COMPUTER TECHNIQUE FOR ACTIVATION ANALYSIS

by

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ABSTRACT

A computer program has been developed for application to rapid routine qualitative and quantitative analysis of atmospheric particulates by thermal neutron activation. The program is designed to automatically analyze samples of material having unknown composition, but a limited number of possible constituents (20 to 30 isotopes). The qualitative analysis depends only on the gamma spectrum peak energies with no half-life determinations. The quantitative analysis is carried out by a matrix synthesis of the composite spectrum using isotopic spectra in a permanent isotopic library on magnetic tape. The method of spectrum synthesis minimizes the amount of computer storage required so that a 1024-channel spectrum containing 20 components can be analyzed using only about 8000 words of core storage. Program input consists of raw data from the spectrometer and experimental conditions, and the output consists of both the isotopic and elemental sample compositions.

Preliminary program tests using synthesized mixture spectra have produced excellent results for mixtures with up to seven components. Errors in the spectrum synthesis are usually on the order of one to two percent for the most abundant constituents.

CHAPTER I

INTRODUCTION

The activation of isotopes by thermal neutron capture provides an extremely sensitive technique for trace element determination. The activation is accomplished by radiative capture (n,γ) type reactions. Many of the nuclides thus produced are unstable with respect to beta emission with accompanying subsequent de-excitation gammas. Each such decay will in general produce gammas at characteristic energies with a characteristic half-life. By studying the γ-ray spectrum emitted by the sample after neutron irradiation it is possible to deduce both the qualitative and quantitative isotopic composition of the irradiated sample.

This method of analysis, thermal neutron activation analysis, presents important advantages over other methods for certain applications and is to be applied to the fast, routine elemental analysis of particulate air pollution samples. This problem is characterized by a list of twenty to thirty elements which are of interest. The sample is unknown in that it may contain any combination of elements from among those of interest, but is known in the sense that it cannot (in theory) contain any element which is outside the list of elements of interest. Thus the sample composition is unknown, but it has a limited number of possible constituents.

In this technique the qualitative analysis of a sample is carried out by measuring the energies of the gamma rays and the apparent half-life of each gamma of interest. The quantitative analysis is obtained by measuring the activity of each component in the gamma spectrum at a given time. From these data and the experimental conditions it is possible to derive the composition of the original sample. Most such analyses are performed by using various manual techniques, but these are usually difficult, time consuming, and rather inaccurate. Furthermore, manual methods tend to fail completely for a sample of any complexity.

Recently many good computer programs have been developed for data reduction in activation analysis. These programs tend to fall into two categories; those used for simple, qualitatively known samples with only one or a few components, and those used for unknown highly complex samples. The former are rather simple and generally produce good results, while the latter much more complex (and, therefore, rarer) programs are many times more difficult to develop. These complex programs can provide great savings in time and are therefore very useful.

A program was developed for application to the analysis of samples of unknown composition but with a limited number of possible constituents. This particular type of sample indicated the use of a type of program intermediate in scope between the two general classes of programs.

This program differs from most other programs in three rather fundamental aspects:

1. The sample is of unknown composition but has a limited number of possible constituents.
2. Component identification is made only on the basis of measured gamma ray energies with no half-life determinations.
3. The program is capable of correcting for instrumental variations which have proven troublesome to previous workers.

Furthermore, in order to make the analysis time as short as possible, the entire analysis is performed with as few human decisions and as little manual data handling as possible. Lastly the program is kept as simple as possible consistant with the above objectives.

CHAPTER II

THEORY

When a sample of material is placed in a nuclear reactor many of the isotopes present in the sample are converted to radioactive products. The gamma radiation from these products can then be analyzed to deduce sample composition.

The basic process of isotope activation is characterized by the following differential equation:

$$\frac{dN(t)}{dt} = P - \lambda N(t) \tag{1}$$

where: N = number of atoms of the radioactive product

λ = decay constant for the radioactive product

P = production rate of product

Solving equation 1 for the case where $N(t=0)=0$, one obtains:

$$N(t) = \frac{P}{\lambda}(1-e^{-\lambda t}) \tag{2}$$

or:

$$A(t) = P(1-e^{-\lambda t}) \tag{3}$$

where A(t) is the activity due to the radioactive product isotope after irradiation of the parent isotope for a length of time t.

The production rate is given by:

$$P = N_o \sigma \phi V \tag{4}$$

where:

N_o = atomic density of parent isotope

σ = effective activation cross-section

ϕ = effective thermal neutron flux.

In the case of thermal reactor irradiation σ is an effective cross-section dependent on the neutron spectrum and the nuclear reaction of interest. The most common activation is produced by radiative neutron capture [(n,γ) reaction].

The atomic density is given by:

$$N_o = \frac{\theta W N_A}{VM} \tag{5}$$

where

θ = isotopic abundance of isotope being activated

W = amount of parent element present in sample (grams)

N_A = Avogadro's number (6.023×10^{23} atoms per gram-mole)

M = Atomic weight of element in question.

A given element may be made up of several isotopes each capable of forming a different radioactive product.

Combining equations 3, 4, and 5 we obtain:

$$A(t) = \frac{\theta W N_A \sigma \phi}{M} (1-e^{-\lambda t}) \tag{6a}$$

or

$$A(t) = \frac{\theta W N_A \sigma \phi S(t)}{M} \tag{6b}$$

where

$$S(t) = (1-e^{-\lambda t}). \tag{7}$$

$S(t)$ is the saturation term, and corrects for decay during irradiation.

Solving for W:

$$W = \frac{MA(t)}{\theta N_A \sigma \phi S(t)} \tag{8}$$

Equation 8 gives the weight of the element of interest in the sample in terms of activity of a particular product radioisotope at the end of an irradiation of duration t.

If the sample is allowed to decay for a time t_1 and then is counted until a time t_2 after the end of an irradiation of duration T, the total count recorded is given by:

$$C = \int_{t_1}^{t_2} gA(T)\exp(-\lambda t)dt \tag{9}$$

where g is the counter efficiency.

Integration yields:

$$C = \frac{gA(T)}{\lambda} [\exp(-\lambda t_1)-\exp(-\lambda t_2)], \tag{10}$$

and solving for A(T):

$$A(T) = \frac{\lambda C}{g[\exp(-\lambda t_1)-\exp(-\lambda t_2)]} \tag{11}$$

Combining equations 11 and 8 for the case of irradiation time T yields:

$$W = \frac{M\lambda C}{\theta N_A \sigma \phi S(T) g[\exp(-\lambda t_1)-\exp(-\lambda t_2)]} \tag{12}$$

Equation 12 gives the weight of the element of interest in the sample in terms of measurable, experimental quantities. In theory W could be obtained directly in this way. In practice, however, some of the quantities needed, particularly σ, ϕ, and g, are not usually known with sufficient accuracy. Therefore this method, known as the absolute

method, is subject to comparatively large systematic errors[14] somewhat compensated for by the simplicity of the procedure. Much greater accuracy can be attained by the comparator method in which a known amount of the element of interest is irradiated along with the unknown sample. Equation 12 also applies to this known sample in the form:

$$W' = \frac{M\lambda C'}{\theta N_A \sigma \phi S(T) g [\exp(-\lambda t_1') - \exp(-\lambda t_2')]} \qquad (13)$$

where the primes refer to the known sample, and the decay constant, λ, is the same for both known and unknown samples. Dividing equation 12 by equation 13 yields:

$$W = W' \left[\frac{C}{C'}\right] \left[\frac{\exp(-\lambda t_1') - \exp(-\lambda t_2')}{\exp(-\lambda t_1) - \exp(-\lambda t_2)}\right] \qquad (14)$$

Equation 14 provides a much more accurate value for W at the expense of the increased experimental complexity of preparing, irradiating, and counting an additional sample. This technique is the one nearly always used in actual analysis work.

This discussion of the theory of activation analysis is highly simplified in that the sample of material was assumed to contain only one monoisotopic element capable of being activated, and that no interfering reactions took place which would also contribute to the activity of the irradiated sample. A complete discussion of the complexities encountered with most real multicomponent samples is given in many places in the literature.[4,10,20,26,27]

In real samples, the principle difficulty is encountered in obtaining the number C in equation 14, i.e. in ascertaining the number

of counts due only to a particular radionuclide in an irradiated sample containing several or many other radionuclides. The gamma radiation emitted by the irradiated sample is mostly due to de-excitation after β^- emission. Since the energy levels in the nuclei are discrete, the gamma rays are monoenergetic, each energy corresponding to an allowed transition. Furthermore, since energy level positions are characteristic of the particular nuclide, the gamma emission energies are unique and characteristic of the decaying radionuclide. It is this monoenergetic character of gamma emission, as well as half-life measurements, which allows the contributions to the count rate of the various isotopic components to be separated.

The resolution of a mixture gamma spectrum into component contributions is made rather difficult by non-ideal performance of the instruments used to obtain the spectrum. Even in principle, however, the problem is not an easy one if the sample is of any complexity. A further disadvantage of the method is the expensive equipment needed, i.e. a high flux neutron source and gamma-ray spectrometer. These disadvantages are more than offset, however, by the great sensitivity of the method which for many elements far surpasses that of any other method which for many elements far surpasses that of any other method of analysis. Depending on the nuclear properties of the particular element of interest, limits of detection range to about 10^{-13} grams with 10^{-8} to 10^{-9} grams being about average. A listing of detection sensitivities for most of the elements by thermal neutron activation has been compiled by H. P. Yule.[34] This technique is a nondestructive analysis capable of detecting and measuring a large number of elements (about 70).

CHAPTER 3

EXPERIMENTAL

Samples of material to be analyzed by use of the computer program developed in this research are irradiated in a General Atomic Triga Mark I reactor and counted in a gamma spectrometer assembled especially for this research. The gamma spectrometer consists of a 4" x 3" flat NaI(Tl) crystal coupled to a 1024 channel Technical Measurement Corporation model CN-1024 pulse height analyzer with standard 8 channel perforated tape output. The detector assembly contains a Harshaw type 16MBS12/5B 4" x 3" NaI(Tl) scintillation crystal coupled to an RCA 8055 5" photomultiplier tube. The detector-shield arrangement is shown in figure 1.

Most gamma ray spectrometry is performed using a NaI(Tl) crystal due to its comparatively high efficiency, although it suffers from rather poor resolution in addition to other problems.

Each time a gamma ray interacts in the crystal a part or all of its energy is lost. The energy of the γ-ray is dissipated as heat and visible light; the latter is detected and the signal amplified by the photomultiplier and preamplifier to give a voltage pulse proportional to the amount of energy the gamma photon lost in the crystal. This pulse is then sorted by pulse height and a count stored in a particular channel in the pulse height analyzer corresponding to this pulse height.

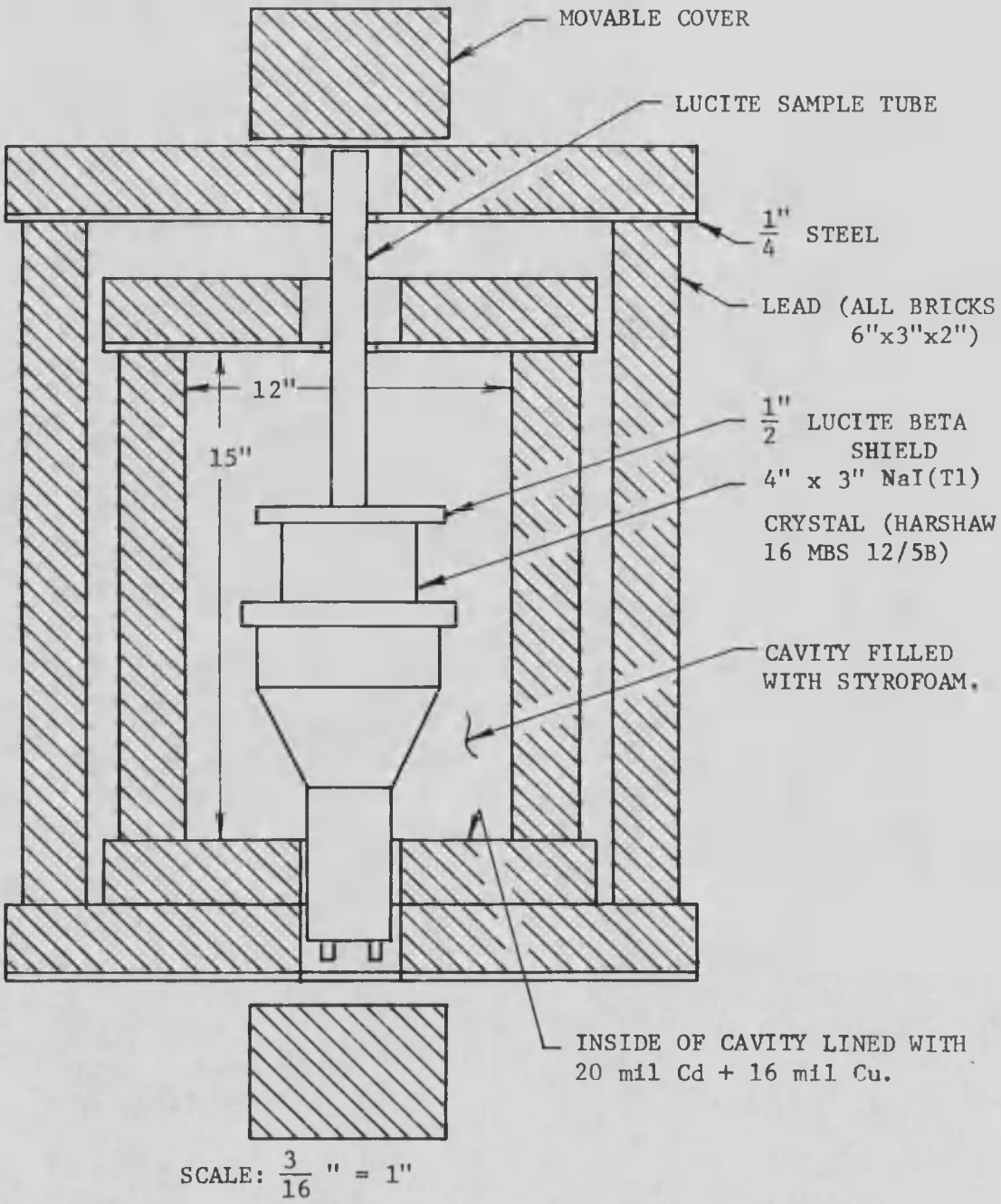

FIGURE 1: Detector-Shield Arrangement

The major gamma photon interactions with the crystal are:

Photoelectric effect, in which the gamma photon is completely absorbed by an atom in the crystal with the production of a photoelectron which is absorbed within a short distance in the crystal. The atom involved is also excited and emits de-excitation x-rays.

Compton scattering, where the gamma photon suffers scattering collision with a bound electron producing a recoil electron and a secondary gamma photon of reduced energy.

Pair production, where the gamma photon may be converted into an electron-positron pair in the vicinity of a nucleus. The electron energy is absorbed and the positron, after slowing down, is annihilated with the emission of a pair of 0.51 MeV gamma rays. Since the energy required to create an electron-positron pair is 1.02 MeV, this is the threshold of the reaction.

These three interactions provide various mechanisms for energy loss in the crystal. First, the gamma photon may be completely absorbed inside the crystal either by photoelectric absorption, Compton scattering where the secondary gamma does not escape, or by pair production where neither annihilation gamma escapes. Complete absorption produces a Gaussian peak in the gamma spectrum centered at the energy of the gamma photon.

Secondly, the gamma photon may suffer a Compton collision after which the scattered gamma escapes from the crystal. Since the energy lost in the crystal varies with scattering angle, this produces

a continuous contribution from low energy up to a maximum corresponding to maximum energy loss by the photon at 180° scattering angle.

Thirdly, the gamma photon (if its energy is greater than 1.02 MeV) may produce an electron-positron pair where either one or both of the annihilation gammas escape from the crystal. This produces a pair of escape peaks at 0.51 and 1.02 MeV less than the energy of the total absorption peak. The escape peaks, however, are usually not very pronounced below a gamma energy of about 2 MeV.

The spectrum formed in this way due to a monoenergetic source will not, therefore, be a single line, but will instead be a rather complicated response function resembling figure 2. The difficulty in separating the contributions due to the various component isotopes is largely due to the complexity introduced when many such response functions of different energies are superimposed. The preceding has only been a rough outline of the theory of spectrum formation which is treated in much more detail in the literature.[4,5,9,19,26,27]

The formation of a relatively wide Gaussian total absorption peak (as shown in figure 2) may result in two peaks close together not being resolved. These will then appear to be a single, perhaps distorted peak.

The most important experimental problem from a programming point of view is the instabilities in the pulse height analyzer. In particular, the energy gain (MeV per channel) and threshold (channel of zero energy) are functions of time over long periods. Most methods

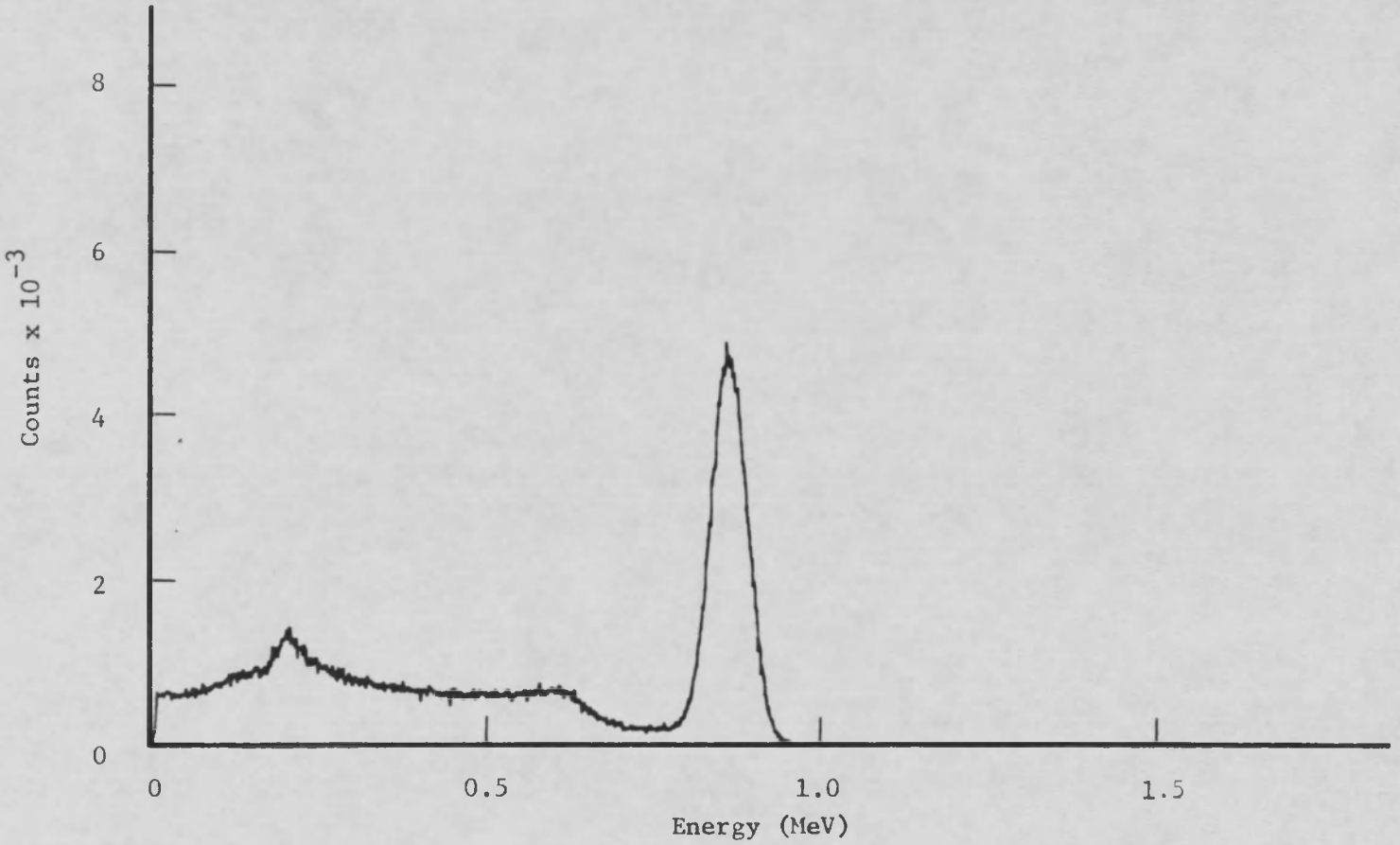

FIGURE 2: Typical Monoenergetic Response

of automatic quantitative analysis depend on the assumption that instrument response is exactly reproducible, and change in the gain or threshold therefore tends to cause large errors in the analysis.[3,15] This problem of gain and threshold shifting has, in fact, been one of the major difficulties in computerizing activation analysis, and several rather elaborate schemes have been tried to stabilize the instruments involved.[7,8,12] The trend within the last few years, however, has been to make the necessary corrections of gain and threshold within the program itself.[21]

CHAPTER 4

METHODS OF ANALYSIS

If the composite spectrum is assumed to be a linear sum of the constituent spectra then the analysis is performed by determining the identities and magnitudes of the component spectra present in the composite. The constituents are determined by identification of γ-ray energies and/or measurement of half-lives. Standard spectra of pure known amounts of the corresponding isotopes are obtained and used to make the quantitative analysis by various comparison methods.

The composite spectrum obtained from the pulse-height analyzer can be represented by a discrete function of the form F(i), where i is the channel number. If $f_j(i)$ is the standard spectrum of the j^{th} isotope, then the composite spectrum, F(i), is assumed to be a linear combination of the N standard spectra:

$$F(i) = \sum_{j=1}^{N} a_j f_j(i) \qquad i = 1,2,\cdots,M \qquad (15)$$

where M is the number of channels in a spectrum, and the a_j's are the weighting constants relating the magnitudes of the standard spectra to the magnitudes of the corresponding component spectra in the composite. Since all variables related to the N standard spectra are known, the determination of the a_j's will yield the quantitative sample analysis. Most analyses, therefore, are simply different methods,

either direct or indirect, of obtaining the values of the a_j's in equation 15, which is equivalent to synthesizing the unknown spectrum using the standard spectra.

Manual Methods

Manual methods of processing gamma ray spectra usually do not attack the analytical problem directly due to the huge amount of calculation involved, but instead usually employ various graphical techniques[5,14,22] where the constants a_j are determined on the basis of some type of measurement of areas under corresponding peaks in the composite and standard isotopic spectra. These graphical methods work quite well in many cases where qualitatively known samples having only one or two component spectra are quantitatively analyzed. There have been some attempts at manual algebraic solution of the analytical problem of spectroanalysis.[2] These methods, however, do not seem to present any great advantage over graphical techniques and are generally much more time consuming.

The manual methods all tend to suffer from several important disadvantages. Since gain and threshold corrections cannot be easily made during analysis, these instrumental parameters must be the same for both the composite spectrum and the standard isotopic spectra. This, in turn, usually requires that the isotopic standards be irradiated with the unknown sample, which again, is not a serious difficulty if only one or two components are present in the unknown sample.

The difficulties of these methods rapidly become overpowering as the number of components in the unknown spectrum increases beyond three or four. Then the manual methods tend to break down (except in ideal cases) due to such complications as overlapping or composite peaks, background, etc. In the more sophisticated methods, able to overcome these difficulties to some extent, the analysis becomes very tedious and time consuming. Furthermore, the accuracy of these methods, limited at best, becomes quite poor when the sample complexity increases even slightly.

Computer Analysis

The obvious solution to this situation is the development of computer programs which will perform all, or at least parts of the analysis. This indeed has been one of the most important developments in activation analysis in recent years.

There are programs which use about the same graphical techniques as in manual analyses with some refinements made possible by the speed of the computer.[1,6] These programs tend to suffer the same disadvantages as the manual methods as sample complexity increases. More commonly, the computer has been used to obtain a direct solution to the purely analytical problem of spectroanalysis, i.e., the solution of equation 15 for the quantities a_j.

Methods of Analytical Spectrum Unscrambling

Equation 15 is set of M equations in the N unknowns, a_j. M, the number of channels, is in general much greater than N, the number of

component spectra present in the composite. This gives (M-N) degrees of freedom in the solution of the problem. To obtain a "best" solution to the full set of M equations in N unknowns, the method of least squares may be used as follows. Define a residual spectrum:

$$R(i) = F(i) - \sum_{j=1}^{N} a_j f_j(i). \tag{16}$$

Then square both sides and sum over all channels:

$$\sum_{i=1}^{M} [R(i)]^2 = \sum_{i=1}^{M} [F(i) - \sum_{i=1}^{N} a_j f_j(i)]^2 \tag{17}$$

For the solution set, a_j, let this sum of the squares of the residuals be a minimum. Then, minimizing equation 17 with respect to a_k is equivalent to:

$$\frac{\partial}{\partial a_k} \{ \sum_{i=1}^{M} [F(i) - \sum_{j=1}^{N} a_j f_j(i)]^2 \} = 0. \tag{18}$$

Equation 18, after some manipulation, leads to a set of N equations in N unknowns, a_j, which uses all available information. This treatment is probably the most powerful yet developed and has been extensively studied and used.[3,11,25,29,32,33]

The solution of equation 15 can be somewhat simplified by dividing the range of channels into L intervals $[i_1, i_2]$, $[i_2, i_3]$, $\cdots$, $[i_L, i_{L+1}]$, and summing over the k^{th} interval:

$$T_k = \sum_{i=i_k}^{i_{k+1}} F(i) = \sum_{i=i_k}^{i_{k+1}} [\sum_{j=1}^{N} a_j f_j(i)], \quad k=1,2,\cdots,L \tag{19}$$

$$N \leq L \leq M$$

where T_k is the total number of counts in the k^{th} interval of the composite spectrum. While this approach may seem undesirable because

of the inherent destruction of information, it offers certain advantages in many cases.

In the system of linear programming developed by Kerrigan,[24] equation 19 is converted to an inequality of the form:

$$T_k \geq \sum_{j=1}^{N} \left[\sum_{i=i_k}^{i_{k+1}} a_j f_j(i) \right] \tag{20}$$

with the additional constraint that the solution set be non-negative, i.e.,

$$a_j \geq 0 \tag{21}$$

This method produces good results with the additional advantage that amounts of components are constrained to be non-negative.

A simpler specialization of equation 19 is that of making L equal to N, thereby producing a set of N equations in N unknowns which can be solved by purely algebraic means as follows.

Define a matrix:

$$g_{kj} = \frac{\text{counts in } k^{th} \text{ interval of } j^{th} \text{ standard spectrum}}{\text{total counts in } j^{th} \text{ standard spectrum}}$$

that is,

$$g_{kj} = \frac{\sum_{i=i_k}^{i_{k+1}} f_j(i)}{\sum_{i=1}^{M} f_j(i)} \tag{22}$$

where $k = 1,2,\cdots,N$. Since the a_j's are constants with respect to i,

$$g_{kj} = \frac{\sum_{i=i_k}^{i_{k+1}} a_j f_j(i)}{\sum_{i=1}^{M} a_j f_j(i)} \tag{23}$$

or

$$\sum_{i=i_k}^{i_{k+1}} a_j f_j(i) = g_{kj} \sum_{k=1}^{M} a_j f_j(i). \tag{24}$$

Reversing the order of summation in equation 19 and substituting equation 24 yields:

$$T_k = \sum_{j=1}^{N} [g_{kj} \sum_{i=1}^{M} a_j f_j(i)] . \tag{25}$$

Letting

$$H_j = \sum_{i=1}^{M} a_j f_j(i) , \tag{26}$$

equation 25 becomes

$$T_k = \sum_{j=1}^{N} g_{kj} H_j . \tag{27}$$

Equation 27 is a set of N equations for the N unknowns, H_j, in terms of known quantities. From equation 26:

$$a_j = \frac{H_j}{S_j} \tag{28}$$

where

$$S_j = \sum_{i=1}^{M} f_j(i) \tag{29}$$

is the total number of counts in the j^{th} standard spectrum (a known quantity). Therefore, the solution of equation 27 for the quantities H_j, the total number of counts in the composite spectrum due to the j^{th} component spectrum, yields, in effect, the quantitative composition of the sample.

An important advantage of this method is the simplicity of the coefficient matrix, g_{kj}, defined by equation 22. Notice that in order to calculate the g_{kj}'s, only one standard spectrum has to be in core storage at any one time. This means that spectra with a relatively large number of channels can be used without running out of core storage in the computer. Using this method, a 1024 channel complex spectrum containing 20 components can be analyzed using only about 2500 words of spectrum and equation working storage.

Starting with the least squares approach (equation 18), it can be shown[3] that the coefficient matrix of the set of N equations resulting is of the form

$$h_{kj} = \sum_{i=1}^{M} \left[\frac{f_j(i) f_k(i)}{F(i)} \right]. \qquad (30)$$

In order to calculate these coefficients it is necessary to have the composite spectrum and all N standard spectra in core storage at one time. Thus analysis of a 1024 channel, 20 component spectrum would require about 22,000 words of working storage. For this reason programs using this method are much more seriously limited as to numbers of channels and components.

All three of the spectrum unscrambling schemes discussed assume that the qualitative analysis has already been performed on the basis of peak energies and/or half-lives. There are other approaches in which these operations are more intimately mixed. One of the most well known is that developed by Heath and others[5,13,16,17,18] in which the assumption is made that each isotopic spectrum (and hence the composite) is due to

a collection of monoenergetic gamma components of various intensities and half-lives. Each standard spectrum, $f_j(i)$, is then a monoenergetic response function (resembling figure 2) which may either be generated by the program or be stored in a response library. Spectra are obtained as a function of time and analyzed in terms of these monoenergetic spectra, thus obtaining a half-life for each monoenergetic component. The components are then grouped according to half-life and the members of each group summed in the proper proportions to obtain the isotopic spectra. A program developed by Hull and Gilmore[31] uses a simplified version of this same sort of approach.

Most computer programs for routine spectroanalysis fall into two general categories. The more common type is designed to provide an accurate determination of the amounts of one or a few elements known to be in the sample by directly stripping the isotopic spectra of the constituents from the composite. The second and much more complex type is employed in qualitative and quantitative analysis of samples of completely unknown composition. Since direct stripping of isotopic components would require a large comprehensive library of standard isotopic spectra, the monoenergetic component treatment is usually applied.

The program developed here uses a type of analysis which seems to have been relatively neglected; namely, the analysis of samples whose composition is unknown, but for which the number of possible constituents is limited (20 to 30 detectable isotopes). The need for a large comprehensive spectral library is avoided in this approach. In order to make the analysis as fast as possible, component identification is made on the basis of peak energies with no half-life measurements.

The advantages of the method are its relative simplicity compared to other programs of similar capabilities, its ability to make a fast analysis based on only one spectrum instead of requiring a whole series of spectra, and its ability to perform a completely automatic analysis. The latter implies that the program should be capable of taking raw data from the pulse height analyzer and producing from it a complete isotopic and elemental analysis of the sample with no intermediate human decisions or manual data handling under as wide a range of circumstances as possible.

CHAPTER 5

THE PROGRAM

The complete analysis consists of a series of separate problems each requiring a solution compatible with all the other solutions. The following is a description of the program detailing these problems and methods of solution along with comparisons of these methods with those already developed or under development by others. More detailed information on the mechanics of the program (flowcharts, listings, etc.) may be found in Appendix A.

Preliminary Spectrum Processing

Before the actual analysis can begin, the raw gamma spectrum must first undergo preliminary processing in preparation for component identification and spectrum synthesis.

Data Smoothing

The count in each channel of the spectrum is subject to a statistical error which introduces random variations in the spectrum. This noise is not too serious if the energy per channel ratio is coarse (i.e., if the spectrum contains relatively few channels). However, the energy per channel here is in general 2.5 KeV/channel, and even for ratios of the order of 15 KeV/channel, noise may be a rather serious problem when analyzing the spectrum. It would be desirable, therefore, to enhance the spectrum signal-to-noise ratio by some analytical means

while avoiding a loss of significant information.

One method commonly used for treatment of continuous numerical data is that of data convolution. This technique adjusts the value of each data point according to the equation,

$$Y_j^* = \frac{\sum_{i=-m}^{m} C_i Y_{j+i}}{N}, \qquad (31)$$

which considers a group of 2m + 1 data points centered on the j^{th} data point. Using a set of 2m + 1 convoluting integers C_i, and a normalizing factor N, yields a new value Y_j^* for the j^{th} data point Y_j which is then placed in a new data table. The entire spectrum is processed by letting j run through the channel numbers in the original data table. The convolution simply represents a moving average of the ordinate values of the data points. The integers C_i are simply a weighting function applied to the points on each side of a data point in determining its new value. Many different sets of integer functions C_i have been tried, but most result in some loss of information.[31]

Perhaps the best possible results would be obtained by applying a least squares fit of a polynomial to the 2m + 1 data points in order to relocate the center point. This would seemingly entail a much more complicated procedure of setting up and solving a set of 2m + 1 equations for each data point, a somewhat lengthy prospect. Fortunately, however, by making two simple assumptions (continuity of the spectrum and equal spacing of data points along the abscissa), this least squares polynomial fit can be shown[31] to be exactly represented by a set of convoluting integers C_i and a normalizing factor N. The polynomial to be fitted may be parabolic, cubic, etc., and the value of 2m+1

(number of points in the fit) may be any odd integer above a minimum determined by the degree of polynomial. A particular set of integers C_i and N is associated with each choice of a polynomial degree and a value of 2m+1. Values of C_i and N for least squares convolutions have been tabulated by Savitzky and Golay.[31]

The question of the combination of polynomial degree and number of points per fit best suited for gamma scintillation spectra has been investigated by H. P. Yule[35] and to some extent in this research. It was found that a quadratic-cubic fit (the $C_{i's}$ and N are the same in both cases) with 2m+1 no greater than the width of a significant peak at half maximum gave best results. The program, therefore, uses a quadratic-cubic convolution with 2m+1 as an adjustable parameter.

Peak Location

Once the spectrum has been processed to remove as much noise as possible, the peaks are located. There may be many meaningless bumps and wiggles in the spectrum caused by Compton effect, low frequency noise, etc. These must be discarded and only meaningful peaks should be recorded for analysis. Furthermore, the center of the peak should be located as exactly as possible in order to determine its energy.

The first step in this procedure is the generation of the first derivative of the spectrum. This is accomplished by fitting a quadratic polynomial to 2m+1 data points to find the first derivative at the center point. It turns out that this operation, also, may be exactly

represented by a data convolution using a particular set of integers C_i and N.[31] The convolution is performed directly on unsmoothed data since the smoothing is accomplished by the fitting of the quadratic.

After the derivative is obtained, the program scans it looking for changes of sign. A change from positive to negative indicates a possible peak while the opposite change may indicate a valley. Due to low frequency noise, etc. there may be many insignificant sign changes. Therefore, to ascertain the validity of a sign change, various statistical tests are applied, several types of which have been previously proposed.[30,35]

The tests made by this program are based on two adjustable parameters, p and h. To be admitted as a valid sign change, the derivative must have at least p successive channels with the same sign after a sign change. If the change is from positive to negative (a peak), the top of the peak must be at least h counts higher than the previous valley to qualify as a valid peak. During the scan of the first derivative, the program first searches for a peak. Once a valid peak is found, a valid minimum is searched for, and the cycle is repeated until the last channel is reached.

The location of the sign change in the derivative provides an estimate of where the peak is, but to obtain the location of the center of the peak more exactly, a linear fit is made to a region of the derivative centered on the apparent sign change and of width 2g, where g is an adjustable parameter. The intersection of the linear fit with the abscissa is then interpreted to be the location of the center of the peak. The peak center does not have to be located with great accuracy since

sloping background and other mechanisms may cause a peak to shift as much as several channels. Accuracy within one-half channel would be ample.

It is also useful to have some measure of the height of the peak above background. Although this can be done in a variety of ways, the program measures the absolute height of the peak (in counts) above the previous minimum.

Energy Calibration

In order to determine the energy of an unknown peak in a complex spectrum, it is necessary to know the gain (MeV/channel) and the threshold (channel of zero energy) accurately. The usual method of accomplishing this is to take spectra of known gamma calibration standards (Co^{60}, Cs^{137}, etc.) before and after the unknown spectrum is produced. Then a plot is made of energy as a function of channel number. The known peaks in the standards are plotted as points on the graph, and a straight line is fitted to the points. The graph is then used to determine the energies of the peaks in the unknown spectrum.

This procedure has been incorporated into the program to speed up the analysis and increase accuracy. Several calibration spectra taken just before or after the unknown spectrum are placed into the program input. Along with each calibration spectrum a list of the energies and approximate locations of known peaks is included. The program then locates all peaks in each spectrum by the method previously described and proceeds to search through the detected peaks to find the ones corresponding to the standard peaks read in. A series of pairs of the form (x_i, E_i) is then formed where x_i and E_i are the location (channel

number) and energy (MeV) of the i^{th} standard peak. The points are fitted by least squares to an equation of the form $E = mx + b$ where it is assumed that the E_i's are exact and the x_i's contain random errors. Having thus found values for k and b, it is easy to determine the energies of the peaks in the unknown spectrum by the use of the above relationship. With this the preliminary data processing is completed.

Gain and Threshold Correction

The problem of instrumental gain and threshold shifting has been one of the most troublesome problems associated with automatic activation analysis, especially when the standard isotopic spectra are stored in a permanent library made up at a time previous to the sample analysis. The various methods of spectrum synthesis discussed previously are all more or less sensitive to changes in gain, and a shift of only a few channels may produce errors so large that the results of an analysis are meaningless. The most common solution to this problem is direct calibration of the instrument for specific values of gain and threshold at the beginning of each analysis. Some rather elaborate schemes have been devised for keeping the instrument calibrated.[12] In this work the corrections for such instrumental instabilities are included in the program itself in the form of a routine capable of changing the gain and threshold of a spectrum to any values desired.

Consider two spectra having different gains and thresholds in which the energy as a function of channel number is given by:

$$E = mi + b \tag{32}$$

$$\text{and } E = m'i' + b' \tag{33}$$

for the unprimed and primed spectra, respectively. Notice that the channel numbers i and i' both correspond to energy E in their respective systems. Equating the right hand sides of equations 32 and 33 and solving for i' yields:

$$i' = \frac{mi + b - b'}{m'} . \tag{34}$$

The threshold channel numbers in the two systems are obtained by setting E = 0 in equations 32 and 33 and solving for i_o and i_o', the channel numbers of zero energy:

$$i_o = -\frac{b}{m} \tag{35}$$

$$i_o = -\frac{b'}{m'} \tag{36}$$

Combining equations 34, 35, and 36 then yields:

$$i' = \frac{m}{m'} (i - i_o) + i_o' . \tag{37}$$

Equation 37 is the basic equation used to transform a spectrum from the primed system to the unprimed system. The program scans the unprimed channel numbers and for each i finds the corresponding i' to obtain the count at that energy. The count at channel i' must, however, be multiplied by the factor $\frac{m}{m'}$ to keep the apparent activity (i.e., the area under the spectrum) of the sample a constant.

Another complication occurs because i' is, in general, not an integer and, therefore, some type of interpolation scheme must be used to obtain the count at a non-integral channel number of the spectrum being adjusted. Since the gain used in this research was small (about 2.5 KeV per channel) a linear interpolution between pairs of adjacent

channels was considered sufficient. For a coarser gain, however, higher order interpolation should be used; parabolic interpolation for this purpose has been tried with good success.[21]

Qualitative Analysis

The first major phase of the analysis is the identification of components. The program has available to it an isotopic spectral library on magnetic tape containing in addition to the spectra, other information associated with the isotopes (half-lives, peak energies, etc.), as well as experimental parameters (sample weights, decay and count times, etc.). Detailed information on the library format may be found in Appendix B.

On the basis of the peak energies found in the unknown spectrum the program must decide which of the isotopes in the library are present in the composite. For this purpose, each entry in the library corresponding to a particular element contains a list of one or more reference peak energies which are chosen so that there will be as few interferences as possible with other elements in the library.

An element usually has only one isotope which activates to an appreciable extent, in which case the element entry in the library will contain only one isotopic spectrum. Some elements will produce more than one isotope when activated and in these cases an elemental entry in the library contains all of the isotopic spectra produced by that element. The first isotopic entry contains all reference peaks corresponding to the element as a whole, and if the element is found to be present all of the corresponding isotope entries are read out.

The program scans through the elemental entries in the library checking to see if all the peaks listed for each element are present in the unknown spectrum within adjustable confidence regions in the energy range. If a particular element is found to be present all the corresponding isotopic entries are read out one at a time along with other associated information; the standard isotopic spectra are smoothed; and the gain and threshold adjusted to match that of the unknown spectrum. Each isotopic entry is then placed onto an intermediate magnetic tape.

Thus, the program scans the library testing for the presence of each element until the end of the library is reached. At that point the isotopic entries corresponding to all the components detected in the complex spectrum are stored on the intermediate tape and the program is ready to determine the actual amount of each one present in the composite spectrum.

Quantitative Analysis

The isotopic spectra on the intermediate tape are used to synthesize the composite spectrum by solving equation 15 for the quantities a_j. The method used, a compromise of accuracy, simplicity, and available computer core storage, is the linear matrix method of equation 27. The standard isotopic spectra are read one at a time from the intermediate tape to calculate the matrix g_{kj} defined by equation 22. The matrix T_k defined in equation 19 is calculated using the composite spectrum.

In order to calculate these matrices the spectra involved must be divided into N intervals $[i_1, i_2]$, $[i_2, i_3]$, $\cdots$, $[i_N, i_{N+1}]$ where N is the number of isotopic components. The program does this so that each such interval in the composite spectrum contains approximately the same number of counts.

Once the matrices are set up, the set of equations 27 could be solved by any of several methods. Since, however, each set is solved only once for a given set of numbers g_{kj}, it was decided to use matrix triangularization and back substitution.[28]

After the spectrum has been synthesized it is subtracted from the composite spectrum to obtain a residual spectrum which can be used to judge the validity of the analysis. In the ideal case, of course, the residual should be identically zero at all channels, but in a real analysis it will be a series of small randomly positive or negative numbers produced by counting statistics and errors in gain shift correction.

Having solved the set of equations 27 for the quantities H_j it is a relatively easy matter to obtain the composition of the sample by using equation 14 where

$$\left[\frac{C}{C'}\right]_j = a_j$$

for the j^{th} isotope. Then assuming the isotopic abundances in the sample to be normal, properly weighted averaging will yield amounts of multi-isotope elements.

CHAPTER 6

RESULTS

All of the major data processing routines have been tested and evaluated, and with few exceptions excellent results have been obtained.

Data smoothing by least squares convolution has been investigated using five, seven, and nine points per quadratic-cubic fit, and the good results obtained by previous workers have been consistently confirmed. Figure 3 shows the results of a seven point quadratic-cubic convolution on a typical peak. As can be seen the shape is considerably improved. A fit over fewer points tends to retain more fluctuations, but as the number of points increases, small but significant peaks tend to be flattened.

The peak location routine produces very good results and seems to be quite reliable when the peak parameters are properly chosen. Figure 4 shows a typical peak along with its derivative generated by a seven point quadratic convolution. The center of the peak as calculated by the program is also indicated. The peak location parameters in this case were $p = 5$, $h = 50$, $g = 8$. The peak detection was generally found to be more reliable than visual examination of plotted data in that valid peaks were often found which were so small as to be overlooked on visual examination.

The energy calibration routine works well and produces results more accurate than could be obtained by the usual graphical methods.

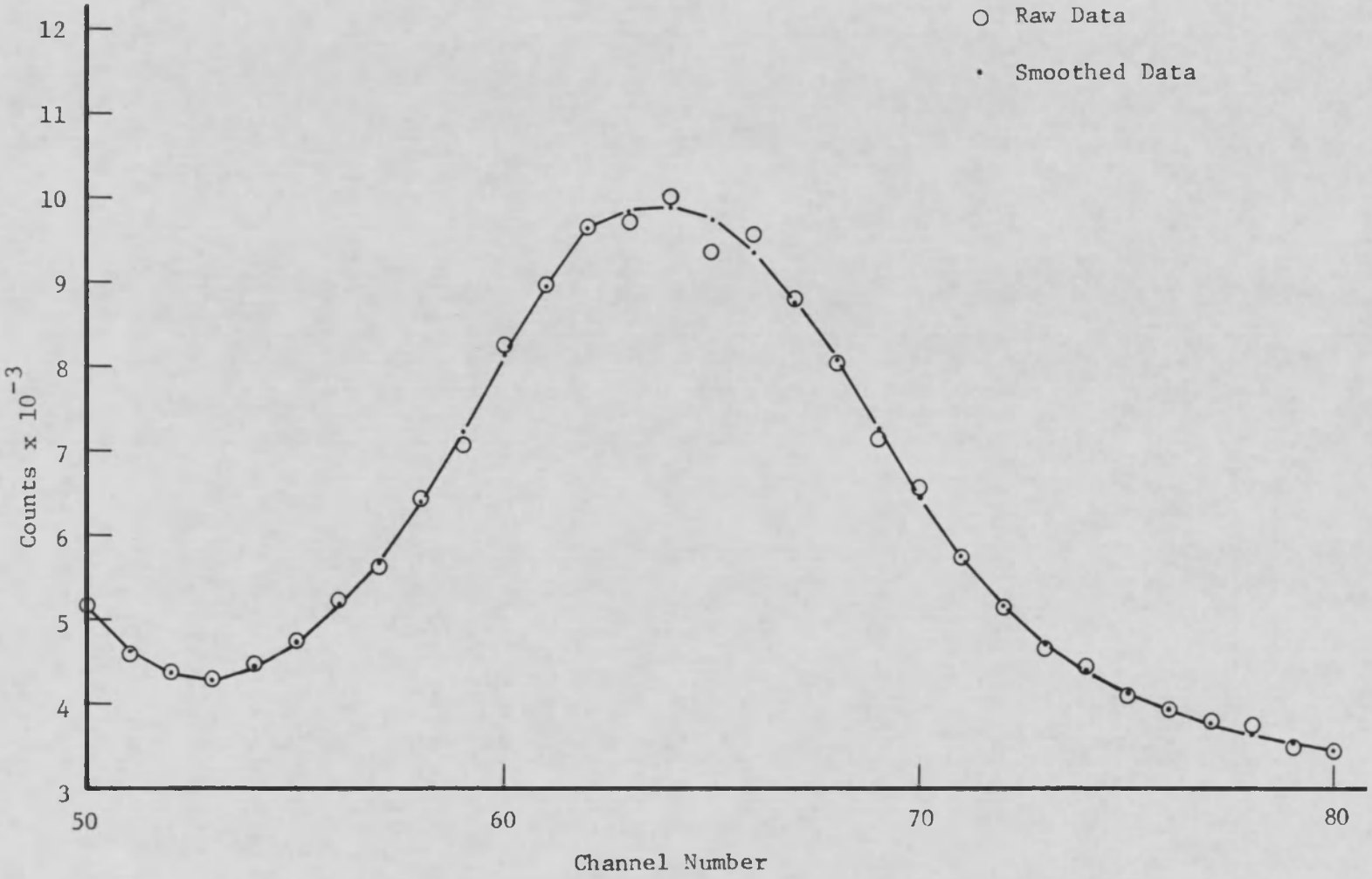

FIGURE 3: Effect of 7-Point Smooth

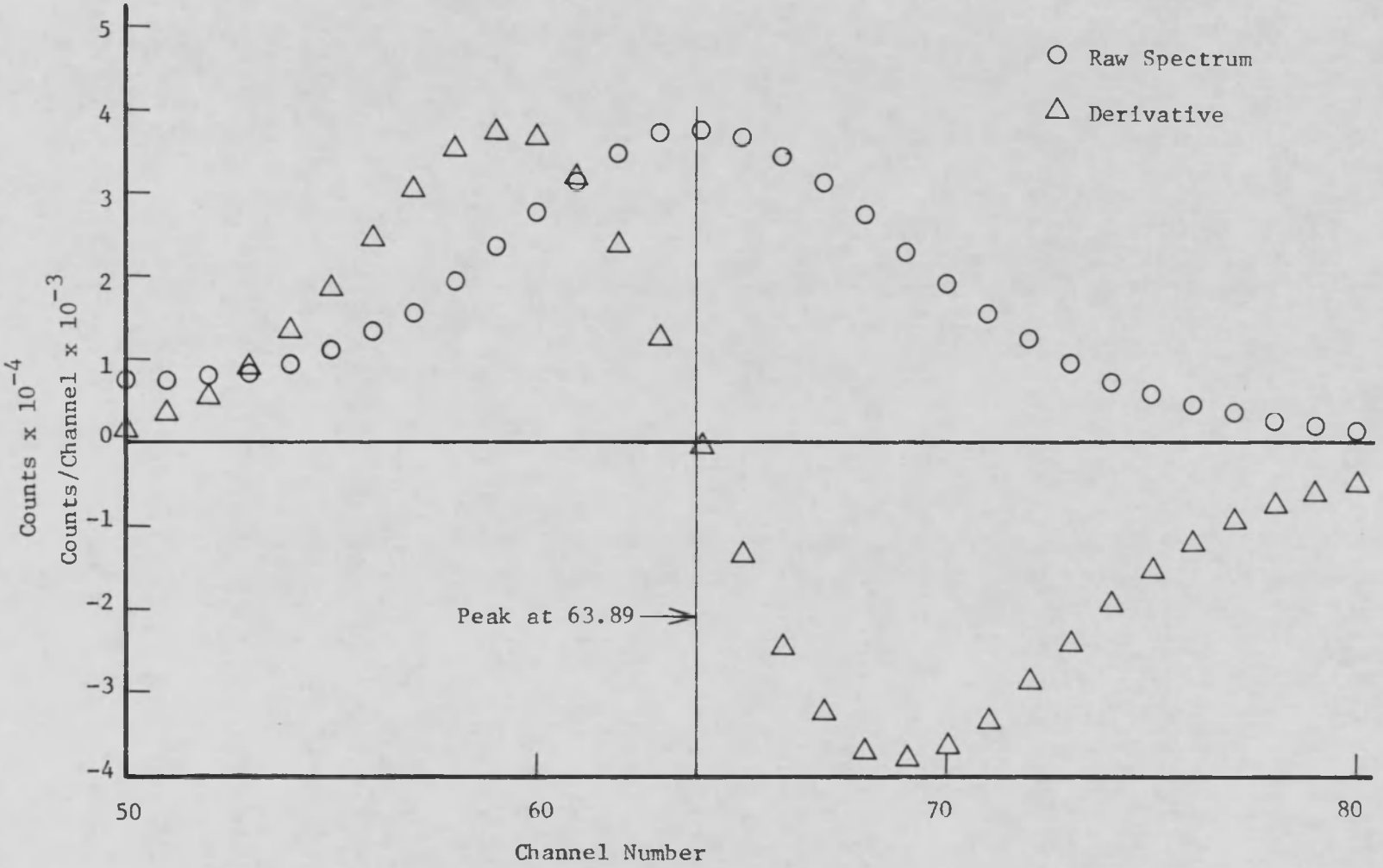

FIGURE 4: Results of Typical Peak Location

Since the program uses least squares fitting its accuracy is limited only by the linearity of the pulse height analyzer. Results of a typical spectrum calibration using several gamma standards are shown in table 1 and figure 5.

Since preliminary tests of the library search and spectral synthesis routines produced acceptable results, a test of the entire integrated program was made using long lived gamma standard sources. The proper information was fed into the program to make the mixture look exactly like a real physical mixture, but containing no errors due to weighing or irradiating samples. The only errors present were due to counting statistics and gain and threshold shifting.

The standard spectrum library contained seven isotopic spectra of which the most important are shown in figures 6 through 9. A total of six mixture spectra were prepared and supplied with the properly consistent synthetic physical quantities (i.e., irradiation times, sample weights, etc.). These mixtures are summarized in table 2. The six mixtures were first analyzed by the spectrum synthesis routine alone as final test of the routine. The output from the analyses were the numbers of counts due to each component in the various mixture spectra. These tests indicated one flaw remaining in the spectrum synthesis routine.

Notice that the spectra shown in figures 8 and 9 (Mn^{54} and Cs^{137}) are both monoenergetic, of the same general shape, and do not differ greatly in energy. The accompanying difficulty in the spectroanalysis appears if both these peaks are included inside the same spectral region

TABLE 1: Peak Locations for Energy Calibration

ISOTOPE	PEAK ENERGY	LOCATION READ IN (CHANNEL NO.)	LOCATION USED BY PROGRAM (CHANNEL NO.)
Co^{57}	0.123	64	63.66
Cd^{109}	0.087	43	43.04
Co^{60}	1.18	683	683.32
	1.33	777	777.00

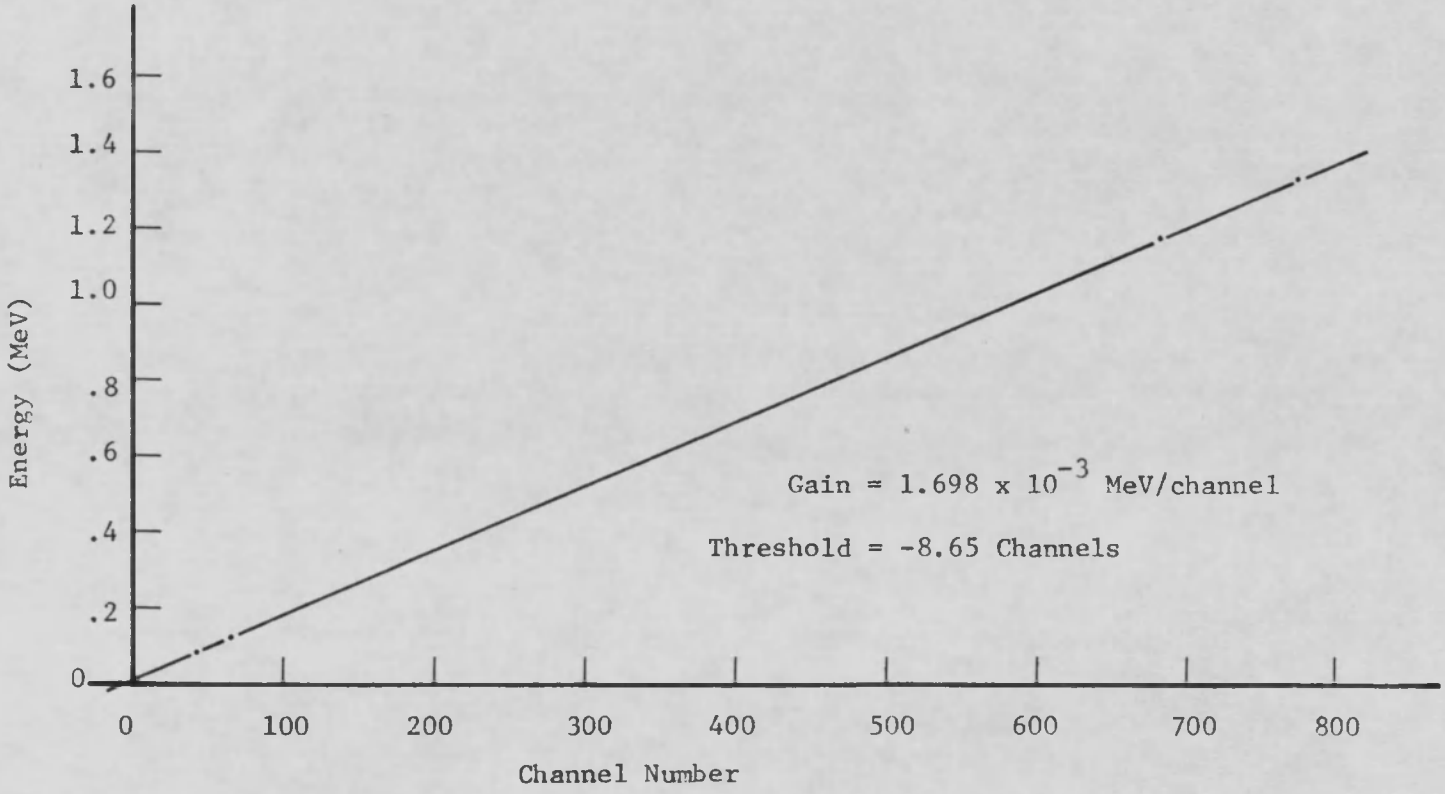

FIGURE 5: Results of Energy Calibration

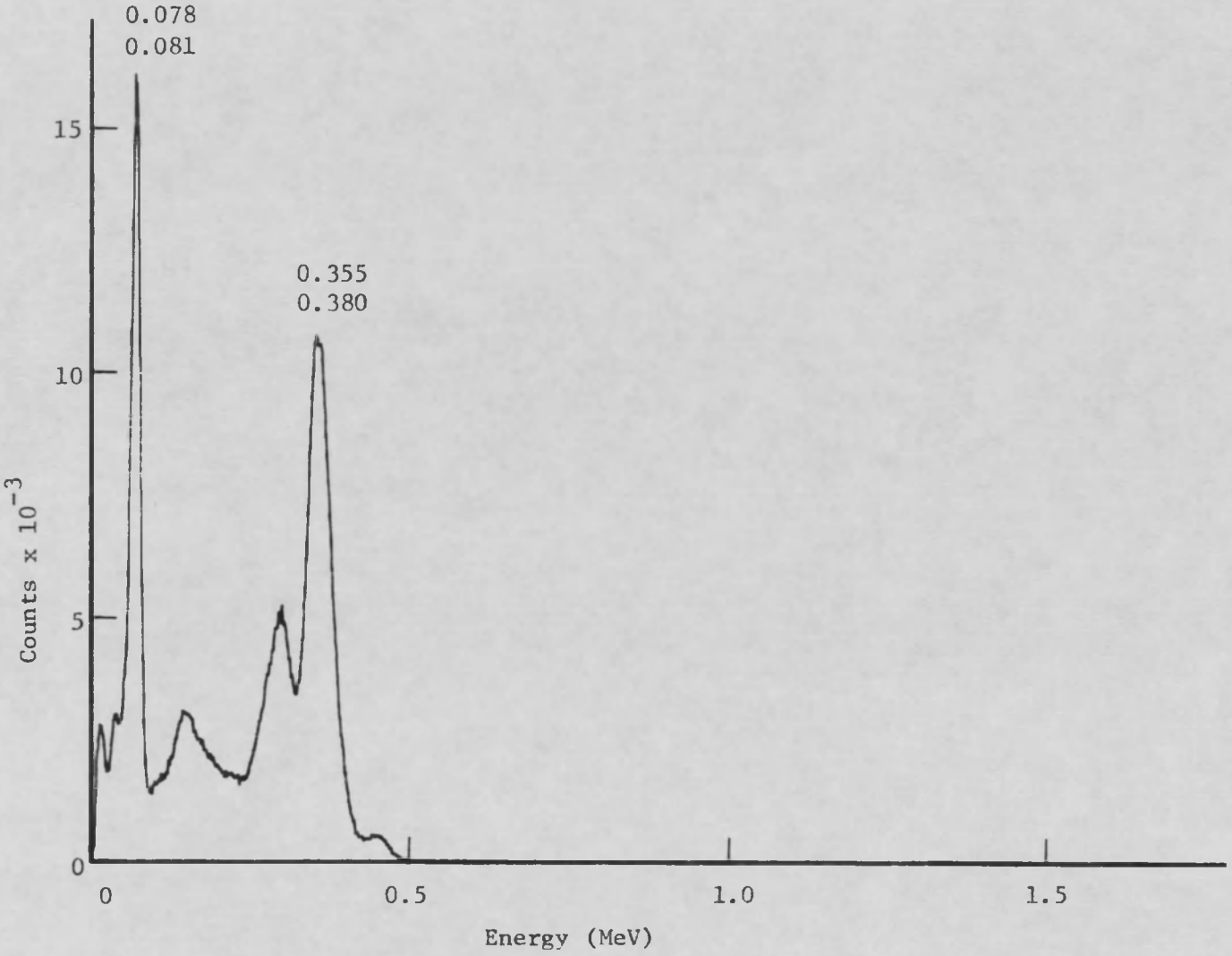

FIGURE 6: Ba^{133} Standard Spectrum

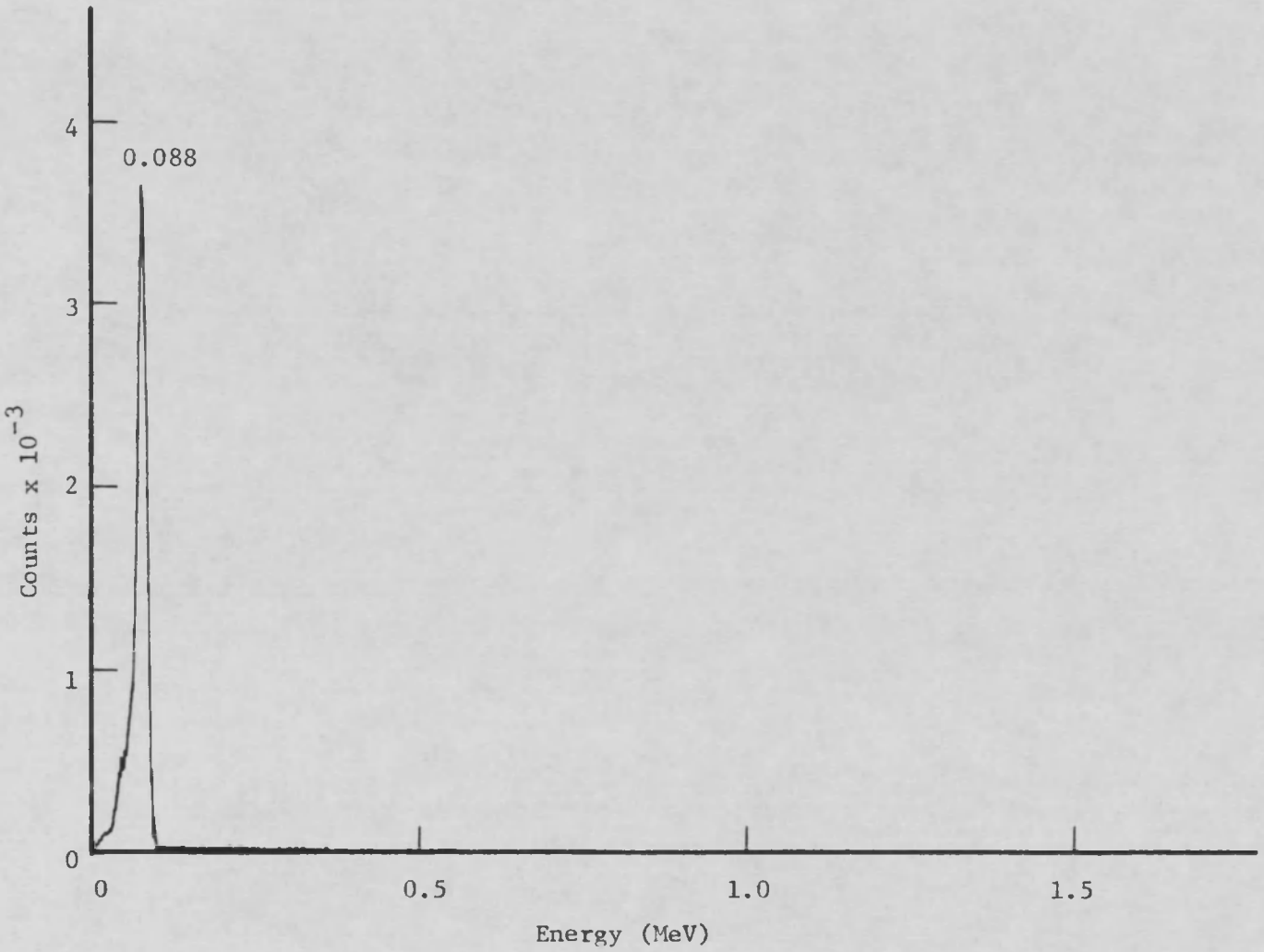

FIGURE 7: Cd^{109} Standard Spectrum

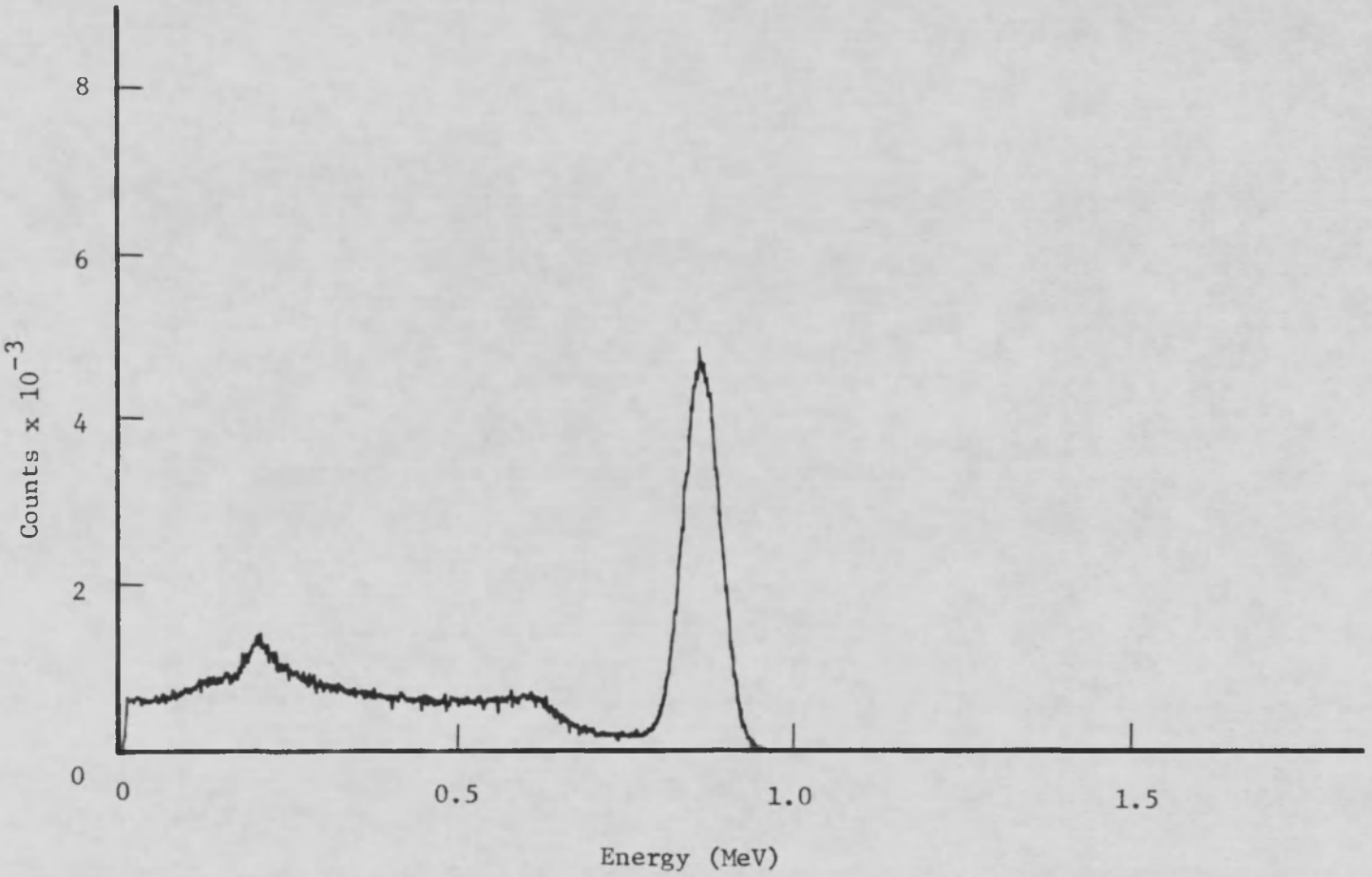

FIGURE 8: Mn^{54} Standard Spectrum

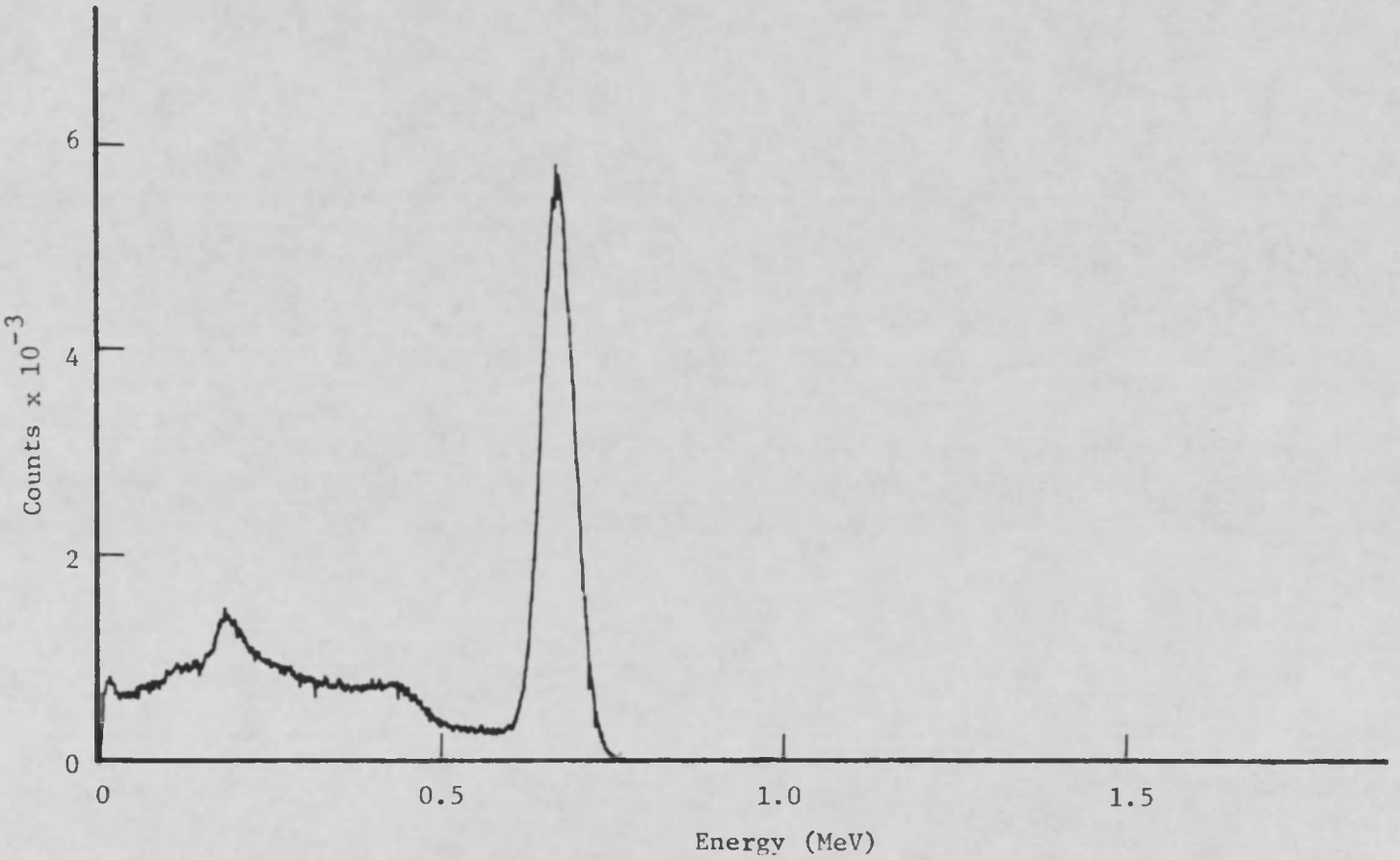

FIGURE 9: Cs^{137} Standard Spectrum

TABLE 2: Weights Supplied to Program for Synthetic Mixtures (μg)

MIXTURE NUMBER	Co^{60}	Co^{57}	Na^{22}	Mn^{54}	Ba^{133}	Cd^{109}	Cs^{137}
1	33.3	23.9	5.93	1.56	0	0	0
2	33.3	23.9	5.93	1.56	3.13	0	0
3	33.3	23.9	5.93	1.56	3.13	694	0
4	33.3	23.9	5.93	1.56	3.13	694	3.86
5	33.3	23.9	5.93	1.56	3.13	694	19.3
6	33.3	23.9	5.93	1.56	3.13	694	38.6

$[i_k, i_{k+1}]$ when the spectrum is divided to calculate the T_k matrix. Since T_k is the sum of the counts in the mixture spectrum in the k^{th} interval, the Mn^{54} and Cs^{137} contributions appear almost identical to the spectrum synthesis routine and very large errors tend to be produced in the analysis. When, however, the spectral divisions were manually supplied to the program so that a division point fell between the Mn^{54} and Cs^{137} peaks, results again became very accurate with errors of no more than a few percent. This difficulty was only present in mixtures 4 through 6 where Mn^{54} and Cs^{137} were both contained in the mixture.

Because of the way in which the mixture spectrum is divided (with an equal number of counts in each division), tests have shown that the division points are more likely to be located on peaks than in regions of lower count rate. A complication occurs when a division point falls near the center of a high sharp peak, and even a small error in gain correction may then have a serious effect on the solutions of equation 27.

The six mixtures were analyzed by the entire integrated program containing all the features previously discussed. The overall results of the six analyses were very similar so that only one typical case (mixture number 3) is shown in detail in figure 10 and tables 3 and 4. Figure 10 shows the mixture spectrum, and table 3 lists the results of the peak location routine on which the spectrum library search was based. Table 4 lists the overall results of the analysis including the errors caused by counting statistics. The program correctly identified the components and calculated their amounts with very acceptable errors. The other five mixture analyses resulted in very similar errors and in

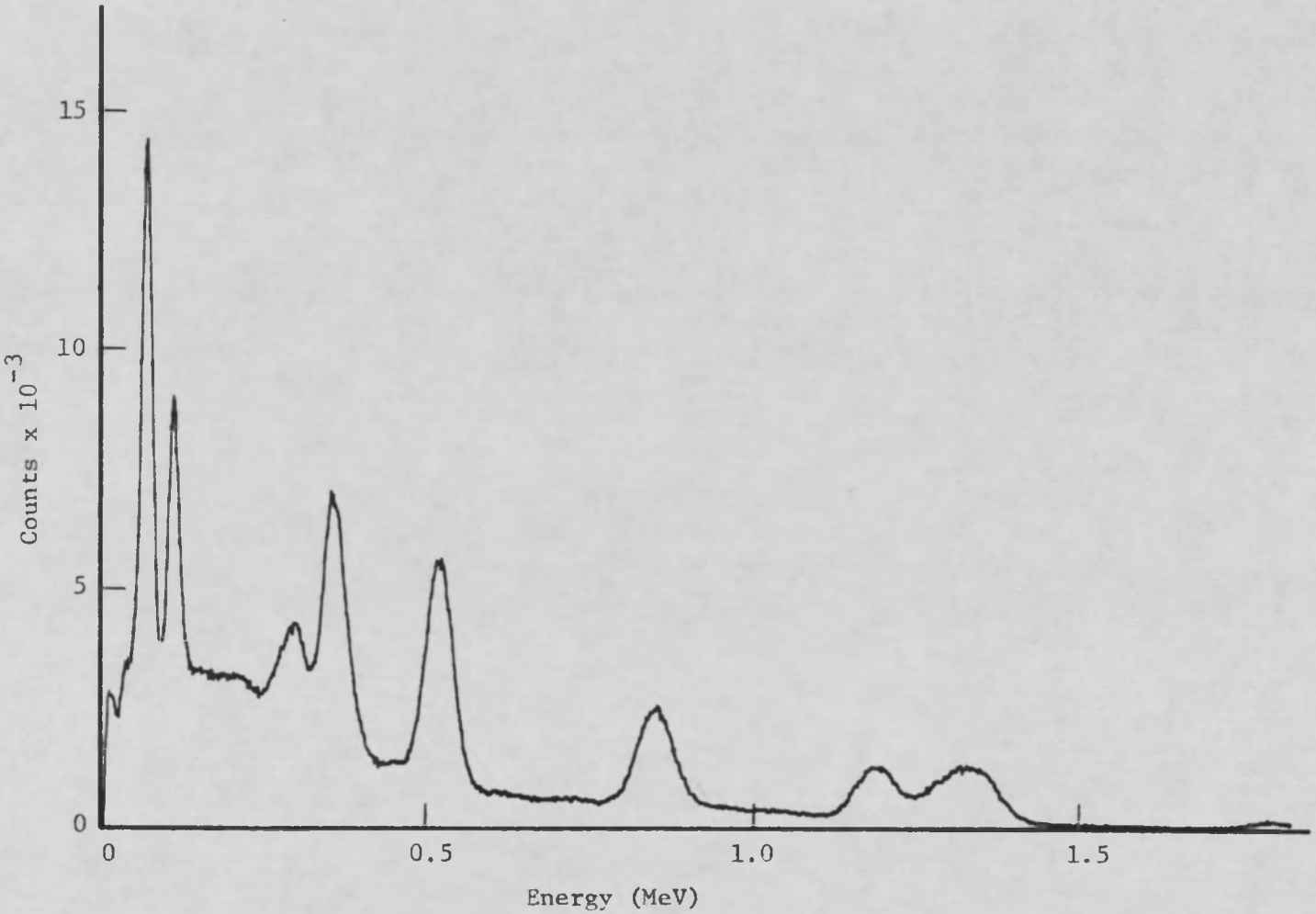

FIGURE 10: Mixture 3 Spectrum

TABLE 3: Results of Peak Location, Mixture 3

CHANNEL NUMBER	ENERGY ASSIGNED (MeV)	TRUE ENERGY (MeV)	ISOTOPES RESPONSIBLE
41.16	0.0846	[0.088 0.079	[Cd^{109} Ba^{133}
63.77	0.1230	0.1220	Co^{57}
170.90	0.3049	0.302	Ba^{133}
205.92	0.3644	0.367	Ba^{133}
299.11	0.5227	0.511	Na^{22}
489.60	0.8462	0.835	Mn^{54}
684.18	1.1766	1.173	Co^{60}
765.64	1.3150	[1.274 1.332	[Na^{22} Co^{60}

TABLE 4: Summary of Analysis, Mixture 3

ISOTOPE	STATUS	COUNTS FOUND ($\times 10^5$)	AMOUNT FOUND (μg)	% ERROR
Co^{60}	Present	3.42	34.3	3.0
Co^{57}	Present	1.30	23.8	0.4
Na^{22}	Present	4.61	5.91	0.3
Mn^{54}	Present	2.30	1.55	0.6
Ba^{133}	Present	4.63	3.08	1.6
Cd^{109}	Present	0.787	690.	0.6
Cs^{137}	Absent			

every case but one, the components were properly identified. The one exception occured in the analysis of mixture number 2 and was the result of the complication of coinciding peaks mentioned earlier. Notice in figures 6 and 7 that the single peak in the Cd^{109} spectrum is effectively at the same energy as the first peak in the Ba^{133} spectrum. These two peaks sum to form the first peak in the mixture spectrum, and the presence of Ba^{133} therefore completely masks the presence or absence of Cd^{109}. If Ba^{133} is present, the presence of Cd^{109} will be indicated whether it is really present or not, and so the analysis of mixture number 2 included a determination of the amount of Cd^{109}. The spectrum synthesis routine, however, attributed only 285 counts to Cd^{109} out of a total of 1.6×10^6 counts in the composite spectrum. In a real analysis this would be considered equivalent to a zero amount.

Table 5 presents the errors which occured in the analyses of the 6 mixtures. Mixtures 4 through 6 were analyzed using manually supplied spectrum divisions due to the complication discussed earlier concerning Cs^{137} and Mn^{54}. The errors associated with the analyses of mixtures 1 through 4 seemed to indicate no dependence of the size of errors on the number of components in the mixture, but mixtures 4 through 6 as well as earlier work suggest a strong dependence of error on the number of counts due to a particular component compared to the numbers of counts due to the other components. Figure 11 shows the error in the determination of Cs^{137} as a function of the number of counts of Cs^{137} found, all else remaining constant. The data shown are for mixtures 4 through 6, but the curve obtained is generally consistent with earlier results obtained in the testing of the program.

TAB:E 5: Summary of Errors in Mixture Analyses

(Percent Errors)

MIXTURE NUMBER	Co^{60}	Co^{57}	Na^{22}	Mn^{54}	Ba^{133}	Cd^{109}	Cs^{137}
1	2.1	0.4	2.7	8.3			
2	1.8	1.7	0.7	1.3	1.0		
3	3.0	0.4	0.3	0.6	1.6	0.6	
4	1.5	1.7	0.3	0.6	1.6	1.2	7.5
5	1.8	1.7	0.3	0.6	1.9	1.7	1.6
6	2.1	1.3	0.3	0.6	1.9	2.9	1.0

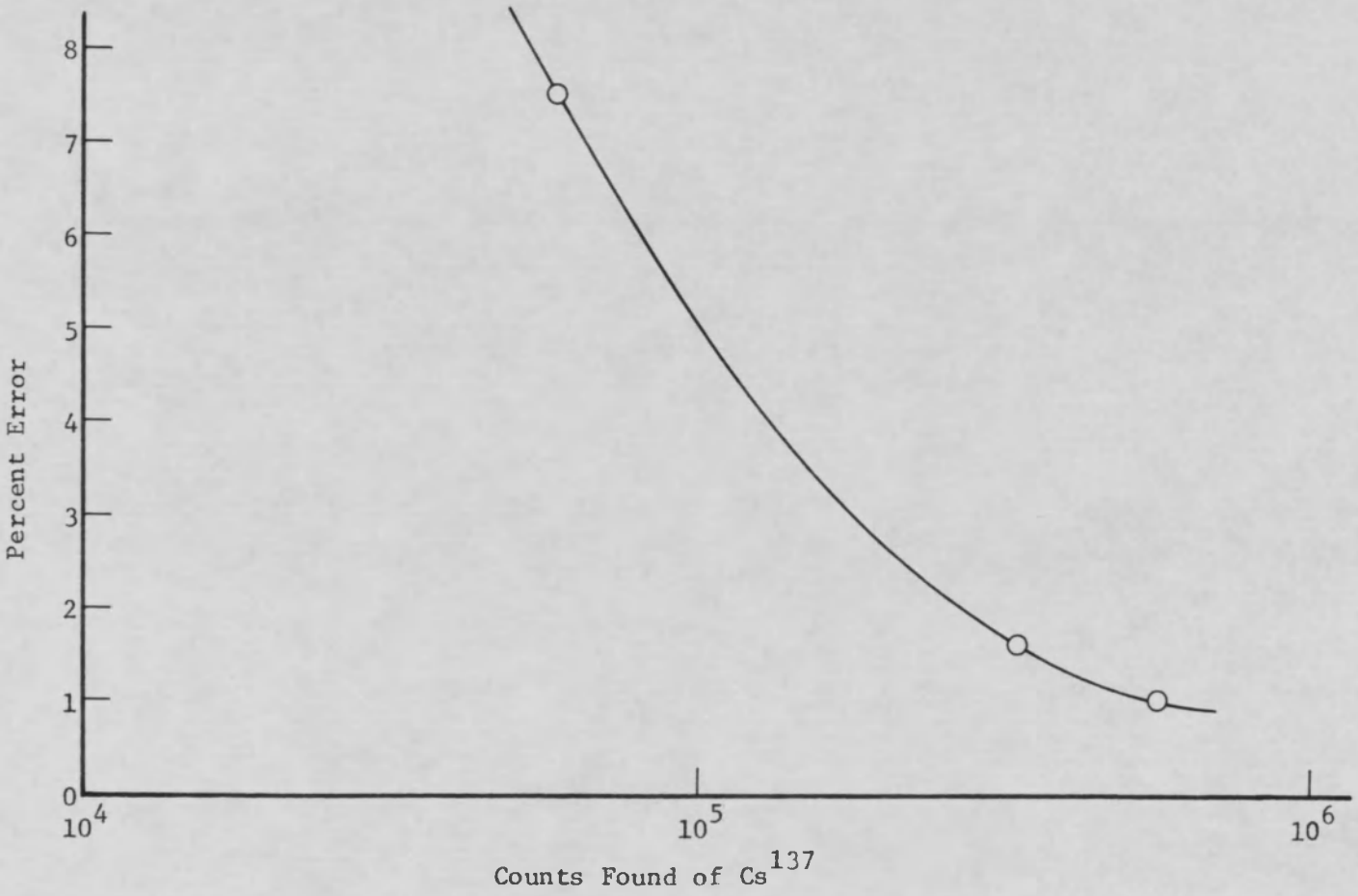

FIGURE 11: Variation of Error in Cs^{137} Determination

CHAPTER 7

CONCLUSIONS

The program as a whole works very well and produces highly acceptable results in tests using synthetic mixtures. The preliminary processing routines are reasonably well refined and can be considered finished.

The library search routine works well, but with the limitations already discussed concerning composite peaks and peak shifting due to steeply sloping background. That part of the routine which tests for the existence of library reference peaks in the composite spectrum could be refined further to take into account neighboring peaks which might shift or suppress the peak being tested for.

The spectrum synthesis routine performs reasonably well, yielding results of highly acceptable accuracy under most circumstances. However, the division of the spectrum into N segments to form the equation 27 matrices has caused trouble in some instances. Three general paths of solution to this problem seem open. First, the routine which locates the spectral divisions could be made more sophisticated so as to take into account peak locations and identities of components. Second, the spectrum synthesis routine could be converted to a linear algebra (equations 20 and 21) or a partial least squares approach (equation 19), thereby reducing the effect of division point

locations. Or, third, the spectral division points could be supplied manually. The first two alternatives would severely increase complexity and required core storage, and the third would necessitate running the program in two parts: the library search, and then the spectral synthesis. The difficulty could be removed completely only by converting to pure least squares (equation 18), but this would require even more core strage than is presently available on the present University of Arizona CDC 6400 computer.

The easiest and most foolproof way to make the program workable on a routine basis appears to be to divide it into two parts: first, the preliminary data processing and library search, and second, the spectral synthesis and quantitative sample analysis. The output from the first part would be used to manually assign spectral division points on the basis of the qualitative analysis. Although this method would not be completely automatic and would add about two hours to the total analysis time, it would be much less subject to failure.

The program as it now stands is completely automatic and produces reasonably good results given reasonably favorable circumstances. It often fails, however, due to some unfavorable combination of circumstances, and past experience both in this research and in the work of others, indicates that further refinement of the program will reduce the chance of failure, but that the chance of failure will always be considerable. This fact is somewhat compensated for, however, by the fact that whenever the analysis does fail, the failure always shows up very clearly in the output of the program, especially in the residual spectrum produced by subtracting the synthesized spectrum from the

composite. There seems to be little possibility that the analysis could appear to be accurate when it, in fact, is not.

For a completely automatic program using, for example, linear algebraic spectral synthesis, the ultimate refinement forseen here could be the addition of half-life determinations in the form of an iterative, self-correcting analysis scheme operating on a series of spectra taken over a period of time from the unknown sample after activation. Such a program would be several times more complex than the present one, and would probably completely fill the CDC 6400 to capacity, but would by no means be impossible and might not be too difficult using the present program as a starting point.

APPENDIX A

FLOWCHARTS AND PROGRAM LISTING

In this section are included the summary flowcharts of the program including the major subroutines (figures 12 through 16). Table 6 shows a detailed format of the input to the program for a typical analysis run. Following table 6 is a complete listing of the program.

MAIN PROGRAM

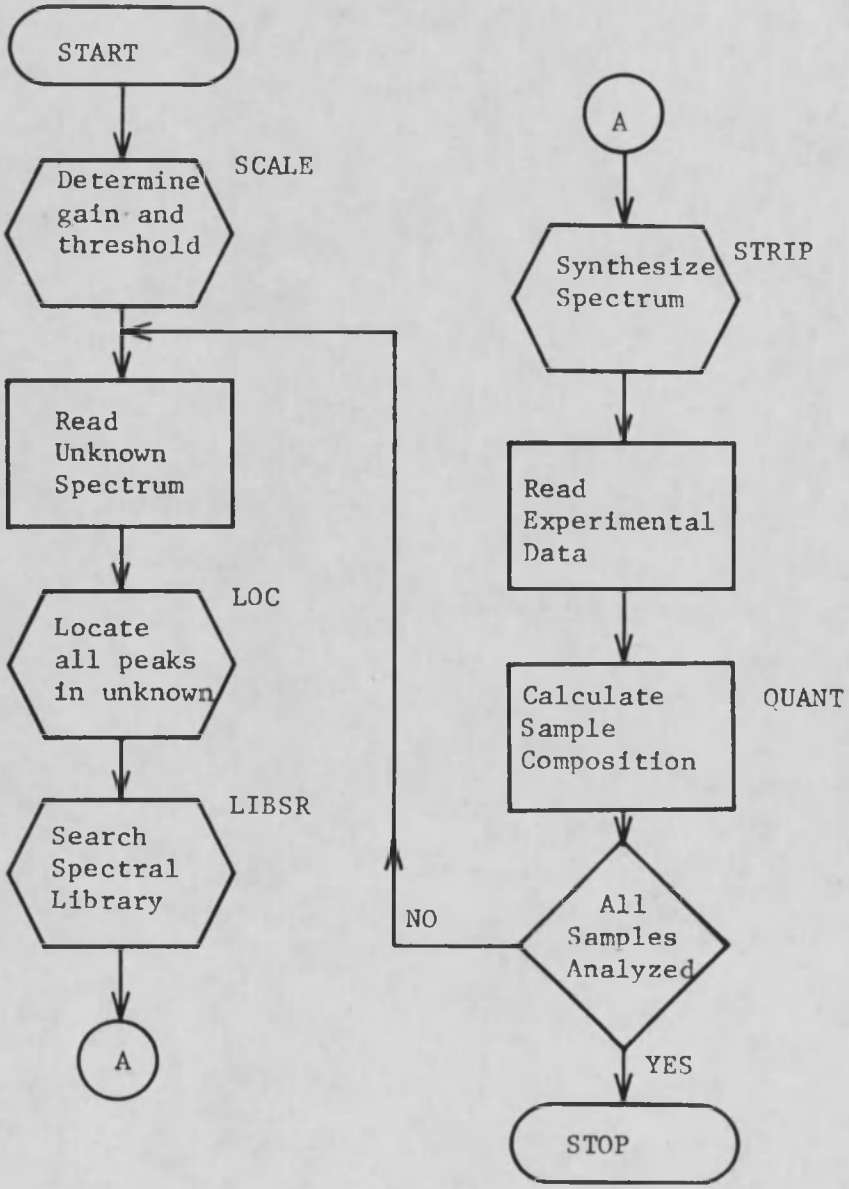

FIGURE 12: Flowchart for Main Program

SUBROUTINE SCALE

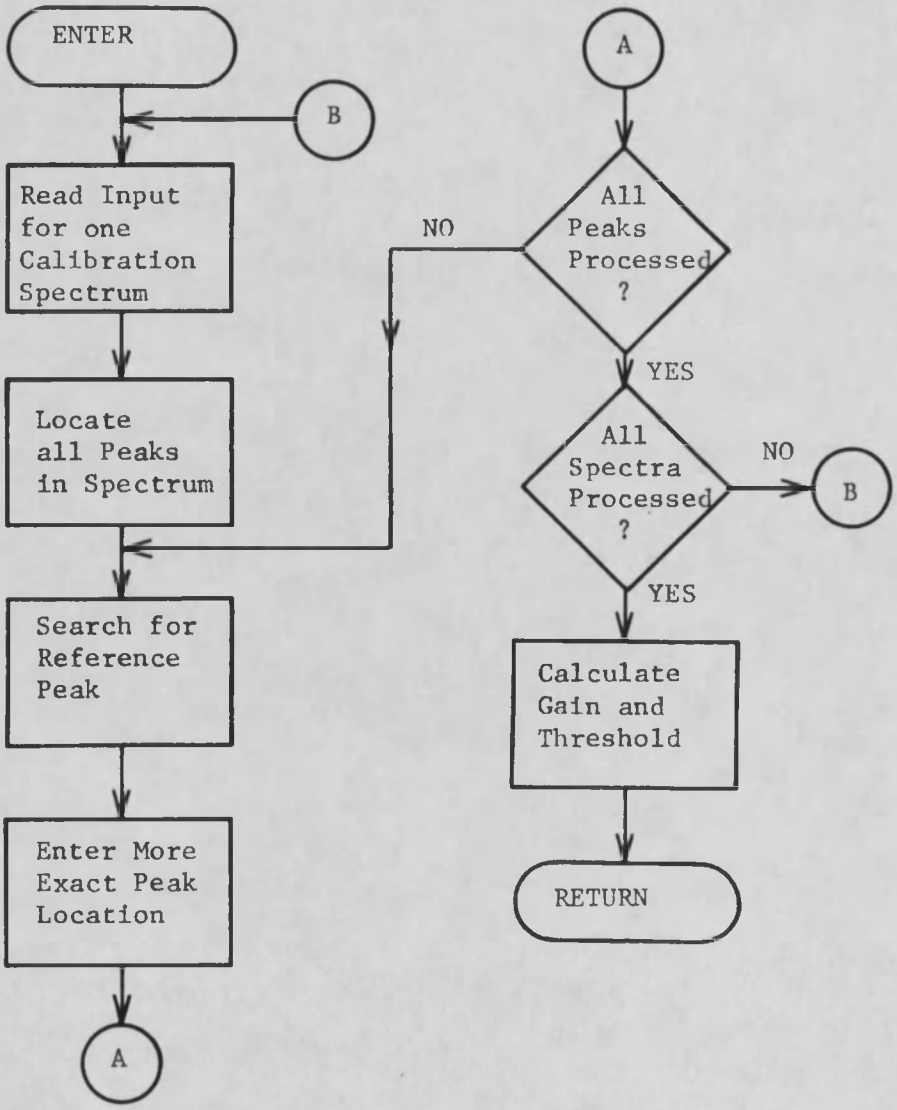

FIGURE 13: Flowchart for Subroutine SCALE

SUBROUTINE LOC

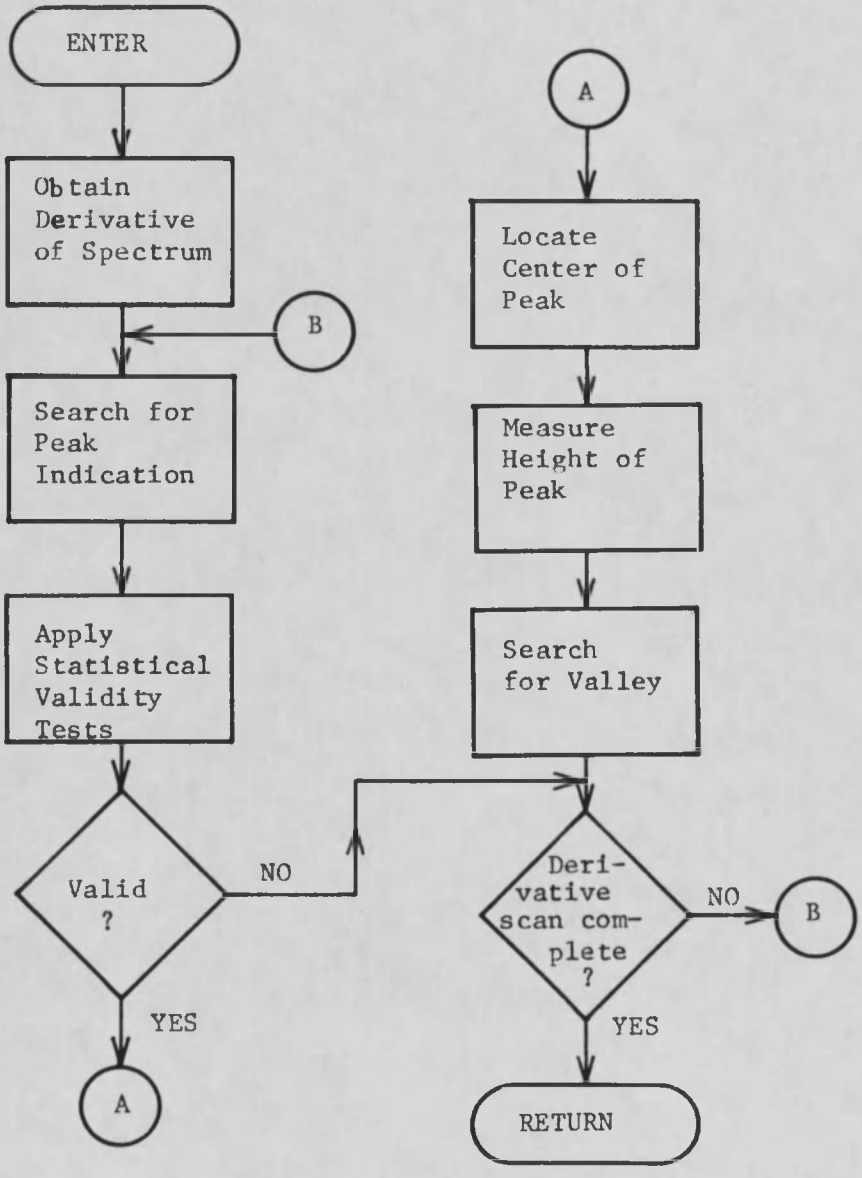

FIGURE 14: Flowchart for Subroutine LOC

SUBROUTINE LIBSR

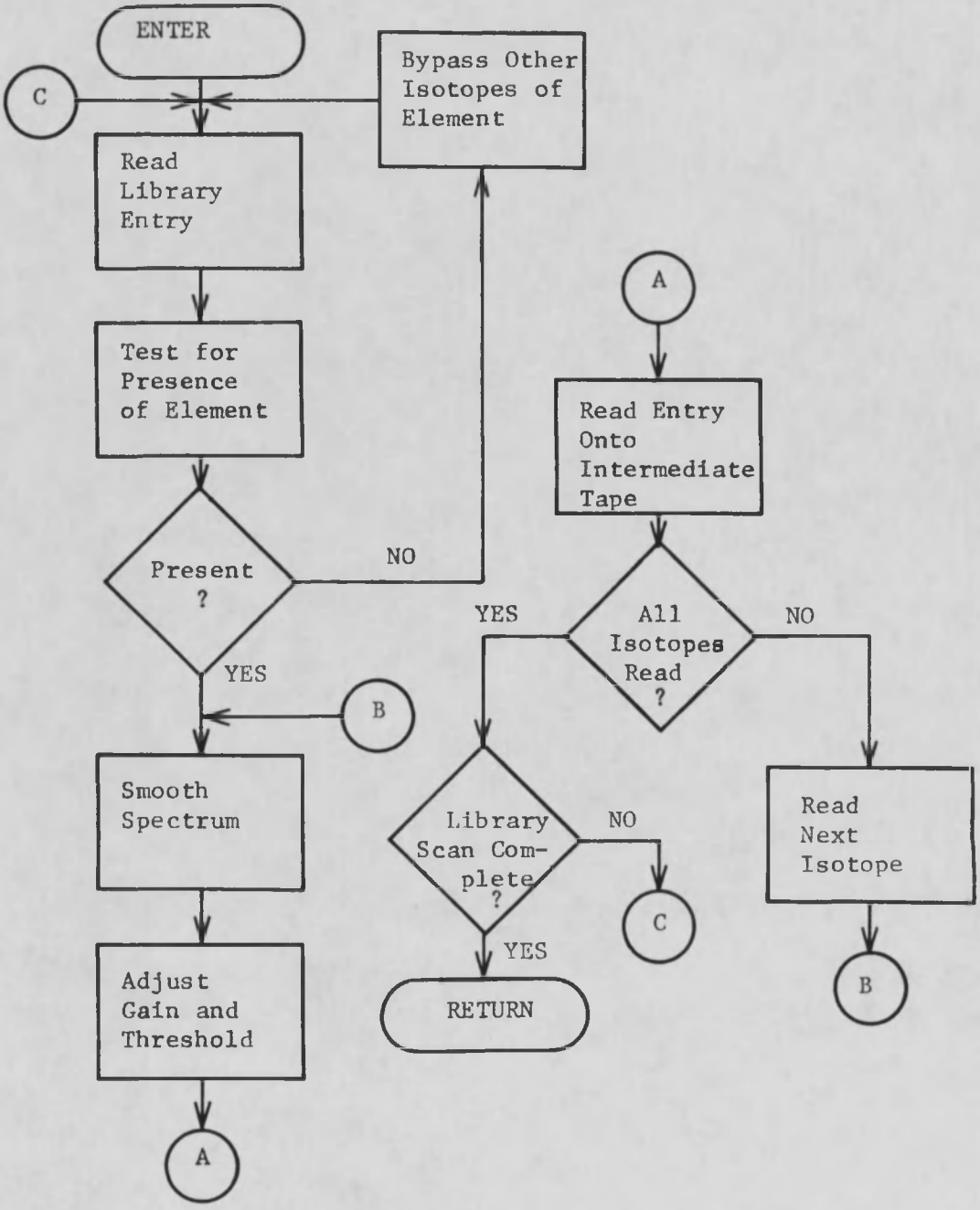

FIGURE 15: Flowchart for Subroutine LIBSR

SUBROUTINE STRIP

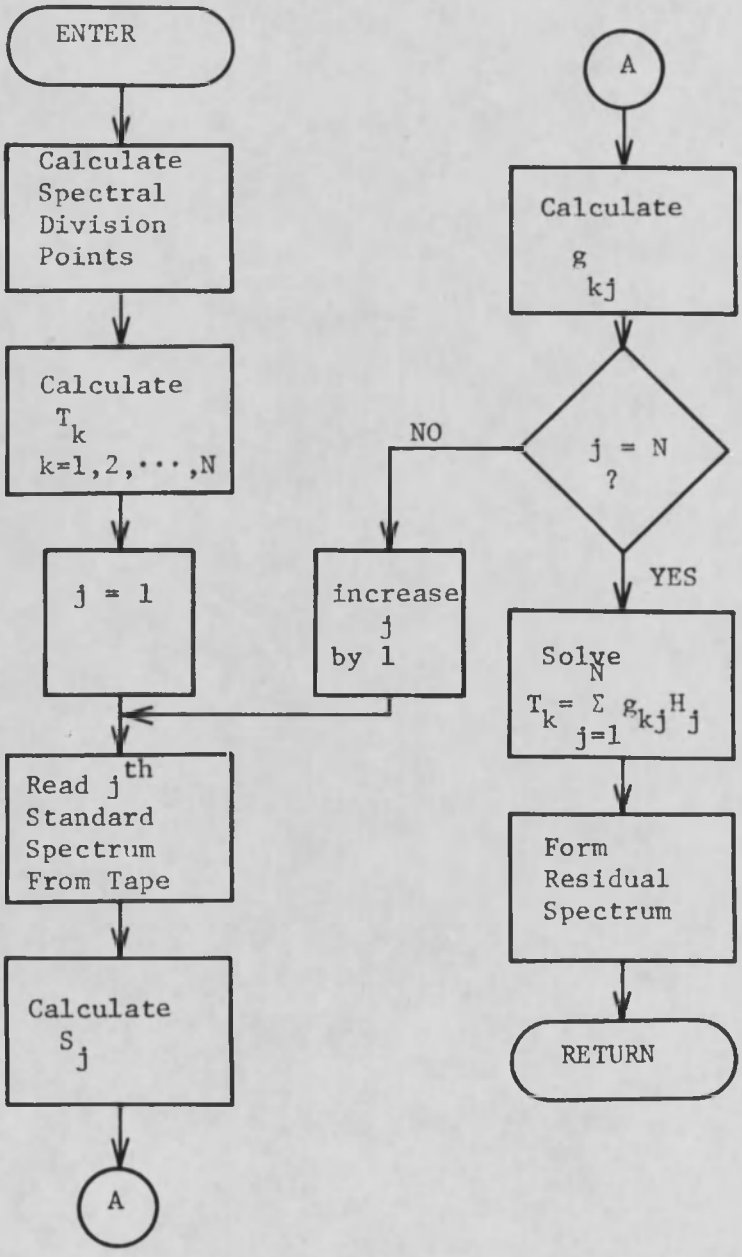

FIGURE 16: Flowchart for Subroutine STRIP

TABLE 6: Input for Program Run

Data	Columns	Field	Repetition
No. of Channels in Calibration Spectra	1-4	I4	1
No. Of Calibration Spectra	1-2	I2	1
Name of Spectrum	1-80	16A5	A
No. of Standard Peaks in Calibration Spectrum	1-2	I2	A
Peak Location (Channel No.)	1-4	F4.0	B, A
Energy of Peak (MeV)	11-18	F8.6	B, A
Calibration Spectrum			
No. Of Mixtures	1	I1	1
No. of Channels in Unknown Mixture Spectrum	1-4	I4	1
Name of Unknown Mixture Spectrum	1-80	16A5	1
Unknown Mixture Spectrum			1
No. of Elements to be stripped automatically	1-2	I2	1
Name of Element to be stripped automatically	1-5	A5	C
Reactor Power (K.W.)	1-10	F10.8	1
Irradiation Time (min)	11-20	F10.8	1
Time to Count Start from end of Irradiation (min)	21-30	F10.8	1
Count time (live Time (min)	31-40	F10.8	1

A: Repeat for Each Calibration Spectrum

B: Repeat for Standard Peak in Spectrum

C: Repeat for Each Element to be stripped automatically

```
C       SUBROUTINE TO READ A SPECTRUM
        SUBROUTINE RD(AX)
        DIMENSION AX(1024),NAP(2,7)
        DO 2 J=1,1024
      2 AX(J)=0.0
        NAP1=0
      4 FORMAT(7(I4,I6,1X))
     20 READ 4,((NAP(I,J),I=1,2),J=1,7)
        NUTS=NAP(1,1)+NAP(1,2)+NAP(1,3)
        IF(NUTS)6,6,8
      6 RETURN
      8 DO 10 J=1,7
        IF(NAP(1,J))10,10,12
     12 IF(NAP(1,J)-NAP1-1)14,16,14
     18 FORMAT(///13H CHANNEL NO. ,I4,16H OUT OF SEQUENCE,/
       ***                                                //)
     14 PRINT 18,NAP(1,J)
     16 NAP1=NAP(1,J)
        AX(NAP1)=NAP(2,J)
     10 CONTINUE
        GO TO 20
        END

C       **********
C       SUBROUTINE TO PRINT A SPECTRUM
        SUBROUTINE PRNT(N,ASPEC)
        DIMENSION ASPEC(1024),NPRNT(2,9)
      2 FORMAT(7H  CHAN-,/5H  NEL,/13H  NO.    COUNT/)
        PRINT 2
        NF=FLOTF(N)/9.0
        DO 4 J=1,NF
        DO 6 I=1,9
        KL=J+NF*(I-1)
        NPRNT(1,I)=KL
      6 NPRNT(2,I)=XFIXF(ASPEC(KL))
      8 FORMAT(1H ,9(1X,I4,1H*,I6,1X))
      4 PRINT 8,((NPRNT(M,L),M=1,2),L=1,9)
        KA=NF*9
        KB=KA+1
        DO 10 J=KB,N
        KR=XFIXF(ASPEC(J))
     12 FORMAT(106X,I4,1H*,I6)
     10 PRINT 12,J,KR
        RETURN
        END

C       **********
C       SUBROUTINE TO SMOOTH SPECTRUM USING QUADRATIC-CUBIC
C       LEAST SQUARES FIT DATA CONVOLUTION (7 POINTS)
        SUBROUTINE SMOT7(M,SPEC)
        DIMENSION SPEC(1024),AXE(7)
```

```
C       INITIALIZE
        DO 2 J=1,7
      2 AXE(J)=SPEC(J)
C       SMOOTH
        NUTS=M-4
        DO 4 I=4,NUTS
        SPEC(I)=(-2.0*(AXE(1)+AXE(7))+3.0*(AXE(2)+AXE(6))+6
     ***                                                  .0*
       1(AXE(3)+AXE(5))+7.0*AXE(4))/21.0
        DO 6 J=1,6
      6 AXE(J)=AXE(J+1)
      4 AXE(7)=SPEC(I+4)
        RETURN
        END

C       **********************
C       SUBROUTINE TO TAKE DERIVATIVE BY QUADRATIC CONVOLUT
C     ***                                                ION
C       (7 POINTS)
        SUBROUTINE DERIV(M,AX,AY)
        DIMENSION AX(1024),AY(1080)
        NUTS=M-3
        DO 2 I=4,NUTS
      2 AY(I)=(-3.0*AX(I-3)-2.0*AX(I-2)-AX(I-1)+AX(I+1)+2.0
     ***                                                *AX
       1(I+2)+3.0*AX(I+3))/28.0
        RETURN
        END

C       **********************
C       SUBROUTINE TO PROVIDE LINEAR LEAST SQUARES FIT FOR
C       SPECTRUM CALIBRATION
C       ERRORS IN CHANNEL NOS.  *  ENERGIES EXACT
        SUBROUTINE LINE(DATA,AM,AB,N)
        DIMENSION DATA(2,30)
C       X=ENERGY, Y=CHANNEL NO.
        SUMXY=0.0
        SUMX=0.0
        SUMY=0.0
        SUMX2=0.0
        DO 2 J=1,N
        SUMXY=SUMXY+DATA(1,J)*DATA(2,J)
        SUMX=SUMX+DATA(2,J)
        SUMY=SUMY+DATA(1,J)
      2 SUMX2=SUMX2+DATA(2,J)**2
C       CALCULATE ZERO ENERGY CHANNEL NO. AND MEV/CHANNEL
C       RATIO
        AB=(SUMY*SUMX2-SUMXY*SUMX)/(FLOTF(N)*SUMX2-SUMX**2)
        AM=(FLOTF(N)*SUMX2-SUMX**2)/(FLOTF(N)*SUMXY-SUMX*SU
     ***                                                MY)
        RETURN
```

```
      END

C     **********************
C     SUBROUTINE TO DETERMINE INTERVALS
C     SUBROUTINE TO DETERMINE INTERVALS
      SUBROUTINE INTER(N,INT,MIN,MAX,AX)
      DIMENSION INT(21),AX(1024)
    2 FORMAT(///19H SUBROUTINE INTER**,//5H MIN=,I4,/5H M
     ***                                          AX=
     1,I4,////12H INTERVALS**,//)
      PRINT 2,MIN,MAX
      TOT=0.0
      DO 6 J=MIN,MAX
    6 TOT=TOT+AX(J)
      AMP=TOT/FLOAT(N)
      INT(1)=MIN
      DO 8 I=1,N
      TOT=0.0
      J=INT(I)
   12 TOT=TOT+AX(J)
      IF(TOT-AMP)10,8,8
   10 J=J+1
      GO TO 12
    8 INT(I+1)=J+1
      IF(INT(N+1)-MAX)14,14,16
   16 INT(N+1)=MAX
    4 FORMAT(I10)
   14 NUTS=N+1
      PRINT 4,(INT(J),J=1,NUTS)
      RETURN
      END

C     **********************
C     SUBROUTINE TO ADJUST ENERGY SCALE OF SPECTRUM
      SUBROUTINE SCADJ(AX,AY,Y1,Y2,M,B1,B2)
      DIMENSION AX(1024),AY(1080)
      DO 4 J=1,M
      GJP=(Y2/Y1)*(FLOTF(J)-B2)+B1
      K=GJP
      IF(K)5,5,7
    5 AY(J)=0.0
      GO TO 4
    7 IF(K-1023)6,6,8
    6 AKK=GJP-FLOTF(K)
      AY(J)=(AKK*(AX(K+1)-AX(K))+AX(K))*(Y2/Y1)
    4 CONTINUE
    8 RETURN
      END

C     **********************
C     SUBROUTINE TO SOLVE N SIMULTANEOUS LINEAR EQUATIONS
```

```
      SUBROUTINE SYMEQ(A,X,B,N)
      DIMENSION A(20,20),X(20),B(20)
   31 FORMAT(///,51H INFORMATION ON THE RESULTING SYSTEM
     ***                                            OF
     1EQUATIONS *)
      PRINT 31
      MM=N-1
      DO 14 L=1,MM
C     DETERMINE LARGEST ELEMENT IN L TH COLUMN FOR PIVOT
C     ( =A(M,L) )
      K=L
    8 M=K
   10 IF(K-N)6,4,4
    6 K=K+1
      IF(A(M,L)-A(K,L))8,10,10
C     TRANSFER PIVOT POW TO FIRST POSITION
    4 DO 12 J=1,N
      C=A(L,J)
      A(L,J)=A(M,J)
   12 A(M,J)=C
      C=B(L)
      B(L)=B(M)
      B(M)=C
C     CALCULATE AND STORE MULTIPLIERS AND ELIMINATE
C     COEFFICIENTS
      NUTS=L+1
      DO 14 I=NUTS,N
      A(I,L)=A(I,L)/A(L,L)
      B(I)=B(I)-A(I,L)*B(L)
      DO 14 J=NUTS,N
   14 A(I,J)=A(I,J)-A(I,L)*A(L,J)
C     BACK SUBSTITUTE TO COMPUTE X(J) MATRIX
      X(N)=B(N)/A(N,N)
      L=N-1
   16 D=0.0
      NUTS=L+1
      DO 18 J=NUTS,N
   18 D=D+A(L,J)*X(J)
      X(L)=(B(L)-D)/A(L,L)
      L=L-1
      IF(L-1)20,16,16
C     COMPUTE DETERMINANT OF MATRIX
   20 DET=A(1,1)
      DO 22 I=2,N
   22 DET=DET*A(I,I)
   29 FORMAT(////,53H DIAGONAL ELEMENTS OF TRIANGULARIZED
     ***                                            MA
     1TRIX (PIVOTS)*,//)
      PRINT 29
   24 FORMAT(     ,(1PE20.7,/))
      PRINT 24,(A(I,I),I=1,N)
```

```
   26 FORMAT(///,36H DETERMINANT OF COEFFICIENT MATRIX =,
     ***                                                 1PE
     115,7,//)
      PRINT 26,DET
   34 RETURN
      END

C     **********************
C     SUBROUTINE TO LOCATE ALL IMPORTANT PEAKS IN SPECTRU
C    ***                                                 M
      SUBROUTINE LOC(M,AX,NUM,PEAK,HITE,AY)
      DIMENSION AX(1024),AY(1080),PEAK(100),HITE(100)
C     ESTABLISH PARAMETERS
      HI=50.0
      NRES=5
      NCEN=8
C     OBTAIN DERIVATIVE
      CALL DERIV(M,AX,AY)
      NUM=0
      K=1
      AMN=0.0
      MM=M-NCEN
      NATZ=NCEN+1
C     SCAN DERIVATIVE TO LOCATE PEAKS
      DO 2 I=NATZ,MM
    8 GO TO(10,12),K
C     SEARCH FOR MAXIMUM
   10 DO 14 J=1,NRES
      NAT=I+J-1
      IF(AY(NAT))14,2,2
   14 CONTINUE
      AMX=(AX(I-1)+AX(I))/2.0
      IF(AMX-AMN-HI) 2,18,18
   18 NUM=NUM+1
C     CALCULATE RELATIVE HEIGHT OF PEAK
      HITE(NUM)=AMX-AMN
C     CALCULATE CENTER OF PEAK
      SUMXY=0.0
      SUMX=0.0
      SUMY=0.0
      SUMX2=0.0
      N=2*NCEN
      DO 20 J=1,N
      NUTS=I-NCEN+J-1
      SUMXY=SUMXY+FLOTF(NUTS)*AY(NUTS)
      SUMX=SUMX+FLOTF(NUTS)
      SUMY=SUMY+AY(NUTS)
   20 SUMX2=SUMX2+FLOTF(NUTS)**2
      PEAK(NUM)=(SUMXY*SUMX-SUMY*SUMX2)/(FLOTF(N)*SUMXY-S
     ***                                                 UMX
     1*SUMY)
```

```
      K=2
      GO TO 2
C     SEARCH FOR MINIMUM
   12 DO 22 J=1,NRES
      NAT=I+J-1
      IF(AY(NAT))2,2,22
   22 CONTINUE
      AMN=(AX(I-1)+AX(I))/2.0
      K=1
    2 CONTINUE
      RETURN
      END

C     **********
C     SUBROUTINE TO DETERMINE ENERGY SCALE FROM CALIBRATI
C    ***                                              ON
C     SPECTRA
      SUBROUTINE SCALE(YK,YB,PEAK,HITE)
      DIMENSION STAN(2,30),PEAK(100),AX(1024),NSTAN(10)
     1 ,HITE(100),AY(1080),NAME(16)
   51 FORMAT(///65H **** DETERMINATION OF ENERGY SCALE FR
    ***                                              OM
     1CALIBRATION SPECTRA ****)
      PRINT 51
    2 FORMAT(I4/I2)
      READ 2,M,NCAL
      LKAP=0.0
      DO 1 J=1,NCAL
C     J TH SPECTRUM READ AND PROCESSED
      READ 35,(NAME(NZ),NZ=1,16)
   35 FORMAT(16A5)
   37 FORMAT(///,1X,16A5)
      PRINT 37,(NAME(NZ),NZ=1,16)
      READ 6,KAP
    6 FORMAT(I2)
      DO 3 I=1,KAP
      NUTS=LKAP+I
    5 FORMAT(F4.0,6X,F8.6)
      READ 5,STAN(1,NUTS),STAN(2,NUTS)
    3 NSTAN(I)=XFIXF(STAN(1,NUTS))
      LKAP=LKAP+KAP
      CALL RD(AX)
      CALL LOC(M,AX,NUM,PEAK,HITE,AY)
C     SEARCH FOR ENERGIES OF DETECTED PEAKS
      NUTS=LKAP-KAP+1
      DO 8 I=NUTS,LKAP
      DO 10 K=1,NUM
      ANIK=2.0+(FLOTF(I)/1024.0)*4.0
      IF(ABSF(STAN(1,I)-PEAK(K))-ANIK)14,14,10
      IF(STAN(1,I)-(PEAK(K)-2.0))10,12,12
   12 IF(STAN(1,I)-(PEAK(K)+2.0))14,14,10
```

```
   14 STAN(1,I)=PEAK(K)
      GO TO 8
   10 CONTINUE
      MP=I-(LKAP-KAP)
   16 FORMAT(    /13H PEAK NUMBER ,I2,32H OF CALIBRATION S
     ***                                                  PEC
     1TRUM NUMBER
     2,I2,21H COULD NOT BE LOCATED/38H LOCATION READ IN U
     ***                                                  SED
     3 FOR CALIBRATION)
      PRINT 16,MP,J
    8 CONTINUE
C     PRINT OUTPUT
   21 FORMAT(  /32H CHANNEL NOS. OF PEAKS DETECTED*,//,(1
     ***                                                  OF1
     10,2,/))
      PRINT 21,(PEAK(JZ),JZ=1,NUM)
   25 FORMAT(///61H STANDARD PEAKS AS PROCESSED FOR CALIB
     ***                                                  RAT
     1ION SPECTRUM NUMBER
     2         ,I2,//28H ENERGY   LOCATION  LOCATION,/26H
     ***                                                   (M
     3EV)    READ IN      USED,//)
      PRINT 25,J
   27 FORMAT(F6.2,5X,I4,F12.2,/)
      DO 29 KK=1,KAP
      KQ=LKAP-KAP+KK
   29 PRINT 27,STAN(2,KQ),NSTAN(KK),STAN(1,KQ)
    1 CONTINUE
C     CALCULATE ENERGY SCALE BY LEAST SQUARES
   55 CALL LINE(STAN,YK,YB,LKAP)
   42 FORMAT(12H CHANNEL NO.,F6.2,28H =CHANNEL NO. OF ZER
     ***                                                  O E
     1NERGY//)
   59 PRINT 42,YB
   41 FORMAT(      15H ENERGY SCALE =,1PE14.7,16H MEV PER
     ***                                                  CHA
     1NNEL,///)
      PRINT 41,YK
      RETURN
      END

C     **********************
C     SUBROUTINE TO SEARCH SPECTRUM LIBRARY FOR COMPONENT
C     OF COMPLEX SPECTRUM
      SUBROUTINE LIBSR'AY,AX,NISO,AUTON,NUM,PEAK,YK,YB,M,
     ***                                                  NAU
     1T)
      DIMENSION AX(1024),AY(1080),AUTON(10),PEAK(100)
   54 FORMAT(25H LIBRARY SEARCH RESULTS**,///)
      PRINT 54
```

```
      NLIBE=7
      DE=0.02
      NISO=0
      N=1
      REWIND N
      REWIND 3
      DO 2 MAD=1,NLIBE
      READ TAPE N,AY
C     TEST FOR AUTO-STRIP
    4 IF(NAUT)42,42,48
   48 DO 8 J=1,NAUT
      IF(AUTON(J)-AY(2))8,10,8
    8 CONTINUE
C     TEST FOR PRESENCE OF ISOTOPE
   42 MCON=0
      NUTS=XFIXF(AY(6))
      DO 12 I=1,NUTS
      DO 14 K=1,NUM
      IF(ABSF(AY(I+6)-PEAK(K))-(DE+(PEAK(K)/2.5)*0.05))20
     1,14
   14 CONTINUE
      GO TO 12
   20 MCON=MCON+1
   12 CONTINUE
   60 FORMAT(16H PEAKS (MEV)*    ,F8.4,/,(16X,F8.4,/),/)
      NAY=AY(6)+6.0
      PRINT 60,(AY(JJ),JJ=7,NAY)
   62 FORMAT(1X,I2,36H PEAKS INDICATED IN UNKNOWN SPECTRU
    ***                                              M,/
     1//)
      PRINT 62,MCON
      IF(MCON-XFIXF(AY(6)))22,10,10
C     ELEMENT ABSENT
   22 NUTS=XFIXF(AY(21))-1
   58 FORMAT(5X,3A5,5X,12H***ABSENT***,//)
      PRINT 58,(AY(JJ),JJ=2,4)
      IF(NUTS)2,2,64
   64 DO 26 J=1,NUTS
   26 READ TAPE N,FAKE
      GO TO 2
C     ELEMENT PRESENT
   10 PRINT 56,(AY(JJ),JJ=2,4)
   56 FORMAT(5X,3A5,5X,13H***PRESENT***,//)
      NUTS=XFIXF(AY(21))
      DO 28 I=1,NUTS
      IF(I-1)68,68,70
   70 READ TAPE N,AY
C     REARRANGE DATA AND ADJUST ENERGY SCALE
   68 DO 30 J=1,M
   30 AX(J)=AY(J+56)
      DO 32 J=1,56
```

```
   32 AY(J+1024)=AY(J)
      CALL SCADJ(AX,AY=AY(1041),YK,M,AY(1060),YB)
C     SMOOTH SPECTRUM
      CALL SMOT7(M,AY)
C     WRITE STANDARD COMPONENT ONTO INTERMEDIATE TAPE
      WRITE TAPE 3,AY
   28 NISO=NISO+1
    2 CONTINUE
      RETURN
      END

C     **********************
C     SUBROUTINE TO STRIP N COMPONENTS FROM COMPOSITE
C     SPECTRUM AND DETERMINE AMOUNTS PRESENT
      SUBROUTINE STRIP(AX,N,M,CR,MIN,MAX,H,AY,G)
      DIMENSION AX(1024),AY(1080),T(20),G(20,20),CR(20),H
     1),TOT(20),INT(21)
      CALL INTER(N,INT,MIN,MAX,AX)
C     DETERMINE COUNTS IN I TH INTERVAL OF COMPOSITE
C     SPECTUM =T(I)
      DO 2 I=1,N
      T(I)=0.0
      NFUN1=INT(I)
      NFUN2=INT(I+1)-1
      DO 2 J=NFUN1,NFUN2
    2 T(I)=T(I)+AX(J)
C     PROCESS J TH STANDARD SPECTRUM
      REWIND 3
      DO 4 J=1,N
      TOT(J)=0.0
C     DETERMINE COUNTS IN J TH STANDARD SPECTRUM
C     (MIN TO MAX)
      READ TAPE 3,AY
      NUTS=MIN+1
      DO 6 I=NUTS,MAX
    6 TOT(J)=TOT(J)+AY(I)
      DO 4 I=1,N
C     CALCULATE COUNTS IN I TH INTERVAL OF J TH STANDARD
C     SPECTRUM
      PART=0.0
      MATT=INT(I)
      MITT=INT(I+1)-1
      DO 8 K=MATT,MITT
    8 PART=PART+AY(K)
C     CALCULATE (I,J) TH COMPONENT OF COEFFICIENT MATRIX
    4 G(I,J)=PART/TOT(J)
C     OBTAIN SOLUTION OF SYSTEM OF EQUATIONS
      CALL SYMEQ(G,H,T,N)
      REWIND 3
      DO 10 J=1,N
C     OBTAIN RATIO OF COUNTS IN J TH COMPONENT (MIN TO MA
C  ***                                          X)
```

```
C       TO COUNTS IN J TH STANDARD SPECTRUM (MIN TO MAX)
        CR(J)=H(J)/TOT(J)
C       STRIP J TH COMPONENT OUT OF COMPOSITE
        READ TAPE 3,AY
        DO 10 I=1,M
   10   AX(I)=AX(I)-AY(I)*CR(J)
   18   FORMAT(////,20H RESIDUAL SPECTRUM**,///)
        PRINT 18
        CALL PRNT(M,AX)
        RETURN
        END

C       **********
C       SUBROUTINE TO CALCULATE AMOUNTS OF ELEMENTS PRESENT
        SUBROUTINE QUANT(H,N,AY,DATA,CR)
        DIMENSION H(20),AY(1080),DATA(20,20),CR(20)
    2   FORMAT(4F10.8)
        READ 2,POW,TR,T1,T2
        T2=T1+T2
        REWIND 3
        DO 4 I=1,N
C       READ ENTRY FROM INTERMEDIATE TAPE
        READ TAPE 3,AY
        DO 30 K=1,35
   30   AY(K)=AY(K+1024)
C       LOAD DATA MATRIX
        DO 6 J=1,4
    6   DATA(I,J)=AY(J+1)
        DATA(I,5)=0.69315/AY(18)
        DATA(I,6)=AY(20)
        DATA(I,7)=AY(21)
        DATA(I,8)=AY(19)
        DO 8 J=9,12
    8   DATA(I,J)=AY(J+23)
        DATA(I,13)=CR(I)
        DATA(I,14)=H(I)
C       CALCULATE AMOUNT OF ISOTOPE AND STANDARD DEVIATION
        CRRAT=CR(I)*((EXPEF(-DATA(I,5)*AY(33))-EXPEF(-DATA(
     ***                                          I,5
     1)*AY(34)))/
     2(EXPEF(-DATA(I,5)*T1)-EXPEF(-DATA(I,5)*T2)))
        DATA(I,15)=DATA(I,8)*CRRAT*((1.0-EXPEF(-DATA(I,5)*A
     12)))/(1.0-
     2EXPEF(-DATA(I,5)*TR)))*AY(35)/POW
        DATA(I,16)=DATA(I,15)*AY(20)
    4   DATA(I,17)=ABSF(DATA(I,16)/SQRTF(ABSF(H(I))))
C       PRINT ISOTOPIC ANALYSIS
   10   FORMAT(20H ISOTOPIC ANALYSIS**,///29X,9HCOUNTS IN,1
     19HAMOUNT IN,
     2/11X,7HISOTOPE,12X,8HSPECTRUM,10X,14HSAMPLE (GRAMS)
     ***                                          ,/)
```

```
      PRINT 10
   12 FORMAT(6X,3A5,I4,5X,1PE9.2,8X,1PE9.2,4H +/-,1PE8.1,
     ***                                                 //)
      DO 14 I=1,N
      NUTS=DATA(I,4)
   14 PRINT 12,(DATA(I,J),J=1,3),NUTS,DATA(I,14),DATA(I,1
     ***                                                 6),
     1DATA(I,17)
C     CALCULATE ELEMENTAL ANALYSIS WITH STANDARD DEVIATIO
C    ***                                                 NS
C     AND PRINT OUTPUT
   15 FORMAT(////)
      PRINT 15
   16 FORMAT(21H ELEMENTAL ANALYSIS**,///29X,9HCOUNTS IN,
     1,9HAMOUNT IN
     2,/10X,7HELEMENT,13X,8HSPECTRUM,10X,14HSAMPLE (GRAMS
     ***                                                 ),/
     3/)
      PRINT 16
   18 FORMAT(6X,3A5,9X$1PE9.2,8X,1PE9.2,4H +/-,1PE8.1,//)
      I=1
   20 NUTS=I+XFIXF(DATA(I,7))-1
      HW=0.0
      HW2=0.0
      DO 22 J=I,NUTS
      HW=HW+DATA(J,14)/DATA(J,15)
   22 HW2=HW2+HW/DATA(J,15)
      WE=HW/HW2
      DELWE=SQRTF(ABSF(1.0/HW2))
      SUMH=0.0
      DO 24 J=I,NUTS
   24 SUMH=SUMH+DATA(J,14)
      PRINT 18,(DATA(I,J),J=1,3),SUMH,WE,DELWE
      I=I+XFIXF(DATA(I,7))
      IF(I-N)20,20,26
   28 FORMAT(/////70H ERRORS GIVEN ARE STANDARD DEVIATION
     ***                                                 S B
     1ASED ONLY ON COUNTING STATISTICS,////)
   26 PRINT 28
      RETURN
      END

C     **********
C     **********
C     START
      DIMENSION NAME(16),AX(1024),AY(1080),PEAK(100)
     1,CR(20),H(20),G(20,20),HITE(100),AUTON(10)
      N=1
    9 FORMAT(////,F20.4,//)
      DO 7 J=1,8
      READ TAPE N,AN
```

```
      7 PRINT 9,AN
C       DETERMINE ENERGY SCALE OF UNKNOWN SPECTRUM
C       USING STANDARD SPECTRA
        CALL SCALE(YK,YB,PEAK,HITE)
     24 FORMAT(I1)
        READ 24,NCYCL
        DO 26 NATZ=1,NCYCL
        NUTS=0.0
C       READ NO. OF CHANNELS IN SPECTRUM AND SPECTRUM
C       DESIGNATION
      2 FORMAT(I4/16A5)
        READ 2,M,(NAME(I),I=1,16)
      4 FORMAT(////13H ANALYSIS OF ,16A5,///)
        PRINT 4,(NAME(I),I=1,16)
C       READ UNKNOWN SPECTRUM AND STORE ON TAPE
        CALL RD(AX)
        REWIND 12
        WRITE TAPE 12,AX
C       LOCATE ALL PEAKS IN UNKNOWN SPECTRUM
        CALL LOC(M,AX,NUM,PEAK,HITE,AY)
     54 FORMAT(///34H PEAKS FOUND IN COMPOSITE SPECTRUM,//3
       11HCHANNEL NO.
       2 ,6X,12HENERGY (MEV),///)
        PRINT 54
     56 FORMAT(1X,F10.2,11X,F7.4,//)
        DO 58 JJ=1,NUM
        ETEMP=YK*(PEAK(JJ)-YB)
        PRINT 56,PEAK(JJ),ETEMP
     58 PEAK(JJ)=ETEMP
C       READ IN ELEMENTS TO BE STRIPPED AUTOMATICALLY
      6 FORMAT(I2)
        READ 6,NAUT
        IF(NAUT)14,14,16
     16 DO 8 J=1,NAUT
      8 READ 10,AUTON(J)
     10 FORMAT(A5)
C       SEARCH LIBRARY FOR COMPONENTS ON BASIS OF PEAK
C       ENERGIES
     14 CALL LIBSR(AY,AX=NISO,AUTON,NUM,PEAK,YK,YB,M,NAUT)
C       STRIP COMPONENTS FROM UNKNOWN SPECTRUM
        REWIND 12
        READ TAPE 12,AX
        MIN=5
        MAX=M
        CALL STRIP(AX,NISO,M,CR,MIN,MAX,H,AY,G)
C       CALCULATE QUANTITATIVE ANALYSIS
        CALL QUANT(H,NISO,AY,G,CR)
     26 CONTINUE
        STOP
        END
```

APPENDIX B

SPECTRAL LIBRARY FORMAT

The standard isotopic spectral library consists of a series of nonformated records on magnetic tape. Each record contains one isotopic spectrum along with all related information and has a length of 1080 words. Each of these records or entries is characterized by an entry number which is the first word in the record.

The following is a list of the information stored in one library entry along with relative locations within the tape record

1. Entry number (1)
2. Name of element (2 - 4)
3. Mass number of isotope (5)
4. Number of standard peaks (6)
5. Energies of standard peaks (7 - 11)
6. Relative heights of standard peaks (12 - 16)
7. Energy scale (MeV/channel) (17)
8. Half-life (18)
9. Mass of sample of standard element (19)
10. Fractional abundance of isotope (20)
11. Number of isotopes in library of this element (21)
12. Entry numbers of other isotopes of this element (22 - 31)
13. Irradiation time (32)

14. Time count started (33)
15. Time count stopped (34)
16. Reactor power during irradiation (35)
17. Threshold channel number (36)
18. Number of channels in standard spectrum (56)
19. Standard spectrum (57 - 1080)

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