13 T = IPR-LP(L)+1
14 F1 = F/10.0
15 Z(J,LL) = R(T) + F1*(R(I+1)-R(I))
T=T+1
J=J+1
IF (I-IPR) 15,15,17
16 IF (J-ITC) 15,15,17
17 IZSTOP(LL) = J - 1
GO TO 23
SUBROUTINE SHIFTR L EQUAL R
18 DO 20 J=1,IPR
20 Z(J,LL) = R(J)
IZSTRT(LL) = 1
IZSTOP(LL) = IPR
GO TO 23
SUBROUTINE SHIFTR P LESS THAN L
300 I=1
IF (IPRE-LRF(L)) 1,2,3
1 F = 10+IPRE-LRF(L)
K = LP(L)-IPR+2
GO TO 5
2 F=0.0
GO TO 4
3 F = IPRE-LRF(L)

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4 K = LP(L) - IPR + 1
5 F1 = F/10.0
  IZSTRT(LL) = K
  J = 1
6 7(I,LL) = R(I) + F1*(R(I+1) - R(I))
  I = I + 1
  J = J + 1
  K = K + 1
  IF (I - IRS) 7,7,8
7 7F(K - ITS) 6,6,8
8 IZSTOP(LL) = K - 1
23 RETURN
  END
  SUBROUTINE FUN(LT)
  ...CALCULATES THE FUNCTION F WHICH IS BEING MINIMIZED...
  REAL LPE
  COMMON/AG1/7(2102,20),SS(2102),IZSTRT(20),IZSTOP(20),R(2102).
1 X(2100),W(2100),E(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2 DEF, F, FREST, LPE(20),LP(20),IRS,IPR,IPFE,I10,ITC,IOFF
  COMMON /DATA/ DIST(2100),COUNTS(2100),PUNID,TODAY,FREQ,OFTEN,
1 NOFTEN,NCHANN,II,IJ,ISPECT,ISMT,IERR,MAXREF,MAXP2
  F=1.0
  DO 60 I=1,ITC
60 E(I) = 0.0
  DO 70 L=1,LT
  I1 = IZSTRT(L+IOFF)
  I2 = IZSTOP(L+IOFF)
  DO 70 I=I1,I2
  J = I - I1 + 1
70 E(I) = E(I) + A(L)*Z(J,L+IOFF)
  DO 80 I=I10,ITC
  F1 = (X(I) - E(I))*W(I)
80 F = F + F1*F1
  RETURN
  END
  SUBROUTINE MATINV(A,MSUB,B,MSUR,DET,NMAX)
  DIMENSION A(NMAX,MSUB),B(NMAX,MSUR)
  DIMENSION PIVOT(100),INDEX(100),IPIVOT(100)
  EQUIVALENCE (PIVOT,INDEX,IPIVOT),(AMAX,T),(IROW,I1,IRC),
1 (TEMP,SWAP)
  DATA (ISHIFT=4000),(MASK=0000000007777777778)
  N=MSUB
  M=MSUR
  INITIALIZATION
  DETERM=1.0
  DO 20 I=1,N
  IPIVOT(I)=0

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20 CONTINUE
   DO 500 I=1,N

   SEARCH FOR PIVOT ELEMENT

   AMAX=0.
   DO 100 J=1,N
   TEMP=IPIVOT(J).AND..NOT.MASK
   IF(TEMP) 100,60
60  DO 100 K=1,N
   TEMP=IPIVOT(K).AND..NOT.MASK
   IF(TEMP) 100,80
80  TEMP=ABS (A(J,K))
   IF(TEMP-AMAX) 100,35,35
85  IROW=J.
   ICOLUM=K
   AMAX=TEMP
100 CONTINUE
105 CONTINUE
   INDEX(I)=INDEX(I)+(ICSHIFT*IROW+ICOLUM)
   J=IROW
   AMAX=A(J,ICOLUM)
   DETERM=AMAX*DETERM

   MATRIX SINGULAR

   IF(DETERM) 110,500

110 PIVOT(ICOLUM)=INDEX(ICOLUM).OR.AMAX.AND..NOT.MASK

   INTERCHANGE ROWS

   IF(IROW-ICOLUM) 140,260
140 DETERM=-DETERM
   DO 200 K=1,N
   SWAP = A(J,K)
   A(J,K)=A(ICOLUM,K)
   A(ICOLUM,K)=SWAP
200 CONTINUE
   DO 250 K=1,M
   SWAP=R(J,K)
   R(J,K)=R(ICOLUM,K)
   R(ICOLUM,K)=SWAP
250 CONTINUE

   DIVIDE PIVOT ROW

260 K=ICOLUM
   A(ICOLUM,K)=1.
   DO 350 K=1,N
   A(ICOLUM,K)=A(ICOLUM,K)/AMAX

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350 CONTINUE
   DO 370 K=1,M
   R(TCOLUM,K)=R(ICOLUM,K)/AMAX
370 CONTINUE

   REDUCE

   DO 350 J=1,N
   IF(J-ICOLUM)-00,350
400 T=A(J,ICOLUM)
   A(J,ICOLUM)=0.0
   DO 450 K=1,N
   A(I,K)=A(J,K)-A(ICOLUM,K)*T
450 CONTINUE
   DO 500 K=1,M
   R(J,K)=R(J,K)-R(ICOLUM,K)*T
500 CONTINUE
550 CONTINUE

   INTERCHANGE

600 DO 710 I=1,N
   T1=N+1-I
   IRC=INDEX(I1).AND.MASK
   K=IRC/ISHIFT
   ICOLUM=IRC-K*ISHIFT
   IF(K-ICOLUM) 650,710
650 DO 705 J=1,N
   SWAP=A(J,K)
   A(J,K)=A(J,ICOLUM)
   A(J,ICOLUM)=SWAP
705 CONTINUE
710 CONTINUE

740 DEF=DETERM
   RETURN
   ENTRY DMATINV
   RETURN
   END
   SUBROUTINE DAVIEN
   ...THIS IS THE CONTROL ROUTINE FOR THE VARIABLE-METRIC PACKAGE...
   COMMON /A30/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
1  GR(20),F,GS,FL,PL,FR,GSF,IG,Z,C,A,CSS,FG,GTP,FG,GTI,GSF,
2  DELTA,E,N,MS,IT,L,IHOLD(20),N1SW1,N2SW2
15 M1=1
   IT = 0
   F=0.0
   CALL FCN(N,G,F,Y,M1)
   TF(N1SW1)20,25,20
20 WRITE(6,8) IT,MS,F
   GO TO 840

```

```

120 M1=2
200 CALL READY
   GO TO (300,300,500,500), L
300 CALL AIM
   GO TO (400,500,500,500), L
400 CALL FIRE
   GO TO (500,500,300,300), L
500 CALL ORDER
   IF (IT-25) 100,500,550
550 M1 = 3
   GO TO 900
800 M1=2
   IF(NSSW1) 22,25,22
   22 WRITE(5,11)
810 DO 920 II=1,N
920 WRITE(5,7) (H(II,JJ),JJ=1,N)
930 WRITE(5,12) DELTA,F,GS
840 IF(NSSW1) 24,25,24
  24 WRITE(5,10) (Y(I),I=1,N)
   GO TO (850,850,850), M1
850 WRITE(5,13) (G(I),I=1,N)
860 WRITE(5,9)
  25 GO TO (120,120,900), M1
900 IF (N.GT.1) CALL ORDER
   CALL FCN(N,G,F,X,M1)
  30 RETURN
  3 FORMAT(6E12.5)
  7 FORMAT(14J8E14.7)
  3 FORMAT(14HIT I4,7H STEP I4,4H F=E14.5)
  9 FORMAT(20H0- - - - -)
 11 FORMAT(24JX=E14.5/(24C 8E14.5))
 11 FORMAT(17H0FINAL VALUES/13H0ERROR MATRIX)
 12 FORMAT(74J0DELTA=F14.5,4H F=E14.5,6H GS=E14.5)
 13 FORMAT(3H0G=E14.5/(3H0 8E14.5))
   END
   SURROUTINE READY
   COMMON /AC00/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
1  GR(20),F,GS,FL,SL,FR,GSP,TD,Z,Q,A,GSS,FO,GTP,FB,GTT,GSR,
2  DELTA,E,N,MS,IT,L,THOLD(20),NSSW1,NSSW2
200 L=1
   CALL MATMPY(N,N,H,G,S)
   DO 205 I=1,N
205 S(I)=-S(I)
   CALL MATMPY(L,N,S,G,GS)
   IF (GS+E) 210,240,240
210 L=2
   FL=2.0
   TL=FL+F/GS
   IF (TJ+FL) 217, 217, 212
217 FL=-TJ
217 SL=-GS

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00 215 I=1,N
215 XP(I)=X(I)+EL*R(I)
    CALL FCON(N,GP,FP,YP,2)
    CALL MATHPY(1,1,0,GP,GSP)
    IF (-GSP) 240,240,220
220 IF (F-FP) 240,240,225
225 L=F
    IF (NSSW1) 100,101,100
100 WRITE(6,1)
101 FR=FP
    00 230 I=1,N
    GR(I)=GP(I)
    T(I)=XP(I)
230 CONTINUE
    IF (EL+2.0) 240,235,240
235 L=0
    DELTA=DELTA+DELTA
    TQ=1.0/SL
240 RETURN
    1 FORMAT(10HUNDERSHOT)
    END
    SUBROUTINE AIM
    COMMON /A00/ H(20,20),X(20),G(20),S(20),YP(20),GP(20),T(20),
    1 GR(20),F,GS,EL,SL,FP,GF,TQ,Z,Q,A,GSS,F0,GTP,FB,GTT,SSB,
    2 DELTA,E,N,MS,IT,L,INCL(20),NSSW1,NSSW2
300 L=1
    Z=7.0/EL*(F-FP)+GS+GSP
    Q=ABS(.7*SQRT(1.0-(GS/Z)+(GSP/Z)))
    A=(Q-Z+GSP)/(Q+Q-Z+GSP)
    TQ=EL/7.0*(Q+Q+Z+GSP)*A+A
    FP=FP-TQ
    CALL MATHPY(N,N,4,GP,T)
    00 305 I=1,N
305 T(I)=(GSP/SL)*R(I)-T(I)
    CALL MATHPY(1,1,T,GP,GTP)
    IF (TQ+TQ+GTP) 315,310,310
310 00 312 I=1,N
312 T(I)=XP(I)+A*(Y(I)-XP(I))
    GO TO 340
315 IF (F+FB+GTP) 310,320,320
320 00 322 I=1,N
322 T(I)=T(I)+YP(I)
    CALL FCON(N,GR,FB,T,2)
    IF (F0-F3) 310,325,325
325 L=7
    IF (NSSW1) 100,101,100
100 WRITE(6,1)
101 00 327 I=1,N
327 S(I)=T(I)-XP(I)
    CALL MATHPY(1,N,S,GR,GTT)
    GTT=GTT-GTP

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      TF (GTT) 340, 330, 330
330 L=0
      GSS=GTT
      GL=-GTP
      FL=1.0
340 RETURN
      1 FORMAT(9H3PI000H77)
      END
      SUBROUTINE FTPE
      COMMON /A00/ H(20,20), X(20), G(20), S(20), XP(20), GP(20), T(20),
      1 GR(20), F, GS, FL, EL, FP, GSP, T0, Z, Q, A, GSS, F0, GPP, FB, GTT, GSB,
      2 DELTA, E, N, MS, IT, L, THOLD(20), NSSW1, NSSW2
      EQUIVALENCE (TE40, GTT)
400 L=1
      TEMP=A/(1.0-A)
      CALL FCN(N, GR, FB, T, 2)
      CALL MATPY(1, N, S, GR, GSP)
      T0=F
      IF (T0-FP) 403, 403, 402
402 T0=FP
403 IF (T0-FB+E) 415, 405, 405
405 GSS=0+0
      T0=GSS*(TEMP-1.0)/TEMP
      IF (ABS (T0)-0) 430, 410, 410
410 L=L+1
      GO TO 440
415 L=L-1
      IF (FP-F) 425, 420, 420
420 IF (NSSW1) 100, 101, 100
100 WRITE(5, 1)
101 FL=(1.0-A)*EL
      FP=FB
      GSP=GSS
      DO 422 I=1, N
      XP(I)=T(I)
      GP(I)=GB(I)
422 CONTINUE
      GO TO 440
425 IF (NSSW1) 200, 201, 200
200 WRITE(6, 2)
201 FL=EL+A
      F=FB
      GS=GSS
      DO 427 I=1, N
      X(I)=T(I)
      G(I)=GP(I)
427 CONTINUE
      GO TO 440
430 GSP=GSS+T0
      DO 435 I=1, N
435 G(I)=(GB(I)-G(I))*TEMP+(GP(I)-GB(I))/TEMP

```

```

441 RETURN
1  FORMAT(10H0MOVE LEFT)
2  FORMAT(11H0MOVE RIGHT)
END
SUBROUTINE DPSS
COMMON /AGC/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
1  CR(20),F,GS,FL,SL,FR,GSR,T0,Z,0,A,GSS,F0,GTP,FR,GTT,GSR,
2  DELTA,E,N,MS,TT,L,THOLD(20),N3SW1,N3SW2
501 GO TO (505,520,530,525), L
505 CALL MATMXY(M,N,H,G,Y)
CALL MATMXY(1,H,X,G,T0)
IF (T0-GSS**2/SL-F) 515,510,510
510 DO 512 II=1,N
DO 512 JJ=1,N
512 H(TT,JJ)=H(II,JJ)-X(II)*X(JJ)/T0
DELTA=DELTA*(FL+GSS/T0)
T0=FL/GSS
GO TO 525
515 IF(N3SW1) 200,520,200
211 WRITE(6,1)
521 DELTA=DELTA*(FL+SL/GSS)
T0=FL/GSS-1.0/SL
525 DO 527 II=1,N
DO 527 JJ=1,N
527 H(TT,JJ)=H(II,JJ)+T0*S(II)*S(JJ)
531 IT=IT+1
C=0
IF(N3SW1) 100,101,100
100 WRITE(6,4) IT,MS,F,GS
101 DO 532 I=1,N
G(I)=G(I)
Y(I)=T(I)
532 CONTINUE
IF(N3SW1) 535,540,535
535 WRITE(6,2) (X(I),I=1,N)
WRITE(6,3) DELTA
540 RETURN
1  FORMAT(9H0COLINEAR)
2  FORMAT(3H0X=,8F14.5/(3H0 ,6E14.5))
3  FORMAT(7H0DELTA=,E14.5/20HC- - - - -)
4  FORMAT(4H0IT ,I4,7H STEP ,I+,4H F=,E14.5,5H GS=,E14.5)
END
SUBROUTINE MATMXY(M,N,H,G,S)
DIMENSION H(20,20),G(20),S(20)
701 DO 720 II=1,M
S(II)=0.0
DO 720 JJ=1,N
720 S(II)=H(JJ,II)*G(JJ)+S(II)
741 RETURN
END

```

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VITA


Richard Steven Hartley was born on 31 August 1954 in Houston, Texas. He graduated from high school in Berkeley Heights, New Jersey in 1972 and attended Texas A&M University from which he received the degree of Bachelor of Science in Physics in May 1976. Upon graduation, he received a commission in the USAF through the ROTC program. While in preparation for graduate school, he was called to active duty. He entered the School of Engineering, Air Force Institute of Technology, in August 1976.

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