

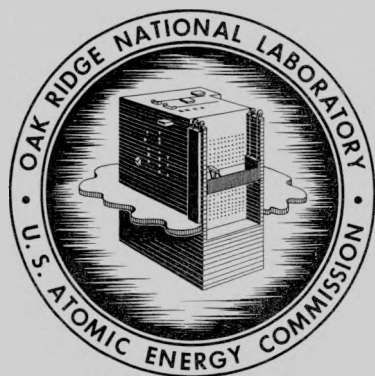
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ALPHA – A COMPUTER PROGRAM FOR THE
DETERMINATION OF RADIOISOTOPES BY
LEAST-SQUARES RESOLUTION OF
THE GAMMA-RAY SPECTRA

E. Schonfeld

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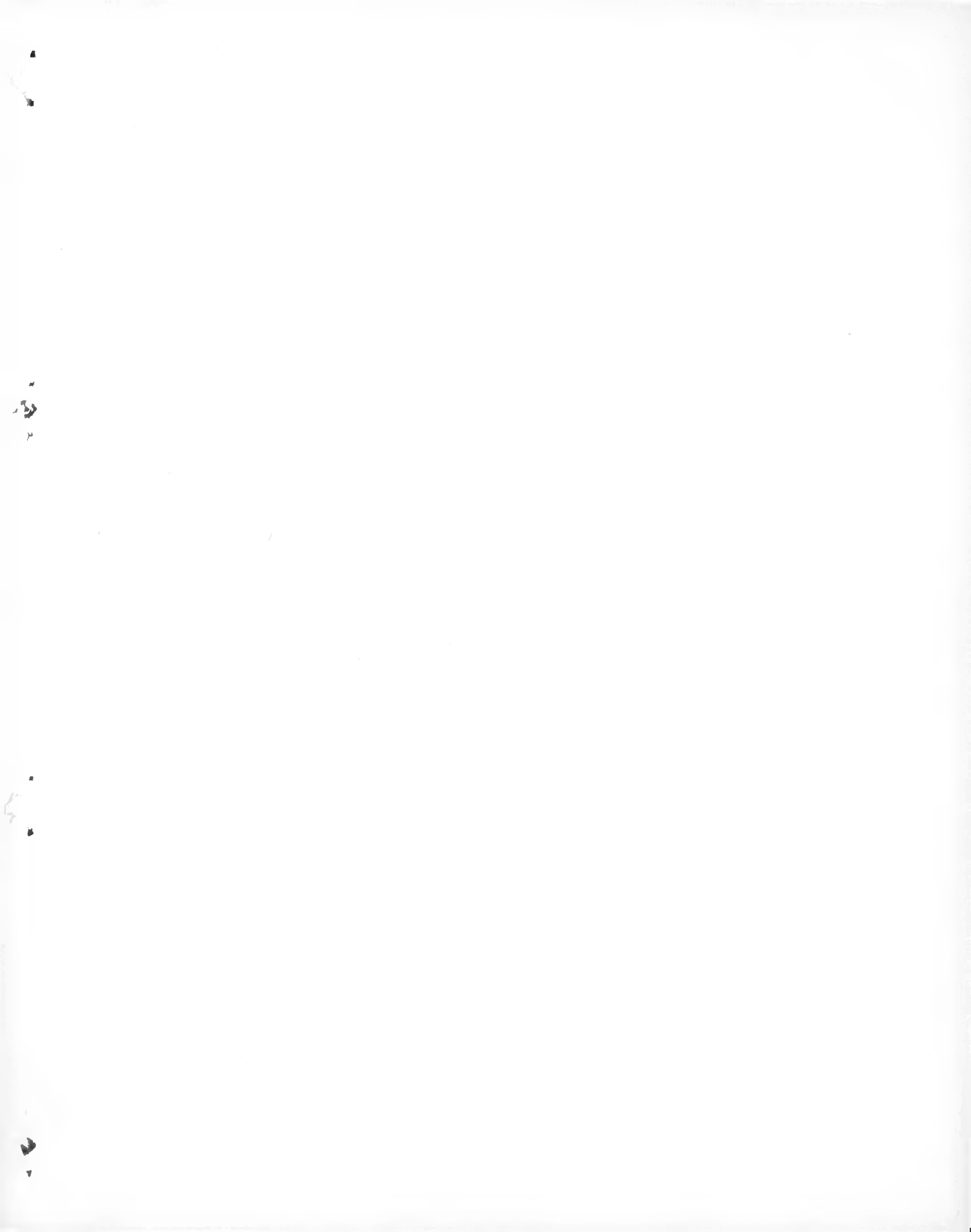
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BY LEAST-SQUARES RESOLUTION OF THE GAMMA-RAY SPECTRA

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ALPHA - A COMPUTER PROGRAM FOR THE DETERMINATION OF RADIOISOTOPES BY LEAST-SQUARES RESOLUTION OF THE GAMMA-RAY SPECTRA

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ABSTRACT

A FORTRAN-63 computer program, ALPHA, was developed for the quantitative analysis of radioactive samples by the least-squares resolution of the gamma-ray spectra. As the result of thousands of analyses, ALPHA was found to be fast, accurate, and relatively inexpensive. This report describes the main features of ALPHA and shows how to use it.

The program was designed to handle a small or large number of samples. The samples can have different radioactivity levels (from 0.1 to 10^4 counts/sec), isotope compositions, and input formats. Also, they can be on cards or magnetic tape. ALPHA takes into account several corrections such as: background subtraction, counting time, decay, dead time, automatic compensation for gain and threshold shifts, sample fraction, volume reduction prior to counting, etc. Typical computation times for samples containing from 6 to 10 isotopes are about 5 to 15 sec. The cost per analysis is about 20 cents (this includes only the CDC-1604 computer charges and not the cost of sample preparation and counting).

1. INTRODUCTION

The purpose of this report is to describe the main features of and show how to use ALPHA, a computer program for the determination of radioisotopes by least-squares resolution of the gamma-ray spectra. This program was written originally for the purpose of greatly reducing the cost of analysis of a large number of samples containing very low radioactivity levels. It has since been found very useful in other phases of the disposal of radioactive wastes, in the processing of reactor fuel, in radiological health physics, in reactor hazards evaluations, in reactor chemistry, and in activation analysis.

As the result of thousands of quantitative analyses, the determination of isotopes by least-squares resolution of the gamma-ray spectra was found to be fast, accurate and relatively inexpensive.¹ In these determinations, the computer program ALPHA was used together with the CDC-1604 digital computer (memory size: 32 K). The program was designed to handle small or large numbers of samples with maximum versatility and simplicity.

The spectrum resolution method requires a library of standards. These are the spectral data of the individual isotopes. In what follows, attention will be first focused on the library of standards, showing the different features available with ALPHA. Then a description of the features available for the samples follows. Finally, the output of the program is discussed.

2. THE SPECTRUM-RESOLUTION METHOD

The mathematical basis and experimental verification of the spectrum resolution method as coded in ALPHA has already been described.¹ A flowsheet of the whole operation is shown in Fig. 1. The computation time for each sample depends on the number of isotopes in the mixture and the amount of spectral shift to be compensated. Typical computing times for samples containing six to ten isotopes are about 5 to 15 sec. The cost of analysis per sample is about 20 cents (this includes only the CDC-1604 computer charges and not the cost of sample preparation and counting).

3. MAIN FEATURES OF ALPHA

The main features of the program ALPHA are shown in Tables 1 and 2. Also in the tables are shown, for comparison, the capabilities of two other programs.^{2,3} A few of the features cannot, for the purpose of comparison, be assigned an absolute yes or no evaluation, for which reason a plus or minus sign was added (yes+, yes-). Here, a yes+ designates a very convenient feature, and a yes- a moderately convenient feature. These features will be discussed in the same order given in Tables 1 and 2.

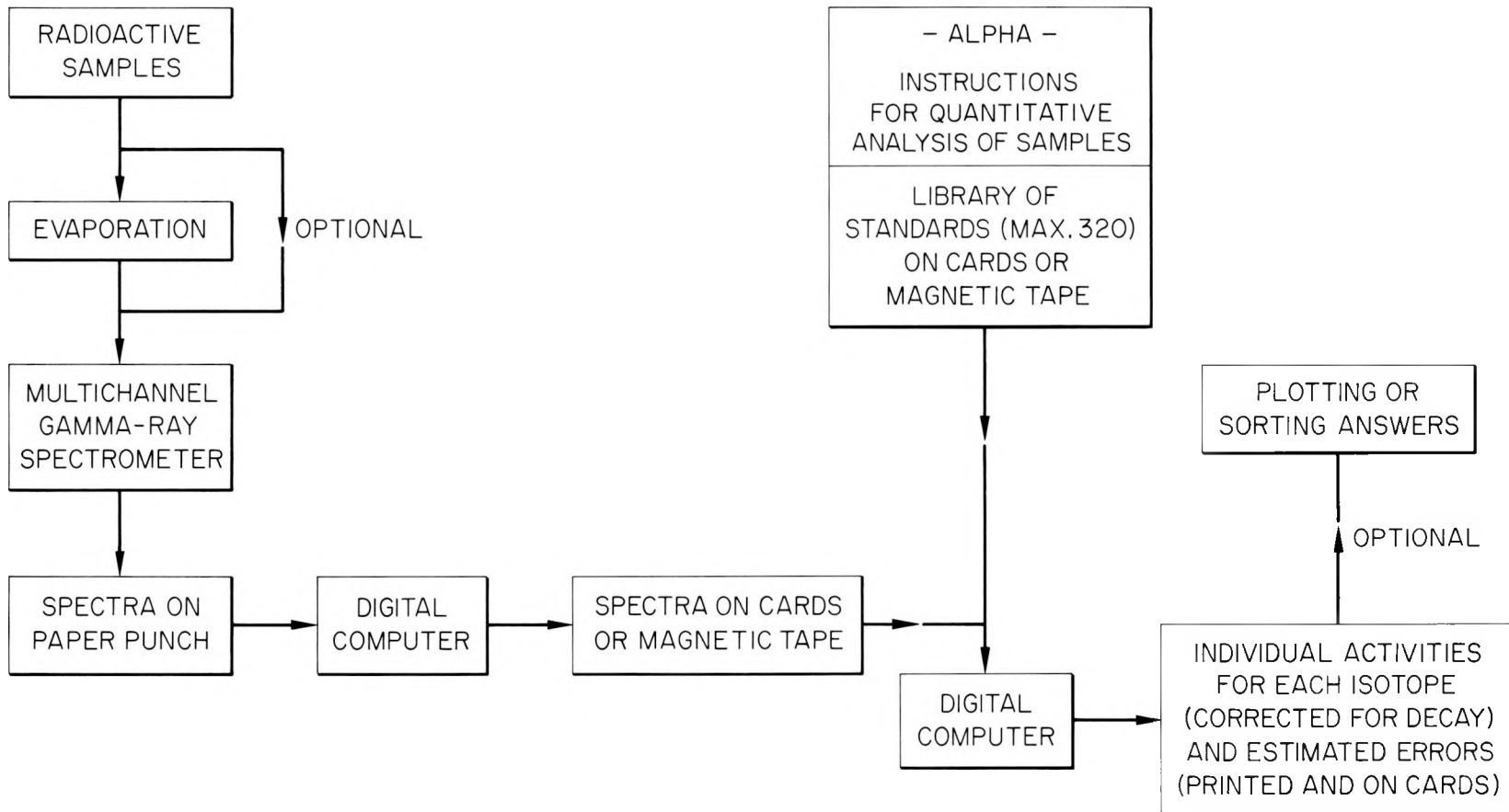


Fig. 1. Steps in the Quantitative Analysis of Samples.

Table 1. Program Capabilities for the Library of Individual Isotopes

Capability	Program		
	ALPHA	II ^a	III ^b
Spectral data can be in any format	Yes	No	Yes
Number of channels	400	400	100
Variable number of channels	Yes	Yes	No
Size of library	300(64 chann) 80(256 ") 50(400 ")	25	20
Can select from the library	Yes	Yes	No
Size of the library if selecting	Same as full size	11	--
Permits use of spectral data on magnetic tape	Yes	No	No
Can subtract background	Yes	No	Yes
Corrects for intensity	Yes	No	Yes
Compensates for gain-shift	Yes	Yes	No
Compensates for threshold-shift	Yes-	Yes-	No
Corrects for complement numbers	Yes	Yes	No

^aSee ref 3.

^bSee ref 2.

Table 2. Program Capabilities for the Samples

Capability	Program		
	ALPHA	II ^b	III ^c
Compensation for spectral shifts			
Corrects automatically	Yes	No	No
Corrects for gain-shift	Yes+	Yes	Yes-
Corrects for threshold-shift	Yes	No	No
Corrects for counting time	Yes	No	Yes
Corrects for decay	Yes	No	Yes-
Corrects for dead time	Yes	No	No
Subtracts background	Yes	Yes	Yes
Several options of computation	Yes+	Yes	No
Permits use of spectral data on magnetic tape	Yes	No	No
Gives results on punched cards and sorts	Yes	No	No
Combines results of several consecutive spectra	Yes	No	No
Computes the α 's for each isotope ^a	Yes	No	No
Rejects "negative" concentrations	Yes+	Yes	No
Corrects for sample fraction	Yes	No	No
Corrects for complement numbers	Yes	No	No
Corrects for other types of errors	Yes	Yes	No

^aSee ref 1 and Sec. 3.2.9.

^bSee ref 3.

^cSee ref 2.

3.1 Library of Standards

3.1.1 Spectral Data Can Be in Any Format. — With ALPHA, the spectral data (on cards or magnetic tape) can be in any kind of format, as long as the standards and samples are in the same format. This is a useful feature because ALPHA can handle data from different multichannel analyzers.

3.1.2 Number of Channels. — The number of channels is variable, but there cannot be more than 400 with the version discussed in this report. This can be changed by simple changes in DIMENSION statements. This variability permits the analyst to use a number of channels consistent with the problem and the available multi-channel analyzer.

3.1.3 Library Size and Ability to Select from It. — This is one of the main features of ALPHA. A large storage allocation for the library and a simple way to select from it allows one to handle samples that contain different kinds of isotopes. Also, since the library is loaded directly into the computer memory at the beginning of the calculation, the computing time for each sample is unaffected. The size of the library (Table 1) can be increased 2.5 times if a 64 K memory is used.

3.1.4 Option for Using the Library Spectral Data on Magnetic Tape. — The user concerned with only a few isotopes or who has a small library may prefer to use cards. But, if a large library is used, it is much simpler and cheaper to store and use spectral data of the standards on magnetic tape. ALPHA can handle either situation. The transfer of cards into magnetic tape is accomplished by use of a short program, TRAMAG.

3.1.5 Units of Concentration. — One can print and/or punch the final results (concentrations or activities) in any convenient units, which is a useful feature when many samples are involved.

3.1.6 Gain- and Threshold-Shift of the Standards. — In general, the standards need not be corrected for spectral shifts unless the main energies of any two isotopes in a sample differ by less than about 5%. Whether corrections must be made depends also on how much care was used in preparing the library. If desired, the spectral-shift compensation can be accomplished with a small program, SHIFT. This program needs, as input numbers, the gain and threshold desired. Then, after shifting the spectrum, SHIFT calls for a new set of cards to be punched.

3.1.7 Subtraction of Background from the Standards. — ALPHA can subtract background from the standards. This feature is especially useful if all the analyzer channels are used for measuring the isotope spectrum.

3.1.8 Correction of Complement Numbers. — If the subtraction of background was done with the multichannel analyzer, the analyzer, instead of writing negative numbers, prints complement numbers, which are incorrect. However, ALPHA "recognizes" such numbers and converts them to the correct values. For example, if a sample count on a channel is 8 and the background count 10, the sample count minus background count is -2. The multichannel analyzer does not print or punch -2; it produces, instead, the complement number 99998, where the number of 9's is dependent on the number of spectrometer levels. ALPHA reconverts this 99998 to -2.

3.2 Samples

3.2.1 Compensation for Spectral Shifts. — During the counting of a sample, gain and threshold shifts may occur (due either to temperature variations or high counting rates^{3,4}); if these shifts are not compensated, incorrect results are obtained. However, ALPHA can compensate for spectral shifts in three different ways.

According to the first way, ALPHA compensates for gain and threshold shifts automatically.¹ Two other programs^{2,3} (see Table 2) require the user to locate a distinct photopeak in the spectrum to compensate properly for gain shift. Such distinct photopeaks do not always exist. Also the other two programs do not correct for threshold shifts unless the value of the threshold of the sample is provided as an input number.

This last requirement is not easily met. The results shown in Table 3 illustrate the ability of ALPHA to determine correctly ^{59}Fe (1.10 and 1.29 Mev) and ^{60}Co (1.17 and 1.33 Mev) in samples containing a mixture of these. As can be seen, very good results and statistical fit were obtained. But, if these shifts are not compensated (ALPHA includes this option), poor results and statistical fit are obtained. The same poor results are obtained with the program of reference 2.

In the second way, ALPHA compensates for gain and threshold shifts semi-automatically. First, the gamma-ray spectrum of a solution containing a single known isotope (one that has a corresponding standard in the library of isotopes) is obtained. This spectrum is analyzed by ALPHA using the automatic gain and shift compensation, as noted above. The resulting estimates of the gain and threshold shifts are stored in the computer's memory and used to shift any subsequent spectrum.

Finally, ALPHA has a third way to compensate for gain and shift. It is called manual because to compensate for spectral shifts, the user must provide, as input parameters, the gain and threshold shifts for the sample.

3.2.2 Counting-Time Correction and Background Subtraction. — ALPHA takes into account the counting time of the sample and can subtract background. As a matter of fact, it is better not to subtract the background from the samples with the multi-channel analyzer because it costs less to do so with ALPHA.

3.2.3 Decay Correction. — ALPHA can give the results corrected for simple radioactive decay in terms of any reference time. This feature is especially useful when many samples are counted at different times.

3.2.4 Dead-Time Correction. — The sensitivity of response of nuclear detection instruments is not constant,⁵ and the fraction of time that they are insensitive or "dead" is called the fractional dead time. Some modern multichannel gamma-ray spectrometers have an indicator that shows this value; others display the fractional live time. The fractional dead-time depends on the energy of the gamma-rays, on the type of analyzer, and on the radioactivity level of the sample. The multichannel analyzer compensates

Table 3. ALPHA Does Not Require a Distinct Photopeak to Determine Correctly the Composition of Samples

Mixture Analyzed	Program	Fit ^a	⁵⁹ Fe		⁶⁰ Co	
			(dis/min)	Error ^c (%)	(dis/min)	Error ^c (%)
1			8.58 × 10 ⁴ (b)		1.390 × 10 ⁶ (b)	
	ALPHA ^d	0.98	(8.11 ± .9) × 10 ⁴	5.5	(1.396 ± .006) × 10 ⁶	-0.43
	LSQ ^e	6.2	(17.3 ± 2.) × 10 ⁴	-101.0	(1.34 ± .013) × 10 ⁶	3.6
	LSQ-G ^f (on 1.10 Mev)	310.0	(241 ± 15.) × 10 ⁴	-2700.0	(0.16 ± .060) × 10 ⁶	89.0
	LSQ-G ^f (on 1.29 Mev)	119.0	(158 ± 10.) × 10 ⁴	-1740.0	(0.60 ± .050) × 10 ⁶	57.0
2			4.30 × 10 ⁶ (b)		6.96 × 10 ⁵ (b)	
	ALPHA ^d	0.94	(4.32 ± .02) × 10 ⁶	-0.47	(6.99 ± .08) × 10 ⁵	-0.43
	LSQ ^e	5.02	(4.54 ± .03) × 10 ⁶	-5.3	(5.86 ± .13) × 10 ⁵	15.8
	LSQ-G ^f (on 1.10 Mev)	23.4	(4.74 ± .06) × 10 ⁶	-10.1	(4.82 ± .26) × 10 ⁵	30.8
	LSQ-G ^f (on 1.29 Mev)	13.4	(4.66 ± .05) × 10 ⁶	-8.4	(5.28 ± .21) × 10 ⁵	24.1

^aChi-square per degree of freedom. This should be close to 1 for a good statistical fit.¹

^bMixture prepared and measured by H. Parker (3 x 3 in. NaI and 10 kev/channel).

^c% error = 100 × [(dis/min in sample) - (calculated dis/min)]/[(dis/min in sample)].

^dALPHA = Least-squares spectrum resolution with automatic gain- and threshold-shift compensation.

^eLSQ = Least-squares spectrum resolution without gain or threshold compensation.

^fLSQ-G = Least-squares spectrum resolution with gain-shift compensation (requires a distinct photopeak²).

automatically for dead-time losses only if the counting time of the sample is much shorter than the half-lives of the isotopes. However, ALPHA can always correct for dead-time, according to the following derivation. Based on the given definition of the fractional dead or live time, the total number of counts collected by the analyzer (with the background subtracted) for isotope s will be:

$$N_s = \int_0^T r_s^*(t) [1 - DT(t)] dt, \quad (1)$$

where $DT(t)$ is the fractional dead-time of the analyzer, $r_s^*(t)$ the "true" counting rate,⁵ and T the counting time interval of the sample (called also clock time). If simple radioactive decay occurs for isotope s , then the value of $r_s^*(t)$ in Eq. (1) can be replaced by the familiar relationship:⁵

$$r_s^*(t) = r_{s,0}^* e^{-\lambda_s t}, \quad (2)$$

where $r_{s,0}^*$ is the true counting rate of isotope s at the beginning of the counting interval, and λ_s is the decay constant. Substituting Eq. (2) into (1) yields:

$$r_{s,0}^* = N_s / \int_0^T [1 - DT(t)] e^{-\lambda_s t} dt. \quad (3)$$

To calculate $r_{s,0}^*$, it is necessary to plot the fractional dead-time of the analyzer versus the counting time (clock) of the sample. Thereafter, the counting time is divided into n equal time increments of length Δt ; the integral in Eq. (3) is then evaluated numerically from this plot by a combination of the Simpson and the trapezoid methods.⁶

ALPHA can correct for dead-time in another way, although it is not as accurate as the previous method. However, it is simpler. According to this procedure, the fractional dead-time is assumed to be constant during the counting time of the sample. Now, the integral in Eq. (3) can be calculated analytically, and the true counting rate for isotope s will be:

$$r_{s,0}^* = \frac{N_s \lambda_s}{(1 - DT) (1 - e^{-\lambda_s T})} \quad (4)$$

The above procedures for correcting for dead-time are independent on the number of isotopes in the sample and can also be applied to correct the library of standards.

3.2.5 Options of Computation. — ALPHA allows one to resolve each sample in many different ways, and there is no limit on the number of ways by which a sample can be resolved. For example, even if some of the isotopes in the mixture are not known, it is still possible to resolve the sample. Here, one uses different isotopic spectra from the library and then, by comparing fit factors (chi-square per degrees of freedom¹), decide the isotopic concentration and composition of the sample. Other possible choices are to use different weighting factors, with or without spectral-shift compensation, etc.

3.2.6 Option for Using the Sample Spectral Data on Magnetic Tape. — ALPHA permits the user to utilize the spectral data of the sample on cards or on magnetic tape. Magnetic-tape operation is very useful when analyzing a large number of samples.

3.2.7 Results Are Printed, Punched, and Sorted. — The output of ALPHA is printed on paper and also punched on cards. The punched-card output is useful when a large number of samples is to be analyzed. Also, the cards can be used for plotting, sorting the answers, etc. A short program, OUTPUT, takes the punched-card output, sorts the six-digit identification numbers of each sample, and prints them in numerical order.

3.2.8 Combining the Results of Consecutive Spectra. — After resolving a group of consecutive spectra, ALPHA can combine all the results (concentrations and estimated errors) in two ways to improve the accuracy of analysis. Either procedure F or H may be used.

Procedure F is used when consecutive spectra are from the same sample but counted at different times to allow for partial decay. The results are combined by a weighted least-squares fit to the familiar equation⁵:

$$r_s = r_{s,0} e^{-\lambda_s t}, \quad (5)$$

where $r_{s,0}$ is the counting rate of isotope s at the reference time. The estimated weighting factors P_s are:

$$P_s = D(r_s)^{-2}, \quad (6)$$

where $D(r_s)$ is the estimated error of the counting rate of isotope s computed by the individual least-squares resolution of each spectrum. ALPHA calculates $r_{s,0}$, the estimated error, and chi-square for each isotope.

Procedure H is used when the consecutive spectra are for similar samples (duplicates, triplicates, etc). ALPHA computes the arithmetic average, the estimated standard error, and the estimated standard error per measurement of each isotope.

3.2.9 Computation of α Values.— ALPHA computes the α values for each isotope in the sample. The definition and application of these α values has already been described.¹ For example, the α values can be used: (1) to determine the optimum counting time, (2) to calculate the optimum ratio of sample-to-background counting time, (3) to compute the optimum time to start counting fast-decaying isotopes, (4) to calculate the effect of volume reduction if the sample was evaporated, (5) to estimate the limits of detection for each isotope, and (6) to calculate the relative effects of the background rates in different locations.

3.2.10 ALPHA Can Reject "Negative" Concentrations.— If the concentration of an isotope in a sample is less than a certain predetermined fraction of the estimated error, then ALPHA repeats the whole least-squares spectrum resolution without calling in the corresponding spectrum from the library. This predetermined fraction is called

the rejection coefficient. Since the estimated error is always positive, the rejection coefficient must be set at zero for ALPHA to reject negative concentrations and restart.

3.2.11 Sample-Fraction Correction. — ALPHA can correct for volume reduction, dilution, or radiochemical yield. This is especially useful when many samples must be analyzed.

3.2.12 Corrections for Other Kinds of Errors. — If the computer detects an error in the transfer of spectral data from paper tape onto cards and magnetic tape, the number 99999 is written instead of the wrong number (wrong parity or length). ALPHA recognizes 99999 and substitutes the interpolated value, which lies between the values of the bracketing channels. This correction feature was tested, and the calculated concentrations were within $\pm 0.1\%$ of the correct ones.

4. HOW TO USE ALPHA

4.1 Input

The program and data are loaded into the computer in the following sequence (Figs. 2 - 5):

1. The program itself, and the computer control cards.
2. The standard library of isotopes — that is, the channel-by-channel spectral data of the individual isotopes — from cards or magnetic tape and appropriate control cards.
3. The spectral data for the samples, on cards or magnetic tape, along with the control and option cards.

The sequence is discussed below.

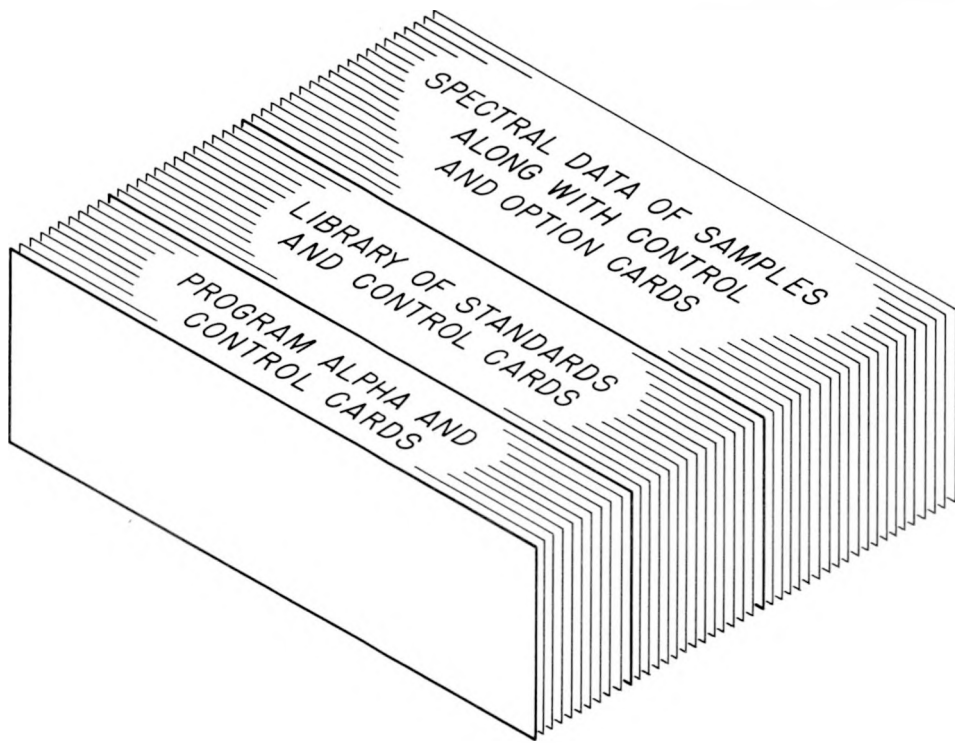


Fig. 2. Complete Input Data Punched on Cards.

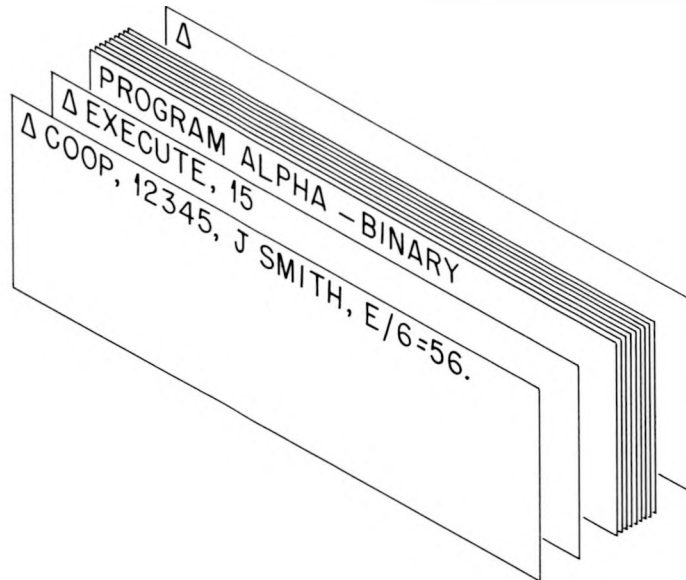


Fig. 3. Program ALPHA and Computer Control Cards.

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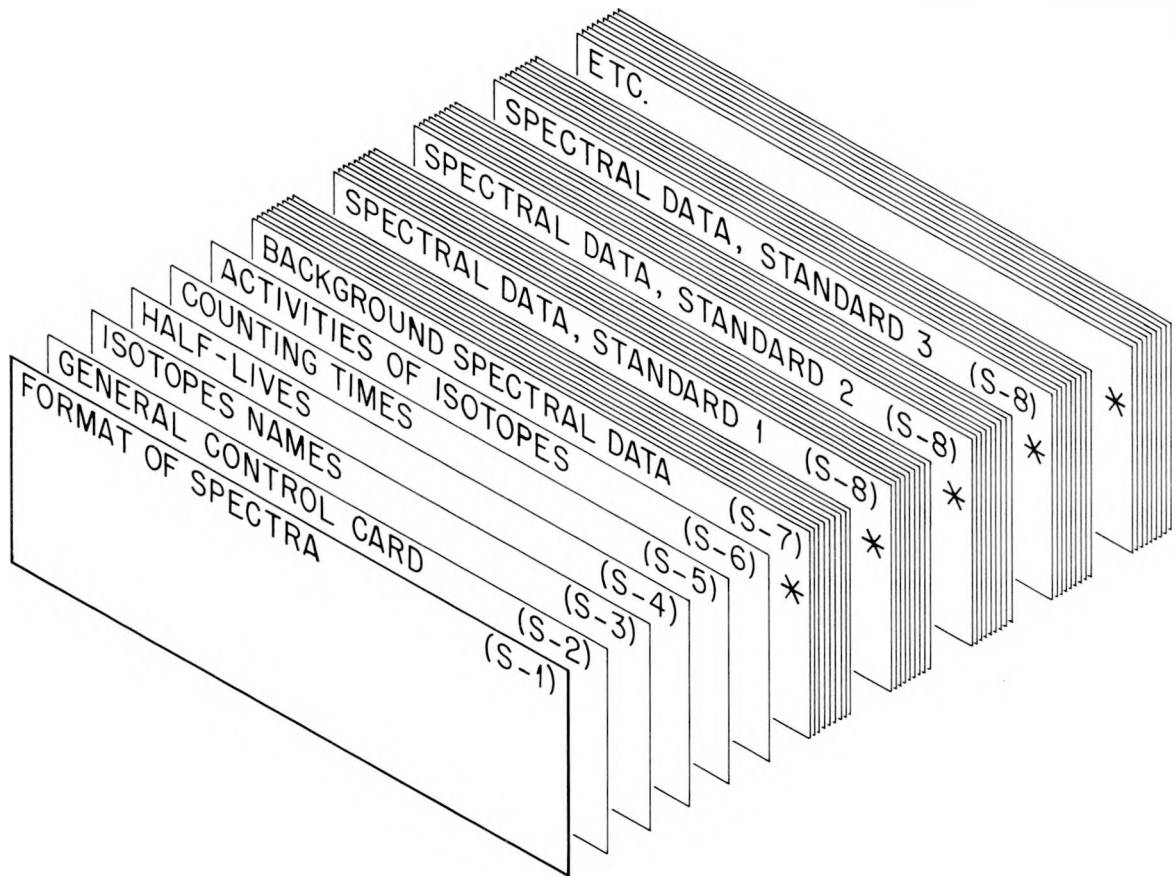


Fig. 4. Library of Standards and Control Cards. If the spectral data are read in from magnetic tape, do not use the cards marked with an asterisk.

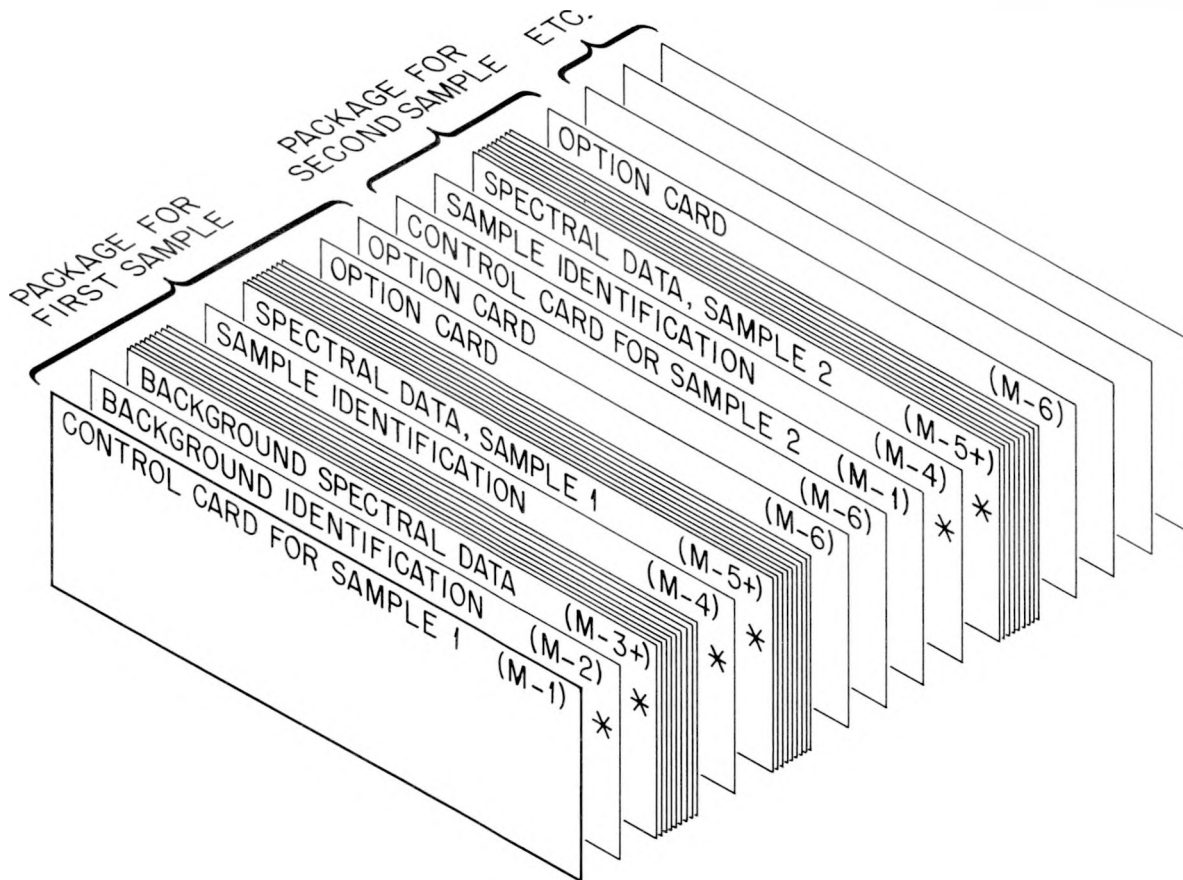


Fig. 5. Spectral Data of Samples Along with Control and Option Cards. If the spectral data are read in from magnetic tape, do not use the cards marked with an asterisk.

4.1.1 Program and Computer-Control Cards.

1. First card (C-1). This is a computer-control card. The user has several choices depending on how the data are fed in.
 - (a) If spectral data of the library and samples are on cards, write, starting in column 1:
 Δ COOP, 12345, MY NAME, E/6 = 56.
 The number 12345 is the individual charge account number.
 - (b) If spectral data of the library and samples are on magnetic tape, write, starting in column 1:
 Δ COOP, 12345, MY NAME, I/7/8/E/6 = 56.
 - (c) If spectral data of library are on magnetic tape, and of samples on cards, write, starting in column 1:
 Δ COOP, 12345, MY NAME, I/7/E/6 = 56.
 - (d) If spectral data of the library are on cards, and of the samples on magnetic tape, write, starting in column 1:
 Δ COOP, 12345, MY NAME, I/8/E/6 = 56.
2. Second card (C-2). This also is a computer-control card. Starting in column 1, write:
 Δ EXECUTE, 15.
3. Program ALPHA in binary cards.
4. Last card (C-3). This is a computer-control card. Write in column 1:
 Δ

4.1.2 Library of Standards

Card	Field ^a	Format ^a	Description
S-1	2-71	A	Write in parentheses the format of the spectral data of both standards and mixtures, e.g., (12F6.0)
S-2			<u>General Control Card</u>
	3-5	I	Number of isotopes in the library (maximum of 80); see Sec 3.1.3
	8-10	I	Number of channels in analyzer (maximum 400); see Sec 3.1.2
	15	I	Number of iterations for gain and threshold compensation; in general, use 2 for 1% gain shift and 4 to 5 for 3-5% gain shift ¹
	20	I	1 Reads background for standards, subtracts, and prints standards 0 Does not read background and does not print standards
	23-25	I	Initial channel for computation
	28-30	I	Final channel for computation
	34	I	Used only when the answers of several consecutive spectra are combined; a 1 punch in this column calls procedure F, a 0 (zero) punch calls procedure H (see card M-1 col 15 and Sec 3.2.8)
	35	I	Always the 6 punch
	39-40	I	50 if the library of standards is on cards 7 if the library of standards is on magnetic tape
	44-45	I	50 if the sample spectrum and identification are on cards 8 if the sample spectrum and identification are on magnetic tape

^aSee glossary (Sec 4.1.4)

Card	Field ^a	Format ^a	Description
S-2 (Cont'd.)	51-60	E	Counting time of the background (use the same units for background, standards, and samples)
	61-70	E	Rejection coefficient: Used only when the option card of a sample calls for it. If this is the case and the concentration of an isotope is less than this number multiplied by its estimated error, then ALPHA repeats the whole computation without that standard (see card M-6, col 10, and Sec 3.2.10)
S-3	1-8, 9-16, etc.	A	Name of each isotope: One name every 8 columns, or a maximum of 10 per card; use as many cards as necessary to list all the isotopes
S-4	1-10, 11-20, etc.	E	Half-lives of the isotopes: Use the same units for all. One every 10 columns, or 8 per card. Use as many cards as necessary to list all the half-lives
S-5	1-10, 11-20, etc.	E	Counting time of each standard (same units as for background and samples): One every 10 columns, or 8 per card; use as many as necessary
S-6	1-10 11-20, etc.	E	Activity or concentration of each standard isotope at the time of counting: May be set at 1.0 (results as fractions), in dpm, in dpm ml ⁻¹ , in dpm gm ⁻¹ or other convenient units; one every 10 columns or 8 per card; use as many as necessary to list all reference activities
S-7 S-7a etc.	See S-1	F	Background spectrum cards for the standards: (Use only if 1 is punched in col 20 of card S-2)
S-8 S-8a etc.			Library of standard spectra (without identification cards): Introduce <u>only</u> if spectra are on cards (if 50 is punched in cols 39 and 40 of card S-2); Standards are numbered 1,2,3, ..., according to their loading order

^aSee glossary (Sec 4.1.4)

4.1.3 Spectral Data of the Samples, Including Control Cards

Card	Field	Format	Description
M-1			<u>Control Card for Each Sample</u>
	2-7	A	Identification, i.e., code number of sample
	9-10	I	Number of option cards (see option card): this sample will be resolved as many times as indicated by the number; see Sec. 3.2.5
	15	I	0 punch means each sample is resolved individually. >1 If the number is, e.g., 5, then the next 5 spectra, including this one, will be resolved individually and the results combined; see col 34 of card S-2 and Sec 3.2.8 Maximum number of spectra that can be combined is 5
	20	I	0 does not read background; the background of the standards can be used here 1 means program reads a background with identification right after this card. This background spectrum will be used for the rest of the samples unless a new one is introduced later on
	30	I	1 program subtracts the background from the sample 0 program does not subtract the background from the mixture
	31-40	E	Counting time of the background (same units as for standards and samples)
	41-50	E	Counting time of the sample (live time): Use same units that were used for counting the background and standards
	51-60	E	Volume reduction, or inverse of the dilution factor
	61-70	E	Decay time (same units as for the half-lives): This is the difference between the beginning of counting time and an arbitrary reference time; if equal to 0.0, then no correction is made for decay

Card	Field	Format	Description
M-2	1-70	A	Identification card for the background: Use only when 1 is punched in col 20 of card M-1 and spectra of samples and backgrounds are on cards
M-3 M-3a, etc.	See S-1	F	Background spectrum: Use only if sample data are on cards, in which case 1 is punched in col 20 of card M-1
M-4	1-70	A	Identification of the sample: Identify only when the sample data are on cards
M-5 M-5a, etc.	See S-1	F	Sample spectrum: Use only if the spectra are on cards
M-6			<u>Option Card for the Sample</u>
			This card indicates in what particular way the computation will take place. There is no limit (up to 99) to the number of option cards for each sample (equal to the value in columns 9-10, card M-1)
	3-4	I	Number of isotopes used from the library (maximum 20)
	5-6	I	0 No threshold and/or gain compensation 1 Gain shift compensation: Automatic procedure -1 Manual shift: The gain and threshold values are computed separately -2 Gain and threshold shift based on the values obtained from a previous mixture (see col 10)
	8	I	1 Weighting factor: 1 -1 Weighting factor: counts ⁻¹ (does not include background) 0 Weighting factor: σ^{-2} (includes background)

Card	Field	Format	Description
M-6 (cont'd)	10	I	1 Applies rejection coefficient (see card S-2, cols 61-70) 0 Does not apply rejection procedure -1 If gain and threshold correction is used (1 punched in cols 6 and 12), ALPHA will store the gain-shift and threshold values in memory and use them to correct another sample when this procedure is called in (when -2 is punched in cols 5 and 6 in another sample). This is the semi-automatic way
	12	I	0 and 0 in col 6, then no gain or threshold compensation occurs 0 and 1 in col 6, then only gain compensation occurs (automatic way) 1 and 1 in col 6, then gain and threshold compensation occurs (automatic way)
	13-18	F	Threshold channel for the standard library spectra ¹
	19-20	I	0 No dead-time correction 1 Dead-time correction according to Eq. (3): Needs cards M-7 and M-8 after this option card -1 Dead-time correction according to Eq. (4): Needs card M-8 after this option card
	21-22, 23-24, etc.	I	Number of library standard in order of desired print-out: Each number occupies 2 cols; the number of an isotope in the library is given by the loading order (see card S-8)

Control Cards for Dead-Time Correction

These cards are used only if a number other than 0 is punched in col 20, card M-6; see Sec 3.2.4

M-7

Use this card only if 1 is punched in col 20, card M-6

1-10

E

Counting time (clock): Use same units as for the live-time

E: Use for numbers that have decimal points. The written decimal point occupies one column, and its position in the field is not important. If numbers have integer exponents (e.g., $1.2309 \times 10^{+2}$), write first, at the left part of the field, the decimal fraction of the number and then the value of the exponent (ending at the last column of the field), preceded by a + sign or - sign, depending on the value of the exponent. For example, the number $1.2309 \times 10^{+2}$ can be written in the field 22-30 in several ways:

1	2	3	.	0	9					1	2	3	.	0	9		1	.	2	3	0	9	+	2											
22						30						22						30						22						30					
0	.	1	2	3	0	9	+	3	1	2	3	0	9	.	-	2	.	1	2	3	0	9		+	3										

F: This format is for decimal fractions only. It is the same kind of number used in format E, but without the exponent.

A: Use any combination of alphabetical, numerical, or punctuational symbols.

Size of numbers: The numbers in the F or E format should be larger than 10^{-308} and smaller than 10^{308} . The numbers in I format should be smaller than 10^{14} .

4.2 Output

There are two kinds of output: One is printed on paper, and the other is written on punched cards. The first one lists most of the input data (spectra corrected for background) and results. The results include activities or concentrations of each isotope, along with the estimated error (1 sigma or about 70% confidence level). The printed output also contains several indexes for locating errors in the data. These indexes include: chi-square per degree of freedom (2 different estimates), the variance of the fit, the sum of the squares of the residuals, the ratio of the residual over the standard deviation per channel, and the estimated gain and threshold shifts. It also includes, separately, the number of "suspicious" channels. This information also helps to detect the presence of unexpected isotopes.¹ The punched cards contain only the identification of the mixture and the results in terms of concentrations and estimated errors.

These punched cards can be used for further calculations in another program (particular

use) or for curve plotting. Two short programs can list the answers from several different jobs. One program lists them in order of appearance, and the other sorts the identification number (6 digits) and prints the answers in consecutive order. These last two programs are especially useful when large numbers of samples are analyzed.

5. ACKNOWLEDGMENT

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7. APPENDIX: PROGRAM ALPHA THROUGH OUTPUT IN FORTRAN 63

```

PROGRAM ALPHA
C
C ** WRITTEN AND TESTED BY E. SCHÖNFELD (GRVL) **
C   FOR INSTRUCTIONS ON HOW TO USE IT SEE GRVL-3810
C
C STD INPUT TAPE=50 ** STD OUTPUT TAPE(PRINT)=51 **
C STD OUTPUT TAPE(PUNCH)=52 ** STD SCRATCH TAPE=56 **
C
C   VERSION GOOD UP TO 96000.0 * LARGER CONVERTED TO ZERO
C   IF IT FINDS 99999. INTERPOLATES BETWEEN NEIB. CHANNELS
C
C DIMENSION A(22,22),Y(257),Z(22),S(82,256),STD(22),B(22),
C 1  R(256),W(256),DER(256),YT(256),IR(256),
C 2  BA(256),SS(80),FM(12),AC(80),HA(80),IS(82), TST(82),HAI(22),
C 3  STDT(22),AT(22),TNAME(12),TISOT(82),TISO(22),IT(22),ZT(22)
C COMMON S,BA,R,IR,DER,W
C TYPE INTEGER FM,TNAME,TISOT,TISO,XI)T
C   CHANGE THIS CARD TO MAX NR OF ISOTYPES IN THE LIBRARY
C
C NSTO=80
C READ INPUT TAPE 50,56,(FM(I), I=1,10)
C WRITE OUTPUT TAPE 51,140,(FM(I),I=1,10)
C READ INPUT TAPE 50,28,NS,M,NIT,NBA,NZ,MF,NH,NF,NTS,NTM,NQ,TB,Q
C WRITE OUTPUT TAPE 51,141,NS,M,NIT,NBA,NZ,MF,NH,NF,NTS,NTM,NQ,TB,Q
C REWIND NF
C READ INPUT TAPE 50,56,(TISOT(I),I=1,NS)
C WRITE OUTPUT TAPE 51,142,(TISOT(I),I=1,NS)
C READ INPUT TAPE 50,58,(HA(I),I=1,NS)
C WRITE OUTPUT TAPE 51,143,(HA(I),I=1,NS)
C READ INPUT TAPE 50,58,(TST(I),I=1,NS)
C WRITE OUTPUT TAPE 51,144,(TST(I),I=1,NS)
C READ INPUT TAPE 50,58,(AC(I),I=1,NS)
C WRITE OUTPUT TAPE 51,145,(AC(I),I=1,NS)
C DO 38 I=1,M
C 38 BA(I)=0.0
C IF (NRA) 118,118,119
C 119 READ INPUT TAPE NTS,FM,(BA(I),I=1,M)
C WRITE OUTPUT TAPE 51,149
C WRITE OUTPUT TAPE 51,22,(BA(I),I=1,M)
C 118 DO 126 I=1,NS
C READ INPUT TAPE NTS,FM,(S(I,J),J=1,M)
C DO 125 J=1,M
C IF(NBA) 122,122,121
C 121 FAT=TST(I)/T3
C S(I,J)=S(I,J)-BA(J)*FAT
C 122 IF(S(I,J)) 124,123,123
C 124 S(I,J)=0.01
C 123 IF(S(I,J)-96000.0) 125,125,120
C 120 S(I,J)=0.01
C 125 CONTINUE
C IF(NBA) 126,126,128
C 128 WRITE OUTPUT TAPE 51,22,(S(I,J),J=1,M)
C 126 CONTINUE
C DO 39 I=1,NS
C SS(I)=0.0
C DO 39 J=NZ,MF
C 39 SS(I)=SS(I)+S(I,J)

```

```

WRITE OUTPUT TAPE 51,164
WRITE OUTPUT TAPE 51,24,(SS (I),I=1,NS)
DO 64 I=1,NS
64  SS (I)=SS (I)**2
    VNN=0
    VD=0
18  WRITE OUTPUT TAPE 51,129
129  FORMAT(14I)
    READ INPUT TAPE 50,25,XIDT,NOPT,NDT,NBR,NBS,TB,TSA,VRED,DAY,VM
    WRITE OUTPUT TAPE 51,140,XIDT,NOPT,NDT,NBR,NBS,TB,TSA,VRED,DAY,VM
    IF (VM) 160,160,161
160  VM=1.0
161  IF (VRED) 162,162,163
162  VRED=1.0
163  IF (TB) 131,131,132
131  FS=0.0
    GO TO 133
132  FS=TSA/TB
133  FX=FS+FS**2
    IF(NBR) 37,37,36
36  READ INPUT TAPE NTM,52,(TNAME(I),I=1,10)
    WRITE OUTPUT TAPE 51,53,(TNAME(I),I=1,10)
    READ INPUT TAPE NTM,FM,(BA(I),I=1,M)
    WRITE OUTPUT TAPE 51,22,(BA(I),I=1,M)
37  READ INPUT TAPE NTM,52,(TNAME(I),I=1,10)
    WRITE OUTPUT TAPE 51,53,(TNAME(I),I=1,10)
    READ INPUT TAPE NTM,FM,(Y(I),I=1,M)
    DO 43 I=2,M
        IF (Y(I)=96000,0 ) 43,43,41
41  IF (Y(I)=99999,0 ) 42, 43,42
42  Y(I)=0.0
43  CONTINUE
    DO 165 I=3,M
        IF (Y(I)=99999,0 ) 165,48,165
48  Y(I)=( Y(I+1)+Y(I-1) )/2.0
165  CONTINUE
    IF (NRS) 45,45,46
46  DO 47 I=1,M
47  Y(I)=Y(I)-BA(I)*FS
45  SB=0.0
    DO 40 I=NZ,MF
40  SB=SB+BA(I)
    WRITE OUTPUT TAPE 51,22,(Y(I), I=1,M)
    S1=0.0
    S2=0.0
    DO 63 I=NZ,MF
63  S1=S1+Y(I)
    S2=S1+SB*FX
    WRITE OUTPUT TAPE 51,147,SB,S1
    DO 130 I=1,M
130  YT(I)=Y(I)
    DO 80 IN=1,NOPT
    READ INPUT TAPE 50,50,N,KT,LW,NEWST,K23D,QH,VDET,(IS(I),I=1,N)
    SH=-QH
    KK=0
    VTT=N

```

```

      DO 91 J=1,N
        DO 92 I=1,NS
          IF (IS(J)-1) 93,93,92
93      TIS0(J)=TIS9T(I)
          GO TO 91
92      CONTINUE
91      CONTINUE
      DO 96 J=1,NTT
96      IT(J)=J
300 WRITE OUTPUT TAPE 51,148,N,KT,LW,NE,ST,K23D,QH,NDET,(IS(I),I=1,N)
      DO 71 J=1,M
71      Y(J)=YT(J)
          FP=1.0
          SMSHC=0.0
          IF (KT) 84,44,44
84      IF (KT+2) 73,83,73
73      IF (KK) 74,74,83
74      READ INPUT TAPE 50,58,FTT,SHCT
          WRITE OUTPUT TAPE 51,58,FTT,SHCT
83      CALL SHIFT (Y,M,SH,FTT,SHCT)
          FP=FTT
          SMSHC=SHCT
44      IS(N+1)=NST0+1
          IS(N+2)=NST0+2
          NT=N
          CHT= 1.0E20
          DO 101 L0=1,NIT
          N = NT
          DO 14 I=1,M
            IF(LW) 29,13,12
12      W(I)=1.0
            GO TO 14
13      T=Y(I)+BA(I)*FX
            IF (T- 1.0) 32,32,34
32      W(I)=1.0
            GO TO 14
34      W(I)=1.0/T
14      CONTINUE
          GO TO 33
29      DO 31 I=1,M
31      W(I)=1.0/(Y(I)+1.0)
33      IF (KT) 26,26,16
16      N=N+1
          I=M-1
          N5=IS(N)
          DO 17 J=2,I
            C=J
            IF(Y(J+1)-1.0 ) 136,136,134
134      IF(Y(J-1)-1.0 ) 136,136,135
135      DER(J)=(Y(J+1)-Y(J-1))/2.0
            GO TO 17
136      DER(J)=0.0
17      S( N5 ,J)=-DER(J)*(C+SH)/100.0
          S(IS(N),1)=S(IS(N),2)
          S(IS(N),M)=S(IS(N),M-1)
          IF(K23D) 26,26,19

```

```

19  V=N+1
    I=M-1
    N5=IS(N)
    DO 27 J=2,I
27  S( N5 ,J)=-DER(J)
    S(IS(N),1)=S(IS(N),2)
    S(IS(N),M)=S(IS(N),M-1)
26  DO 1 L=1,N
    N5=IS(L)
    DO2 K=L,N
    N6=IS(K)
    SA=0.
    DO 3 I=NZ,MF
3    SA=SA+S(N6,I)*S(N5,I)*W(I)
    A(K,L)=SA
    A(L,K)=A(K,L)
2    CONTINUE
1  CONTINUE
    DO 4 K=1,N
    N6=IS(K)
    SX=0.
    DO 5 I=NZ,MF
    SX=SX+S(N6,I)*Y(I)*W(I)
5    CONTINUE
4  B(K)=SX
    CALL INVERT (A,N)
    DO 7 J=1,N
    SUM=0.
    DO 8 I=1,N
    SUM=SUM+A(J,I)*B(I)
8    CONTINUE
7  Z(J)=SUM
    CH=0.0
    VY=0.
    CHS=0.0
    VU=0.0
    DO 11 J=NZ,MF
    SV=0.
    DO 9 I=1,N
    N5=IS(I)
9    SV=SV+S(N5,J)*Z(I)
    RE=Y(J)-SV
    T=RE**2
    VY=VY+W(J)*T
    VU=VU+T
    TMP=ABSF(0.1+SV+BA(J)*FX)
    RT=T/TMP
    CH=CH+RT
    TMP=SQRTF(TMP)
    R(J)=RE/TMP
    TE=Y(J)+BA(J)*FX
    IF (TE=1.0) 65,65,66
65  TT=T
    GO TO 67
66  TT=T/TE
67  CHS=CHS+TT

```

```

11 CONTINUE
    DN=MF-N-VZ+1
    CHDF=CH/DN
    VY=VY/DN
    CHDFS=CHS/DN
    DO 15 I=1,N
        F=A(I,I)*VY
        STD(I)=E
15 CONTINUE
    IF (KT) 500,500,100
500 WRITE OUTPUT TAPE 51,155,CHDF
    GO TO 90
100 IF (K23D) 104,104,103
103 NU=N-1
    SH=SH-Z(V)
    SHC=-1,0*Z(N)
    GO TO 105
104 NU=N
    SHC=0,0
105 F=1.0-Z(NU)/100,0
    FP=FP*F
    SMSHC=SMSHC+SHC
    WRITE OUTPUT TAPE 51,155,CHDF,SMSHC,FP
    T=(CHT-CH)/CH
    IF (T+0,05) 90,90,97
97 IF (T-0,05) 90,90,111
111 IF (CHDF > 1,2) 90,90,107
107 CHT=CH
    CALL SHIFT(Y,M,SH,F,SHC)
101 CONTINUE
90 DO 49 I=1,NT
    A(I,I)=SS(IS(I))*A(I,I)*VY/NU
49 AT(IT(I))=SQRTF(A(I,I))
    WRITE OUTPUT TAPE 51,156
    WRITE OUTPUT TAPE 51,24,(AT(J), J=1,NT)
    DO 95 I=1,NT
        HAT(I)=HA(IS(I))
        FD=EXP(0.693*DAY/HA(IS(I)))
        FAT=TST(IS(I))/TSA
        STD(I)=FAT*AC(IS(I))*FD*SQRTF(STD(I))*VM/VRED
95 Z(I)=Z(I)*FAT*AC(IS(I))*FD*VM/VRED
        IF (NDET) 98,99,98
98 CALL DTIME (A,STD,Z,HAT,TSA,NT,KK,NDET)
99 DO 94 J=1,NT
        ZT(IT(J))=Z(J)
94 STDT(IT(J))=STD(J)
    WRITE OUTPUT TAPE 51,157
    WRITE OUTPUT TAPE 51,21,(TISO(I),ZT(I),STDT(I),I=1,NT)
    IF (NEWST) 35,79,72
72 KK=KK+1
    IF(KK-2) 75,79,79
75 DO 78 I=1,NT
    IF(Z(I)/STD(I)=0) 77,77,78
77 IS(I)=0
78 CONTINUE
    KR=0

```

```

      DO 76 J=1,NT
        IF (IS(J)) 76,76,81
81      KR=KR+1
        IS(KR)=IS(J)
        IT(KR)=J
76      CONTINUE
        IF (KR) 127,79,127
127     IF (KR-NT) 82,79,82
82      V=KR
        QH=-SH
        GO TO 300
35      FTT=FP
        SHCT=SMSHC
79      IF (NDT) 150,150,151
150     IF (ND) 152,152,151
152     WRITE OUTPUT TAPE 52,153,(TNAME(I),I=1,10),NTT,ND
        WRITE OUTPUT TAPE 52,54,(TISO(I),ZT(I),STDT(I),I=1,NTT)
        WRITE OUTPUT TAPE 51,158
151     WRITE OUTPUT TAPE 51,57,(R(J),J=1,MF)
        K=0
        V2=MF-2
        DO 85 J=NZ,N2
          T=ABSF(R(J))
          IF (T-10.) 89,89,88
89          IF (R(J)-2.0) 85,86,86
86          IF (R(J)+2.0) 85,87,87
87          IF (R(J+1)-2.0) 85,88,88
88          K=K+1
          IR(K)=J
85          CONTINUE
        WRITE OUTPUT TAPE 51,159
        WRITE OUTPUT TAPE 51,51,(IR(I),I=1,K)
80          CONTINUE
          IF (NDT) 106,106,108
108         ND=NDT
106         IF (ND) 117,117,109
109         WRITE OUTPUT TAPE NF,154,(ZT(I),STDT(I),I=1,NTT)
          VNN=VNN+1
          IF (ND-VNN) 110,110,117
110         END FILE NF
          REWIND NF
          CALL DECAY (TISO,NTT,VD,NF,NH,TNAME)
          VNN=0 $ VD=0
          REWIND NF
117        GO TO 18
10         FORMAT(5I10,3F10,5)
20         FORMAT(10F6,1)
21         FORMAT(12X,3(4X,A8,E13.4,E11,2))
22         FORMAT(15F8,0)
23         FORMAT(13,2X,4E10,2,E12,2,E12,4,3X,2E10,2,5X,2E10,2)
24         FORMAT(1X,E11,4,9E12,4)
25         FORMAT(1X,A6,1X,12,15,15,110,5E10,3)
28         FORMAT( 6I5,3X,2I1,3I5,E10,3,E10,2)
30         FORMAT(110,2F20,0)
50         FORMAT(14,4I2,F6,2,12,30I2)
51         FORMAT(30I4)

```

```

52  FORMAT(10A7)
53  FORMAT(1X,10A7)
54  FORMAT(3(A8,E10,3,E9,1))
55  FORMAT(12F6,0)
56  FORMAT(10A8)
57  FORMAT(15(1X,F7,1))
58  FORMAT(8E10,3)
59  FORMAT(8E15,4)
140 F9RMAT(12H CARD S-1 10A8)
141 F9RMAT(12H CARD S-2 5I5,2I1,3I5,2E12,3)
142 F9RMAT(12H CARD S-3 10A8)
143 F9RMAT(12H CARD S-4 8E12,4)
144 F9RMAT(12H CARD S-5 8E12,4)
145 F9RMAT(12H CARD S-6 8E12,4)
149 F9RMAT(25H BACKGROUND AND STANDARDS)
146 F9RMAT(12H CARD M-1 A6,I3,2I5,I10,5E11,3)
147 F9RMAT(12H BACKGD SUM=E12,3,16H SAMPLE SUM=E12,3)
148 F9RMAT(12H CARD M-6 I4,4I2,F6,2,3I12,/)
155 F9RMAT( 5H FIT=E11,3,11H THR SHIFT=F5,2,12H GAIN SHIFT=F6,4)
156 F9RMAT(14H ALPHA FACTORS)
157 F9RMAT(47H RESULTS=CONCENTRATIONS AND EST STANDARD ERRORS,/)
158 F9RMAT(47H RATIO OF RESIDUALS OVER STD DEV PER CHANNEL )
159 F9RMAT(20H SUSPICIOUS CHANNELS)
153  FORMAT(10A7,2I5)
154  FORMAT(4(E11,3,E9,1))
164 F9RMAT(17H SUM OF STANDARDS)
END ALPHA

```

```

SUBROUTINE SHIFT(Y,M,S4,F,SHC)
DIMENSION X(257),Y(257),XC(257),YC(257)
DO 7 I=1,M
7  XC(I)=I
  DO 8 J=1,M
  Z=J
  X(J)=Z*F+ SH*(F-1.)
8  X(J)=X(J)+SHC
  DO 60 I=1,M
  DO 40 J=1,M
  IF (XC(I)-X(J)) 50,45,40
45  YC(I)=Y(J)/F
  GO TO 60
40  CONTINUE
50  YC(I)=(Y(J)-Y(J=1))/(X(J)-X(J=1))
  YC(I)=Y(J=1)+YC(I)*(XC(I)-X(J=1))
  YC(I)=YC(I)/F
60  CONTINUE
  DO 80 I=1,M
80  Y(I)=YC(I)
  Y(1)=0.0
  RETURN
END

```

```

SUBROUTINE DECAY (TISO,NT,NK,NF,NH,TNAME)
DIMENSION Z(10,5),W(10,5),A(10),S(10),SUMA(10),V(10),TISO(10)
1      ,TNAME(12)
TYPE INTEGER TISO,TNAME
DO 12 J=1,NK
12  READ INPUT TAPE   NF,5,(Z(I,J),W(I,J), I=1,NT)
    IF (NH) 21,21,20
20  WRITE OUTPUT TAPE 51,10
10  FORMAT(1H /15H   PROCEDURE F/)
DO 1 I=1,NT
    SUM=0.0
    SUM1=0.0
    DO 2 J=1,NK
        W(I,J)=1.0/W(I,J)**2
        SUM=SUM+W(I,J)
2    SUM1=SUM1+W(I,J)*Z(I,J)
    A(I)=SUM1/SUM
1  SUMA(I)=SUM
DO 3 I=1,NT
    SUM=0.0
    DO 4 J=1,NK
4    SUM=SUM+W(I,J)*(Z(I,J)-A(I))**2
    T=NK-1
    V(I)=SUM/T
3  S(I)=SQRTF(V(I)/SUMA(I))
GO TO 100
C    PROCEDURE H
21  WRITE OUTPUT TAPE 51,28
28  FORMAT(1H /15H   PROCEDURE H/)
    T=NK
DO 23 I=1,NT
    SUM=0.0
    DO 24 J=1,NK
        IF (Z(I,J)) 25,25,24
25    Z(I,J)=0.0
24    SUM=SUM+Z(I,J)
23  A(I)=SUM/T
DO 27 I=1,NT
    SUM=0.0
    DO 26 J=1,NK
26    SUM=SUM+(A(I)-Z(I,J))**2
    V(I)=SQRTF(SUM/(T-1.0))
27  S(I)=V(I)/SQRTF(T)
100 WRITE OUTPUT TAPE 51,6,(TISO(I),A(I),S(I),V(I),I=1,NT)
    WRITE OUTPUT TAPE 52,7,(TNAME(I),I=1,10),NT,NK
    WRITE OUTPUT TAPE 52,8,(TISO(I),A(I),S(I),I=1,NT)
    RETURN
5    FORMAT(4(E11.3,E9.1))
6    FORMAT(3(2X,A8,E11.3,E9.1,E9.1))
7    FORMAT(10A7,2I5)
8    FORMAT(3(A8,E10.3,E9.1))
9    FORMAT(2I5)
END

```

```

SUBROUTINE DTIME (A,STD,Z,HAT,TSA,NT,KK,NDET)
DIMENSION A(22,22),STD(22),Z(22),HAT(22),D(30)
IF (NDET) 31,31,30
30 IF (KK) 9,9,10
9 READ INPUT TAPE 50,20,TC,DT,NP,NSI
WRITE OUTPUT TAPE 51,22,TC,DT,NP,NSI
READ INPUT TAPE 50,21,(D(I),I=1,NP)
WRITE OUTPUT TAPE 51,23,(D(I),I=1,NP)
10 IT=NP-2
   DTT=TC-IT*DT
   NEX=NP-NSI
   LT=NP-1
   DO 2 I=1,NT
     T=-DT
     DO 1 J=1,LT
       T=T+DT
       A(I,J)=(1.0-D(J))*EXP(-0.693*T/HAT(I))
1     CONTINUE
     T=T+DTT
     A(I,NP)=(1.0-D(NP))*EXP(-.693*T/HAT(I))
2   CONTINUE
     V=(NSI-1)/2 -1
     DO 7 I=1,NT
       SUM=0.0
       DO 3 J=1,N
         SUM=SUM+4.0*A(I,2*J)+2.0*A(I,2*J+1)
3     CONTINUE
     AR=A(I,1)+SUM+4.0*A(I,NSI-1)+A(I,NSI)
     AR=AR*DT/3.0
     IF (NP=NSI-1) 4,5,6
5     AR=AR+(A(I,NSI)+A(I,NSI+1))*DTT/2.0
     GO TO 4
6     AR=AR+(A(I,NSI)+A(I,NSI+1))*DT/2.0+(A(I,NSI+1)+A(I,NSI+2))*DTT/
2.0
4     TE=TSA/AR
     Z(I)=Z(I)*TE
     STD(I)=STD(I)*TE
7   CONTINUE
     GO TO 100
31 IF (KK) 32,32,33
32 READ INPUT TAPE 50,21,DET
WRITE OUTPUT TAPE 51,23,DET
33 TC=TSA/(1.0-DET)
   DO 34 I=1,NT
     TEM=0.693*TC/HAT(I)
     TEM=TEM/(1.0-EXP(-TEM))
     Z(I)=Z(I)*TEM
     STD(I)=STD(I)*TEM
34 CONTINUE
20   FORMAT(2E10,3,2I5)
21   FORMAT(8E10,3)
22   FORMAT(12H CARD 4=7   2E11,3,2I5)
23   FORMAT(12H CARD 4=8   8E11,3)
100 RETURN
END

```

```

SUBROUTINE INVERT (A,N)
      GAUSS-JORDAN METHOD * VERSION BY
      M H LIETZKE ET AL (ORNL-3430)
      DIMENSION A(22,22),B(22),C(22),LZ(22)
      D9 10 J=1,N
10  LZ(J)=J
      D9 20 I=1,N
      K=I
      Y=A(I,I)
      L=I-1
      LP=I+1
      IF(N-LP)14,11,11
11  D9 13 J=LP,N
      W=A(I,J)
      IF(ABSF(W)-ABSF(Y))13,13,12
12  K=J
      Y=W
13  CONTINUE
14  D9 15 J=1,N
      C(J)=A(J,K)
      A(J,K)=A(J,I)
      A(J,I)=-C(J)/Y
      A(I,J)=A(I,J)/Y
15  B(J)=A(I,J)
      A(I,I)=1.0/Y
      J=LZ(I)
      LZ(I)=LZ(K)
      LZ(K)=J
      D9 19 K=1,N
      IF(I-K)16,19,16
16  D9 18 J=1,N
      IF(I-J)17,18,17
17  A(K,J)=A(K,J)-B(J)*C(K)
18  CONTINUE
19  CONTINUE
20  CONTINUE
      D9 200 I=1,N
      IF(I-LZ(I))100,200,100
100 K=I+1
      IF(I=N)800,200,200
800 D9 500 J=K,N
      IF(I-LZ(J))500,500,500
600 M=LZ(I)
      LZ(I)=LZ(J)
      LZ(J)=M
      D9 700 L=1,N
      C(L)=A(I,L)
      A(I,L)=A(J,L)
700 A(J,L)=C(L)
500 CONTINUE
200 CONTINUE
      RETURN
      END

```

```

PROGRAM TRAMAG
C TRANSFERS STANDARDS IN 1216 FORMAT INTO MAGTAPE
C ALSO INTEGRATES TOT COUNTS FROM CHANNELS 5 TO 256
C DIMENSION NS(300)
C ND IS THE NUMBER OF CHANNELS ** CHANGE ACCORDING CASE
  ND=256
  IN=0
  DO 100 KK=1,500
    IN=IN+1
C     CHANGE CARD FOR DIFF FORMAT
    READ INPJT TAPE 50,10,(NS(I),I=1,12)
    IF(NS(1)) 3,2,2
C     CHANGE CARD FOR DIFF FORMAT
    2 READ INPJT TAPE 50,10,(NS(I),I=13,ND)
      NS(I)=IN
      NSUM=0
      DO 6 I=5,256
        6 NSUM=NSUM+NS(I)
        WRITE OUTPUT TAPE 51,15,IN,NSUM
        WRITE OUTPUT TAPE 51,20,(NS(I),I=1,ND)
C     CHANGE NEXT TWO CARDS DIFF FORM
        WRITE OUTPUT TAPE 6,10,(NS(I),I=1,ND)
        WRITE OUTPUT TAPE 7,10,(NS(I),I=1,ND)
100 CONTINUE
    3 END FILE 6
      END FILE 6
        END FILE 7
          END FILE 7
            WRITE OUTPUT TAPE 51,25
              10 F9FORMAT(1216)
                11 F9FORMAT(1018)
                  15 F9FORMAT( //15,110/)
                    20 F9FORMAT(1218)
                      25 F9FORMAT( TAPE 6 AND 7 LOADED OK )
                        END TRAMAG

```

PROGRAM TRAMMM

C
C
C
C

THIS PROGRAM ALLOWS TO TAKE THE MASTER LIBRARY OF
STANDARDS ON MAGNETIC TAPE AND SELECT FROM IT
A SMALLER LIBRARY OF STANDARDS ON A DIFFERENT MAGNETIC TAPE
TRANS FROM ONE MAGTAPE TO ANOTHER UR=6,NEW=7,NIS=N

DIMENSION NS(256),IN(300)

READ INPUT TAPE 50,10,NIS,(IN(J),J=1,NIS)

DO 100 J=1,NIS

1 READ INPUT TAPE 6,20,(NS(I),I=1,12)

IF(NS(I)=IN(J)) 2,3,2

3 READ INPUT TAPE 6,20,(NS(I),I=13,256)

WRITE OUTPUT TAPE 51,26,J

WRITE OUTPUT TAPE 51,25,(NS(I),I=1,256)

WRITE OUTPUT TAPE 7,20,(NS(I),I=1,256)

GO TO 100

2 READ INPUT TAPE 6,20,(NS(I),I=13,256)

GO TO 1

100 CONTINUE

END FILE 7

END FILE 7

10 FORMAT(40I2)

20 FORMAT(12I6)

25 FORMAT(10I8)

26 FORMAT(/I4//)

30 FORMAT(////////////////////)

END TRAMMM

PROGRAM SHIFT

WRITTEN BY E SCHÖNFELD*** ORNL **
 SHIFT SLOPE AND ORIGIN BY LINEAR INTERPOLATION
 SH IS ORIGINAL SHIFT
 AND SHC THE AMOUNT TO BE INCREASED
 F IS THE CHANGE IN THE SLOPE

```

DIMENSION Y(257),YC(257),X(257),XC(257)
1 READ INPUT TAPE 50,15,M,NOP
WRITE OUTPUT TAPE 51,15,M,NOP
READ INPUT TAPE 50,10,(Y(I),I=1,M)
WRITE OUTPUT TAPE 51,30,(Y(I),I=1,M)
DO 2 K=1,NOP
READ INPUT TAPE 50,20,F,SH,SHC
WRITE OUTPUT TAPE 51,20,F,SH,SHC
CALL SHIFY(Y,YC,M,SH,F,SHC)
WRITE OUTPUT TAPE 51,30,(YC(I),I=1,M)
WRITE OUTPUT TAPE 52,10,(YC(I),I=1,M)
2 CONTINUE
GO TO 1
10 FORMAT(12F6,0)
15 FORMAT(4I10)
20 FORMAT(4E20,10)
30 FORMAT(1X,10F8,0)
END SHIFT

```

```

SUBROUTINE SHIFY(Y,YC,M,SH,F,SHC)
DIMENSION X(257),Y(257),XC(257),YC(257)
DO 7 I=1,M
  IF(Y(I)=90000,.)7,6,6
6   Y(I)=1.0
7   XC(I)=1
  DO 8 J=1,M
    Z=J
    X(J)=Z*F+SH*(F-1,.)
8   X(J)=X(J)+SHC
  DO 60 I=1,M
    DO 40 J=1,M
      IF (XC(I)=X(J)) 50,45,40
45   YC(I)=Y(J)
      GO TO 60
40  CONTINUE
50  YC(I)=(Y(J)-Y(J-1))/(X(J)-X(J-1))
    YC(I)=Y(J-1)+YC(I)*(XC(I)-X(J-1))
    YC(I)=YC(I)/F
60  CONTINUE
    YC(I)=1.0
  RETURN
END

```

PROGRAM OUTSIM

C
 C TAKES THE RESULTS ON PUNCHED CARDS FROM THE SPECTRUM
 C RESOLUTION PROGRAM (CONCENTRATIONS AND ERRORS) AND
 C PRINTS THEM IN CONSECUTIVE ORDER
 C UP TO 16 ISOTOPES AND 10000 SAMPLES PER GROUP
 C CAN HANDLE ANY AMOUNT OF GROUPS OF DATA
 C NEEDS TWO IDENTIFICATION CARDS (COLS 2-80) IN FRONT AND
 C A CARD WITH A -10 PUNCH ENDING ON COLUMN 10 AT THE
 C END OF EACH GROUP OF DATA *****

```

DIMENSION ISOT(20),Z(20),STD(20),NAME(24)
100 WRITE OUTPUT TAPE 51,18
    READ INPUT TAPE 50,19,(NAME(I),I=1,24)
    WRITE OUTPUT TAPE 51,19,(NAME(I),I=1,24)
    WRITE OUTPUT TAPE 51,22
      DO 1 K=1,10000
        READ INPUT TAPE 50,20,ID,KK,NIS,ND
        IF (KK) 100,2,2
      2   READ INPUT TAPE 50,21,(ISOT(I),Z(I),STD(I),I=1,NIS)
        WRITE OUTPUT TAPE 51,23,ID,ND,(ISOT(I),Z(I),STD(I),I=1,NIS)
      1   CONTINUE
18  FORMAT(IH1)
19  FORMAT(IX,10A7,A2,A7)
20  FORMAT(I6,I4,6DX,2I5)
21  FORMAT(3(A8,E10.3,E8.1))
22  FORMAT(///. SAMPLE  A                               COMPOSITION AND ESTIMATED ERROR
      IS. /)
23  FORMAT( /I7,I3,4(IX,A8,E10.3,E8.1)/10X,4(IX,A8,E10.3,E8.1)/
      1      10X,4(IX,A8,E10.3,E8.1)
      2      /10X,4(IX,A8,E10.3,E8.1))
END OUTSIM

```

PROGRAM OUTPUT

```

C      WRITTEN BY E SCHONFELD *B-21 4500N ORNL JAN 1965
C
C      TAKES THE RESULTS ON PUNCHED CARDS FROM THE SPECTRUM
C      RESOLUTION PROGRAM (CONCENTRATIONS AND ERRORS ) AND
C      ARRANGES THEM IN ORDER(SORTING)
C      PUNCHES ORIGINAL DATA CARDS IN SORTED ORDER
C      THIS VERSION FOR JP TO 11 ISOT AND 700 CASES PER GROUP
C      CAN HANDLE SEVERAL GROUPS OF CASES ** START EACH ONE WITH TWO
C      IDENT CARDS (COL 2=80) IN ALPHANUMERIC TYPE ***
C      AT THE END OF JOB PUT A CARD WITH A -10 ENDING ON COL 10 ****
C      SORTS ONLY BY 6 DIGIT NUMBER
C      ISOT=NAME * Z=ANSWER * STD=STD ERROR
C      NT=NR OF CASES * KK=INDEX FOR FINISHING
C
C      DIMENSION ISOT(11,700),Z(11,700),STD(11,700),NIS( 700),ID( 700),
C      1      NAME(24),ND( 700)
C      NC IS THE NR OF COPIES PER CASE THIS TIME SET TO 2      (OUTPUT)
C      NC=1
100 READ INPUT TAPE 50,19,(NAME(I),I=1,24)      $      NT=1
      DO 1 K=1,1600
      READ INPUT TAPE 50,20,      ID(NT),KK,NIS(NT),VD(NT)
      IF (ND(NT)) 9,10,9
10      ND(NT)=1
9      IF (KK) 5,2,2
2      NT=NT+1
      NN=NIS(NT-1)
      READ INPUT TAPE 50,21,(ISOT(J,NT-1),Z(J,NT-1),STD(J,NT-1),J=1,
      NN)
1      CONTINUE
5      NQ=NT-2
      NI=NT-1
DO 4 K=1,NQ
      MIN=10000000
DO 3 J=K,NI
      IF (ID(J)-MIN) 7,7,3
7      MIN=ID(J)
      IM=J
3      CONTINUE
C      *SWITCHING*
      ITEM=ID(K)
      ID(K)=ID(IM)
      ID(IM)=ITEM
C
C      ITEM=NIS(K)
      NIS(K)=NIS(IM)
      NIS(IM)=ITEM
C
C      ITEM=ND(K)
      ND(K)=ND(IM)
      ND(IM)=ITEM
C
C      SELECTS THE LARGEST NR OF ISOTOPES FOR SWITCHING
C      IF (NIS(K)-NIS(IM)) 12,12,11
11      NN=NIS(K)

```

```

      GO TO 13
12   NN=NIS(IM)
13   DO 8 J=1,NN
      ITEM=ISOT( J,K )
      ISOT( J,K )=ISOT( J,IM)
      ISOT( J,IM)=ITEM
C
      TEM=Z( J,K )
      Z( J,K )=Z( J,IM)
      Z( J,IM)=TEM
C
      TEM=STD( J,K )
      STD( J,K )=STD( J,IM)
      STD( J,IM)=TEM
8   CONTINUE
4   CONTINUE
C   ***** NC IS THE NR OF COPIES OF EACH SAMPLE *****
      DO 40 KK=1,NC
      WRITE OUTPUT TAPE 51,18
      WRITE OUTPUT TAPE 51,19,( NAME(I),I=1,24)
      WRITE OUTPUT TAPE 51,22
      DO 6 J=1,NI
      NNN=NIS(J)
      WRITE OUTPUT TAPE 51,23, ID(J),ND(J),(ISOT(I,J),Z(I,J),STD(I,J),
      I=1,NNN)
      PJNCH 24, ID(J),NIS(J);ND(J)
      PJNCH 21,(ISOT(I,J),Z(I,J),STD(I,J),I=1,NNN)
6   CONTINUE
40  CONTINUE
      GO TO 100
18  FORMAT(IH1)
19  FORMAT(IX,10A7,A2,A7)
20  FORMAT(16,14,60X,215)
21  FORMAT(3(A8,E10.3,E8.1))
22  FORMAT(///% SAMPLE A           COMPOSITION AND ESTIMATED ERROR
      IS=/)
23  FORMAT( /17,13,4(1X,A8,E10.3,E8.1)/10X,4(1X,A8,E10.3,E8.1)
      /10X,4(1X,A8,E10.3,E8.1))
24  FORMAT(16,64X,215)
      END OUTPUT

```

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