COMPUTER PROGRAM
FOR
ANALYSIS OF GAMMA SPECTRA

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July 1974

Prepared for
Contract Number AT(11-1)-3015

ATOMIC ENERGY COMMISSION
CHICAGO OPERATIONS OFFICE

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SAMPO is a general-purpose semiconductor spectral analysis code written by J.T. Routti and S.G. Prussin.¹⁾ The code has been tested and revised over a period of years, and seems to provide a reliable and consistent procedure for analysis of a wide variety of Si(Li) and Ge(Li) semiconductor detector X-ray, γ -ray and under certain conditions, conversion electron spectra.

The procedure employed by SAMPO is termed the "photopeak" method by the program authors, because a prerequisite for analysis of spectral data is an exact mathematical representation of the photopeaks and the continua in their vicinity. The program itself is capable of determining the necessary peak shape parameters, provided the user can supply strong, "clean", singlet photopeaks in the region of interest so that the empirical peak shapes may be reduced to functional form. The general formalism presumed to describe semiconductor detector photopeaks consists of a central Gaussian with smoothly joined high and low-energy exponential tails. The peak shapes are normally found to vary continuously as a function of energy; therefore the exact shape parameters at each point in a spectrum can in principle be obtained by interpolation between points for which the standard peak shapes have been determined. The theory and method are described in detail in Ref. 1.

At present, it is necessary only that we know which functions can be performed by the program, and the limitations that presently exist in the routine.

Data can be read in any desired FORMAT, from cards and IBM-compatible magnetic tapes. For rapid, essentially "automatic" analysis of relatively simple spectra, a peak-search algorithm scans the raw data to locate statistically significant events. The program then performs peak-shape, energy, and intensity calibrations, fits the peaks found in the spectrum (FITDO), and provides complete statistical and calibration error estimates in summarizing the results.

Limitations of the routine are both quantitative and qualitative. At present, the program dimensions allow up to 1024 channels of data to be read and analyzed at one time. Up to 100 peaks can be "found" and analyzed before the "RESULT" arrays are filled and must be read out or cleared. As many as 30 each shape, energy, and efficiency calibration data points may be read into core for each analysis run. The "automatic" peak-fitting routine (FITDO) will select intervals such that up to five peaks may be fitted simultaneously. The user-controlled fitting routine (FITS) will accept multiplets containing up to six components in a single specified fitting interval.

The qualitative limitations of the code arise, as might be expected, from the form and statistical quality of the data. The user himself will quickly become familiar with the situations the program will and will not handle. Naturally, it is important to supply peak shape parameters that accurately describe the photopeaks throughout the region of interest. Given accurate peak shape parameters, the program is easily capable of resolving very close-lying multiplets that could be visually detected only with great difficulty. On the other hand, because of the quality of the fit is tested using a chi-square convergence criterion, it is not surprising that very weak lines in the vicinity of much stronger photopeaks are often overlooked by the fitting algorithm, and even if the user explicitly specifies the locations and intensities of the lines in question (FITS), a satisfactory fit to the data is sometimes obtained only after repeated "juggling" of the fitting parameters, if indeed it is obtained at all. Nevertheless, the user will find that, for most applications, the successes of the code far outnumber the failures, and the precision in analysis afforded by SAMPO will, to a large extent, render old "hand" analysis techniques obsolete. The original program was written for a CDC-6600 machine which was adapted for use on IBM-7094 at Yale University by Frederick Bernthal.

The minor errors in the Yale version were rectified and further changes were incorporated, conforming to the FORTRAN IV language convention, particularly in regard to initialization of and transfer between subroutines of common block variables. Also provisions were made to introduce new values for variables through CODEWORDS, IOFILE and PARAM. There are, however, two major changes introduced into the program. One change is the new facility to analyze batches of spectra using CODEWORDS TAPEIN and SAMPO, and the other, probably a more useful change, is an addition to the subroutine RESULT for performing decay calculations encountered in the analysis of neutron activated samples. The necessary input data for isotope identification, based on photopeak energy, can be provided along with other control cards with each spectrum or alternatively, a single data set on a direct access facility can be used repeatedly. The details are explained under the respective CODEWORDS and its application is described in the following section.

There are two different versions of the program available for analyzing 1024 Channel Spectra (this can be changed easily however) differing in their printed output of the details of analysis. PROGA output for each spectrum analyzed contains selected regions of the peak locations and background subtractions along with calculated area under each selected region compared to the spectral data read in that region of the spectrum. PROGB printed output for each selected region of the spectrum contains in addition to the output of PROGA, all the constants used in the analysis along with a graphical representation of the calculated and input spectral data.

Both PROGA and PROGB were compiled on an IBM FORTRAN H compiler using optimization option (OPT = 2) and the load modules were stored and catalogued at Boston College Computer Center. These load modules are available for use on other compatible systems while the source programs can be recompiled for

use at any other installation. The users are requested to communicate to the undersigned any other desirable modifications to the program and difficulties encountered.

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REFERENCES

1. J. T. ROUTTI and S. G. Prussin, Lawrence Radiation Laboratory Report UCRL-17672; Nucl. Instr. and Meth. 72, 125-142, 1969.

II. Illustrative Runs

The logical manner in which the analysis of a gamma spectrum proceeds is seen in the following sets of control cards for some typical runs. The program will recognize any legal data input cards; it obviously cannot perform a SHAPEDO function until the spectral data have been read in. Similarly, FITDO must be preceded by PEAKFIND so that the program knows the approximate locations of the peaks it is being asked to fit. In general, the program will ignore any unreasonable request, and proceed to the next CODEWORD data card. The common FORMAT for all data input cards is (A10,6E10.0) except the DATE and comments card read in the FORMAT (4A4,14A4), and which is required every time the program is invoked.

The complete analysis of a gamma spectrum can be accomplished in a number of ways as indicated in the first 3 runs. The last run, RUN 3, is not usually required except in cases of complex spectra with unresolved or barely resolved multiplets; under normal conditions the calibration data obtained in RUN 1 can be utilized in the same run or can be read in on cards and used in later runs for the analysis of spectra acquired under the same conditions as the standard spectrum. The latter method is indicated in RUN 2 in which additional detector efficiency data is also included.

A number of simple spectra can be analyzed as a batch using the CODEWORDS SAMPO or TAPEIN. The spectral data can be provided either on cards or on a magnetic tape with CODEWORD SAMPO while spectral data are read from a tape with CODEWORD TAPEIN. The analysis of spectra in batches using these two CODEWORDS is shown in RUN 4.

The card output from the analysis of spectra can be used with the CODEWORD FITIN as seen in RUN 5, to recalibrate peak energies and intensities using new energy and detector efficiency calibrations, to apply decay corrections to the various photopeaks found, and to perform ppm calculations of the parent isotopes in the analysis of gamma spectra of neutron activated samples. These latter calculations are based on the identification of the radioactive isotope from photopeak energies. It is, however, possible to combine RUN 4 and RUN 5 in to a single run when recalibrations of energies and/or detector efficiencies are not needed or anticipated in which case the necessary information is supplied following the cards for spectral analysis. A typical control card setup for the analysis of a batch of spectra using the previously determined calibration and isotope identification information libraries is shown in RUN 6.

The objective of the first run is to determine peak shape parameters and locations of peaks that will be sensed by the automatic peak finding routine. The fitting intervals that will be later selected by the program will be obtained so that the user can avert possible problems that may arise when the actual fitting is performed in later runs. In the event that fitting intervals are not critical, which is generally the case with the peaks located far apart in the spectrum, the peak shape parameters and energy calibration points determined in this run can be used to analyze additional spectra. The control cards appropriate for this run are as follows:

RUN 1 Control cards for spectral data on cards or magnetic tape

Col. 1	11	21	31	41	51	61	71
CODEWORD	WHAT(1)	WHAT(2)	WHAT(3)	WHAT(4)	WHAT(5)	WHAT(6)	
DATE of Analysis (col. 1 - 16) and comments (if any) (col. 17 - 72)							
OPTIONS	2.	2.					

A DATAIN $(\frac{1}{2})^1$
 (12X,F4.0),130(F4.0))⁵

B DATAIN 0. 0. ³ 101. -1. ⁴
 1. 0.
 2. 1.
 2. 2.
 (120(2X,F4.0),130(F4.0))⁵

5/74 THIS CARD IDENTIFIES THE DATA AND SUPPLIES NUMBER OF CHANNELS 1024⁶

SHAPEDO 110. 90. 120. 1.
 C ENDO 165.1 0.2 1.
 SHAPEDO 352. 339. 366.
 C ENDO 528.4 0.2
 SHAPEDO 722. 708. 741.
 C ENDO 1083.4 0.2
 PEAKFIND
 FITTEST

D CALDATA 2. 2.

E DATAIN Appropriate parameters depending on card or tape input ANAL⁷
 (Spectral Format card if required)
 SPECTRAL DESCRIPTION CARD

F PEAKFIND
 PEAKADD 84. 233. 524. 528.
 PEAKDROP 526.
 F FITDO
 F RESULT 1.
 STOP

- A,B One or the other DATAIN card set is required. Set A for spectral data on cards and set B for spectral data on magnetic tape
 C These cards are required only when the preceding peak is used for energy calibration

- D This card prints out the shape parameters and energy calibration points determined
- E The spectral data read in by this card are analyzed using the calibration constants determined by above cards. Any number of spectra can be analyzed by reading in the spectral data and the necessary CODEWORDS
- F These cards can be avoided as in footnote 7
- 1 One value must be indicated for card input of spectral data
- 2 If the value in footnote 1 is 2, spectral data FORMAT must be specified on this card
- 3 If this value $\neq 0$ spectral data are reproduced on Unit 3 for which the necessary JCL card must be provided. If this value is 2 the spectral data FORMAT must also be provided on the next card
- 4 Control for print out of spectral data. For a significance of this value refer to CODEWORD DATAIN (magnetic tape) parameters
- 5 This card is required only when the value in footnote 3 is 2
- 6 The default value is 1024. This value need not be coded when spectral data consist of 1024 channels
- 7 This parameter inserts all the cards marked F. If CODEWORDS like PEAKADD, PEAKDROP, PEAKLIST are not required this parameter is adequate for a complete analysis of the spectrum, otherwise this parameter should be avoided.

The user has now obtained standard peak shapes for the spectrum, as well as an indication of how the program will try to analyze spectra. We shall assume also that the detector efficiency data is known. The actual analysis of spectra might then proceed as follows:

RUN 2: Automatic fitting of peaks in spectra

Col. 1	11	21	31	41	51	61	71
CODEWORD	WHAT(1)	WHAT(2)	WHAT(3)	WHAT(4)	WHAT(5)	WHAT(6)	
Date and comments card							
OPTIONS	2.	2.	2.				
SHAPEIN	100.	3.5	4.4	1.8	1.		
SHAPEIN	500.	3.8	4.6	2.1			
SHAPEIN	700.	4.0	4.8	2.25			
SHAPEIN	850.	4.1	4.95	2.4			
SHAPEIN	1000.	4.3	5.1	2.5			
ENIN	109.952	88.95	0.1		1.		
ENIN	352.374	175.45	0.15				
ENIN	704.75	350.95	0.3				
EFIN	100.	0.0325	5.0		1.		
EFIN	500.	0.0115	7.5				
EFIN	1000.	0.005	10.				
DATAIN	Appropriate parameters depending on card or tape input						ANAL
	(Spectral Format card if necessary)						
6/74	SPECTRAL DESCRIPTION CARD						
DATAIN	Appropriate parameters depending on card or tape input						ANAL
	(Spectral Format if necessary)						
6/74	SPECTRAL DESCRIPTION CARD						
.							
.							
.							
STOP							

The data are now fitted and may be inspected for regions where the analysis is not satisfactory. The punched card output allows the user to carry out any further manipulations with regard to energy and efficiency calibration and decay corrections to photopeaks and ppm calculations at a later time without having to repeat the time-consuming fitting process. This is a rather valuable safeguard against possible calibration errors. Next, the user may wish to "clean up" one or more unsatisfactory fits as follows:

RUN 3 -- "Cleanup run" control cards

Col. 1	11	21	31	41	51	61	71
CODEWORD	WHAT(1)	WHAT(2)	WHAT(3)	WHAT(4)	WHAT(5)	WHAT(6)	
Date and comments card							
:	etc., same as RUN 2						
:							
EFIN	1000.	0.005	10.				
DATAIN Appropriate parameters depending on card or tape input (Spectral Format card if necessary)							
SPECTRAL DESCRIPTION CARD							
FITS	2.						
3	507	545	519	525	529		
6	802	865	820	828	837	850	855
CALDATA	2.	2.	2.				
RESULT							1.
STOP							

In the above illustrative runs each spectrum is treated individually with the appropriate CODEWORDS following the reading in of the spectral data. However, as indicated in RUN 2 a routine analysis of a batch of spectra can be accomplished without the need of using the same CODEWORDS with each spectrum. The use of this facility is illustrated in RUN 4.

RUN 4: Batch analysis of spectra

Col. 1	11	21	31	41	51	61	71
CODEWORD	WHAT(1)	WHAT(2)	WHAT(3)	WHAT(4)	WHAT(5)	WHAT(6)	
DATE and comments card							
:	etc., same as RUN 2						
:							
EFIN	1000.	0.005	10.				

IOFILE					1. ¹		ANAL
SAMPO	1. ²					1. ³	
DATAIN Appropriate parameters depending on card or tape input (Spectral Format card if necessary)							
SPECTRAL DESCRIPTION CARD							
DATAIN Appropriate parameters depending on card or tape input (Spectral Format card if necessary)							
SPECTRAL DESCRIPTION CARD							
DATAIN							
:							
:							
:							
:	etc.,						

TAPEIN	3. ⁴		10. ⁵				
Tape description card. Contents used as spectral description when digital print out is not requested (WHAT(3) = 0.)							
A	1001.1000.1003.2000.1009.4000.						

CALDATA	2.	2.	2.				
STOP							

A	Tag number and counting times of spectra to be analyzed.						
1.	Average CW parameter used to determine the peak region.						
2.	Number of spectra to be analyzed, equal to the number of DATAIN cards						

3. RESULT arrays reset (if number of peaks found is ≤ 100) after this many spectra. Should be less than or equal to the value in footnote 2.
4. Number of spectra to be analyzed. Should be less than or equal to 20.
5. (This value - 10.) is the same as WHAT(6) of DATAIN by magnetic tape used for digital print out control.

The user may now want to change the energy calibration, or examine a polynomial fit to energy or efficiency calibration, normalize the relative intensities to a specific peak, apply decay corrections to various photopeaks and calculate the concentrations of nucleides which through neutron activation give rise to various photopeaks. These functions can now be performed using FITIN option together with the punched card output from the previous runs. This is shown in RUN 5.

RUN 5: Use of card output of analysis with FITIN option

[illegible]

RUN 5 cont.

Col.	1	11	21	31	41	51	61	71
	CODEWORD	WHAT(1)	WHAT(2)	WHAT(3)	WHAT(4)	WHAT(5)	WHAT(6)	
C	RESULT		2. ¹	2. ²			10. ³	
	5/74	(₁) ⁰ 4	2. E+13 8.456	210.	8.	1.	11. ⁵	2. ⁶ 0. ⁷
								1. 2.
D	Fe 59	2 ⁸	1.1 E-24 3.	1094.	58.	0.33		
			192. 2.8 1099.56.2 1292.43.5					

.
. .
. .
. .
. .
. .
. .

E FITIN

.
. .
. .

RESULT

Sample-Flux card

Element constants cards.

STOP

A New set of calibration points

B Card output from spectrum analysis

C Sample-Flux card

D Element constants cards. Should be added if the value of footnote 5 is 0

E Same as starting at B

1,2 Energy efficiency recalibration request

3 Number of element to be searched for using element constants cards

4 If this value is 1 the element constants cards used are printed

- 5 Unit number for reading in the element constants cards from a library created earlier. If this value is 0 element constants cards should follow sample Flux card
- 6 Energy tolerance for identification of isotopes based on photo-peak energy. Default value is 3.0 keV.
- 7 If this value is not 0 detector efficiency as a function of energy is created. A value of 1. creates absolute efficiency using true ppm of the isotope in the sample, otherwise relative efficiencies are created and stored for print out by CALDATA CODEWORD.

The use of the FITIN option shown in RUN 5 can be carried out along with the regular analysis of spectra when the energy or efficiency recalibrations are not needed or anticipated. This method of analysis in a single step is shown in RUN 6.

RUN 6: Complete analysis of a batch of spectra including decay corrections.

Col.	1	11	21	31	41	51	61	71
	CODEWORD	WHAT(1)	WHAT(2)	WHAT(3)	WHAT(4)	WHAT(5)	WHAT(6)	
	DATE and comments card							
	IOFILE	1. ¹				1.		ANAL
	PARAM						15. ²	
	SAMPO	1.					1.	
A	DATAIN Appropriate parameters depending on card or tape input (Spectral Format card if necessary)							
	SPECTRAL DESCRIPTION CARD							
	Sample Flux card (see RUN 5 or card marked B)							
	TAPEIN	8.					15. ²	
	Analysis of 8 spectra on tape xxx in filexxx							
	100.400.125.800.133.200.150.1000.255.4000.560.1000.680.2000.840.8000.							
	5/74	2.	E+13	8.456	210.	8.	1.	11. ³
	:	Other sample Flux cards						
	:							
	STOP							

- A Any number of DATAIN card sets can be added
- B This is an example of a sample Flux card. The total number of such cards should be equal to the number of spectra analyzed, WHAT(1) of CODEWORD TAPEIN.
 - 1 The calibration data for shapes, energy, and efficiency are read on Unit 1 from a library created earlier.
 - 2 This value is the number of elements to be searched among the peaks found
 - 3 The element constants are read on Unit 11 from a library already created

The analysis of one or a number of spectra is now complete and unless some peaks are not identified or fitted all the necessary information about various photopeaks in a spectrum is contained in the card output. In general RUN 6 can be considered a standard method of analysis when once the shape parameters are determined and included in a library of energy and efficiency calibrations along with another library of constants for anticipated elements. Thus, by establishing a standard method of spectral analysis and creating some procedures the number of cards to be punched for each run can be minimized and a routine analysis of gamma spectra achieved efficiently and economically.

III. Index of Program Commands

The program options are listed on the following pages according to the most likely programming sequence, i.e. OPTION is first, STOP is last. These two cards will occupy those positions in the data input deck, following the DATE and comments card in FORMAT (4A4, 14A4). For convenience, the program options are also indexed below alphabetically.

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OPTIONS

Specify internal calibrations and options

- WHAT (1) Specifies shape calibration, initialized at 2
- = 1. Use Arrays stored in program DATA statement
 - = 2. Use arrays generated or read in
- WHAT (2) Specifies energy calibration initialized at 2
- = 0. No energy calibration
 - = 1. Use arrays stored in DATA statement for linear interpolation
 - = 2. Use arrays generated or read in for linear interpolation
 - = 3. Use polynomial stored in DATA statement
 - = 4. Use polynomial generated or read in
- WHAT (3) Specifies efficiency calibration initialized at 2
- = 0. No efficiency calibration
 - = 1. Use arrays stored in DATA statement for linear interpolation
 - = 2. Use arrays generated or read in for linear interpolation
 - = 3. Use function stored in DATA statement
 - = 4. Use function generated or read in
- WHAT (4) Specifies when linear background instead of parabolic is used. Whenever the fitting interval measured in units of CW parameter, initialized at 15., only linear background is used.
- = 0. Use existing value for this parameter
 - ≠ 0. Change the parameter to WHAT (4).

DATAGRAPH

		Make printer graph of the spectrum
WHAT	(1) = 0.	Semilogarithmic scale
	≠ 0.	Linear scale
WHAT	(2)	Plot every WHAT (2) channel, if blank, every channel
WHAT	(3)	Starting channel, if blank, the first channel
WHAT	(4)	Stopping channel, if blank, the last channel
WHAT	(5)	Channels in each subdivision, if blank, 100 channels

DATAIN (card input)

		Read indicative and spectral data on cards.
WHAT	(1) = 0.	Search and read in the spectrum NAME from input tape (User must supply appropriate tape-reading subroutine).
	= 1.	Card input, spectral data in FORMAT (10 F 7.0). Maximum number of channels presently 1024.
	= 2.	Card input, spectral data in FORMAT specified on next card, for example (5(5x, F 8.0))
WHAT	(2) = 0.	Erase previous spectrum
	≠ 0.	Add previous spectrum multiplied by WHAT (2) to new spectrum
WHAT	(2) = 0.	Erase previous spectrum
	≠ 0.	Add previous spectrum multiplied by WHAT (2) to new spectrum
WHAT	(3) = 0.	Nothing
	≠ 0.	Multiply new spectrum by WHAT (3) (before addition)

With card input, DATAIN (and FORMAT card) must be followed by one card containing the indicative data as follows:

-run number, columns 1-6, alphanumeric-indicative NAME data, columns 7-66, alphanumeric-number of channels columns 76-80, integer. The spectral data must follow this card.

DATAIN (magnetic tape)

This subroutine is for reading spectral data from IBM compatible magnetic tapes created on a KENNEDY tape drive. The spectral data are written either as 256 or 1024 channel blocks. Each block of data has two, six digit words in front and the first word contains a four digit tag number.

WHAT	(1) = 0.	Read in spectral data from magnetic tape.
WHAT	(2) = 0.	Read spectral data, in standard format (2X, 14, 16, 128F6.0, 128F6.0, 128F6.0, 128F6.0)
	= 1.	Reproduce spectral data read on Unit 3 in standard format.
	= 2.	Read spectral data according to Format specified on next card and reproduce spectral data read on Unit 3 in standard format.
WHAT	(3) =	Tag number of spectrum to be read.
WHAT	(4) = 0.	Erase previous spectrum.
	≠ 0.	Multiply previous spectrum by WHAT (4) and add to new spectrum.
WHAT	(5) = 0.	Same as WHAT (5) = 1. (No data multiplication).
	= 0.	Multiply new spectrum by WHAT (5) (before addition to old spectrum, if specified).
WHAT	(6) = -1.	Digital data NOT Printed 256 Channel blocked unput.
	= 0.	Digital data Printed.
	= 1.	Digital data NOT Printed 1024 Channel blocked input.
	= 2.	Digital data Printed.

SHAPEDO

Perform shape calibration fit. This should be done using strong single lines in the spectrum under analysis or data taken under identical conditions. The resulting shape parameters will be stored and interpolated to fit all peaks in the spectrum. These parameters need to be computed only once for each experimental set-up; the values will remain unchanged till specified, and can be read in rather than recomputed for later runs.

WHAT (1) Approximate center channel of the calibration peak

WHAT (2) Lower limit of fitting interval

WHAT (3) Higher limit of fitting interval

In specifying fitting interval include enough channels to cover both tails, but do not over-extend or include fluctuations due to other peaks.

WHAT (4) = 0. Nothing
= 1. Use this peak for energy calibration by adding ENDO card with energy and calibration error after SHAPEDO card.
= 2. Use this peak for efficiency calibration by adding EFDO card with the peak area and calibration error.
= 3. Energy and efficiency calibration as above

WHAT (5) = 0. Add resulting shape parameters to the present table of parameters
= 1. Start new shape parameter table with the resulting parameters

WHAT (6) Initial guess for CW-parameter, if blank set to 1.8 (2.355 CW = FWHM).

SHAPEIN Read in and store shape parameters computed previously

WHAT (1) Exact peak center in channels

WHAT (2) CL-parameter specifying the lower tailing

WHAT (3) CH-parameter specifying the higher tailing

WHAT (4) CW-parameter specifying peak width ($2.355 \text{ CW} = \text{FWHM}$)

WHAT (5) = 0. Add these values to the present table
 = 1. Start new table with these values

ENDQ Assign energy calibration value for linear interpolation to a peak fitted under FITDO or FITS

WHAT (1) Approximate channel location, accuracy tolerance 3 channels or as specified by WHAT (4)

WHAT (2) Energy in keV

WHAT (3) Calibration error in keV

WHAT (4) = 0. Use previous accuracy tolerance, initialized at 3.

WHAT (5) = 0. Add values to existing energy calibration table
 = 1. Start new table with these values

ENIN Read in energy calibration point to be used through linear interpolation (see OPTIONS)

WHAT (1) Exact channel location

WHAT (2) Energy of channel WHAT (1) in keV

WHAT (3) Calibration error in keV

WHAT (5) = 0. Add values to existing energy calibration table
 = 1. Start new table with these values

ENFITDO

Perform a polynomial fit to the points read in under ENDO or ENIN. The resulting curve may be used for subsequent energy determinations if specified on OPTIONS card. Calibration error will be the same as in linear interpolation.

WHAT (1) Number of terms in the polynomial fit, that is 1 + degree of polynomial

ENFITIN

Read in polynomial coefficient and calibration error point

What (1) Value of polynomial coefficient

WHAT (2) Energy value for calibration error point

WHAT (3) Calibration error in kev

WHAT (4) Number of the coefficient, that is degree + 1.
If 1, start a new coefficient list

WHAT (5) = 0. Add energy calibration error point to existing list
= 1. Start new energy calibration error list

EFDO

Assign efficiency calibration value for linear interpolation to a peak fitted under FITO or FITS

WHAT (1) Approximate energy of the point, accuracy tolerance 3 keV or as specified by WHAT (4)

WHAT (2) Number of disintegrations corresponding to that energy peak (peak area)

WHAT (3) Calibration error in per cent

WHAT (5) = 0. Add values to existing efficiency calibration table
= 1. Start new table with these values

EFIN

Read in efficiency calibration point to be used through linear interpolation

- WHAT (1) Energy of calibration point
- WHAT (2) Efficiency
- WHAT (3) Calibration error in per cent
- WHAT (5) = 0. Add values to existing table
= 1. Start new table with these values

EFFITDO

Perform a functional fit to the points read in under EFDO or EFIN. The resulting curve may be used for subsequent energy determination if specified on OPTIONS card. Calibration error will be the same as in linear interpolation. The function used is of the following form

$$\text{Efficiency} = C_1 (E^{C_2} + C_3 e^{C_4 E})$$

where C_1 , C_2 , C_3 , and C_4 are parameters to be determined and E is energy in keV

- WHAT (1) Initial guess for parameter C_1

Note: This program option does not seem to be very satisfactory, except in regions where the efficiency function is essentially linear, hence deleted in PROGA

EFFITIN

Read in parameter for functional fit above and calibration error point.

- WHAT (1) Energy value for calibration error point in keV.
- WHAT (2) Value of the parameter
- WHAT (3) Calibration error in per cent
- WHAT (4) The index of the parameter, that is 1, 2, 3, or 4
- WHAT (5) = 0. Add calibration error pair to existing list
= 1. Start new calibration error list with these values

EFFITADJ

Adjust the coefficient C_1 in the functional form stored to data or generated by EFFITDO or EFFITIN

- WHAT (1) Energy of adjustment point
- WHAT (2) Efficiency at that energy
- WHAT (4) = 1. Adjust parameters stored in program DATA statement
= 2. Adjust parameter generated

PEAKFIND Search and list statistically significant peaks. Maximum number, 100 per data block.

WHAT (1) Starting channel, if blank, channel 50

WHAT (2) Stopping channel; if blank, last channel

WHAT (3) Significance limit for listing the peaks, if blank use the existing value, initialized at 2

WHAT (4) Significance limit for fitting the peaks, if blank, use the existing value, initialized at 5

WHAT (5) Average value for CW-parameter, if blank use the value obtained in shape calibration (2.355 CW = FWHM)

PEAKADD Add peak to the list of found peaks. Use this option to correct the list of found peaks during the second run. The search routine should be done (PEAKFIND) before this

WHAT (I) I = 1,6 The channel numbers of the peaks to be added, in any order

PEAKDROP Drop peak from the list of found peaks. See comments regarding PEAKADD.

WHAT (I) I = 1,6 The channel numbers of the peaks to be dropped

PEAKLIST Print the corrected list of peaks found

FITTEST Determine and print the channels limiting the fitting intervals and the peaks included for each fit. The fitting is not performed.

FITIN

Read in fitting results from punched cards.
The FORMAT is the same as used in punching
results. (Option WHAT (4) of RESULT)

WHAT (1) Number of peaks to be read in
WHAT (2) $\neq$ 0. Read data identification card next
WHAT (5) = 0. Add results to existing list of fitted peaks
 = 1. Start new list of fitted peaks

This card is followed by WHAT (1) cards with

Columns 2-8 F8.3 Energy
 15-23 F9.3 Exact channel location
 30-35 F6.3 Energy error
 36-46E11.4 Peak area
 53-63E11.4 Peak intensity
 69-74 F6.2 Intensity Error
 75-80 A6 Run number

FITSLINEAR

Perform fast linear fit of peaks specified on
cards, according to the options described under
FITS

FITLINEAR

Perform fast linear fit of peaks found (similar
to FITDO)

FITDO

Perform complete nonlinear fits of peaks found by the search algorithm. Selection of the fitting intervals and the peaks included in each fit is done automatically as in FITTEST. The results include the exact channel locations, peak area, energies, intensities, and statistical and calibration errors for each peak. The energy and efficiency calibration performed as specified on OPTIONS card.

- WHAT (3) = 0. Initial guesses for peak search, peak fitting parameters, comparison of FIT and other details are NOT printed
- = 4. Comparison of FIT is printed
- = 5. All details of analysis are printed

FITS

Perform complete nonlinear fits of peaks specified on the following cards. The computation is the same as performed under FITDO, only complete control over the selection of intervals and peaks is possible. Special weighting and/or initial guess for peak amplitudes may be used.

- WHAT (1) = Number of special cases specified by following WHAT (1) cards
- WHAT (2) = 0. Normal weighting, that is $1/YDATA$
- = 1. Special weighting, $1/YDATA^2$
- = 2. Special weighting as read in for each data point specified in FORMAT (8 E 10.0)
- WHAT = 0. Automatic initial guess
- = 1. Initial guess read in for each peak amplitude in FORMAT (8 E 10.0) after the card specifying the channels
- WHAT (5) = 0. Add results to existing list of fitted peaks
- = 1. Start new list of fitted peaks with these results

The FITS card is followed by cards specifying WHAT (1) cases in FORMAT (16I5) as follows:

1.	column 1-5	Number of peaks in the fit
2.	6-10	Channel defining the lower limit of fitting interval
3.	11-15	Channel defining the higher limit of fitting interval
4.	16-20	Control of the parabolic correction in the background polynomial, if blank assigned to the peak channel for single peaks and the centroid of fitting interval for multiplets
5.	21-25	Channel in first peak in the fit
6.	26-30	The other peaks in the fit
7.	31-35	.
.	.	.
.	.	.
.	.	.

etc.

If special weighting (WHAT (2) = 2.) or initial guess (WHAT (3) = 1.) are specified, they must follow each case, both in FORMAT (8 E 10.0). Up to 200 numbers may be specified in FORMAT (16I5) and stored to be reused under FITREPEAT

FITREPEAT

Repeat the cases specified by last FITS card. Only channel numbers read in under FORMAT were stored, not the special weighting or initial guesses. WHAT (2), WHAT (3), and WHAT (5) have the same meaning as under FITS.

FITSTRIP

Subtract the last fit from spectrum

IOFILE

WHAT (1) $\neq$ 0. INPUT Unit Number (Initialized at 5 in BLOCK DATA)

WHAT (2) $\neq$ 0. IOUTAP Unit Number (Initialized at 6 in BLOCK DATA)

WHAT (3) $\neq$ 0. PKDEV (Significance for Peak Search, initialized at 2 in MAIN)

WHAT (4) $\neq$ 0. PKFIT (Significance for peak fitting, initialized at 5 in MAIN)

WHAT (5) $\neq$ 0. CW (Parameter to determine peak region for background and fitting the peaks)

WHAT (6) $\neq$ 0. IPUNCH Unit Number (Initialized at 7 in BLOCK DATA)

Columns 71-74 RNM - Used when spectral data are read by DATAIN codeword. Initialized BLANK, $\neq$ Blank - PEAKFIND = ANAL, PEAKFIND and FITDO

RESULT

Tabulate fitting results accumulated and compute relative intensities in analysis of the spectrum

WHAT (1) Approximate channel of the reference peak in relative intensity calculations

= 0. Use biggest peak as reference

$\neq$ 0. Use peak in channel WHAT (1) as reference for relative intensities

WHAT (2) = 0. No new energy determination

$\neq$ 0. New energy determination using OPTION as specified by WHAT (2), (see OPTIONS)

WHAT (3) = 0. No new intensity determination

$\neq$ 0. New intensity determination using OPTION as specified by WHAT (3), (see OPTIONS)

WHAT (4) = 0. No punch requested

= 1. Write results on punch tape for punched card output

FORMAT (F9.3, F5.3, F9.3, F6.3, E11.4, F6.2, E11.4, F6.2, E11.4, A6)

WHAT (5) $\neq$ 0. Counting Time (if zero set to 1.)

WHAT (6) = 0. Decay corrections NOT required

$\neq$ 0. # Elements provided as input for Decay Corrections. To be followed by ONE card per spectrum containing SAMPLE-FLUX etc. information and TWO cards per element; one card containing element constants and the other with information of peak energies and intensities in FORMAT (16 F 5.0). Max. of 8 peaks per element. SAMPLE-FLUX and ELEMENT CONST. cards are in the format (A8,I2,E10.3,5F10.0,2F5.0). The variables for Sample-flux card are: SAMPLE, IPT, FLUX, SUNITS, TDECAY, TIRR, DOG, TP, ETEST, SNO. These variables are self explanatory. The names that are not so evident are:

IPT = 0. Table of Results to be printed.

$\neq$ 0. Table of Results NOT to be printed

SUNITS Sample wt Mg. if Zero set to 1.

DOG Gamma Intensity = (Gamma Intensity READ) $\times$ DOG.

TP $\neq$ 0. Unit number for INPUT of Element Constants.

= 10. or 12. Read Element Constants to be printed

= 10. Element constants to be used once

10. Element constants to be used repeatedly. (Should be in a library)

ETEST $\neq$ 0. E for peak identification. Initialized at 3 keV.

SNO $\neq$ 0. Detector efficiency to be stored (can be printed out by CALDATA)

= 1. Absolute efficiency of the detector. PPM of the isotope in the sample should be provided

= 2. Relative efficiency of detector.

The Variables of Element Constants Are:

ELEMENT, IREF, SIGMA, PKS, THALF, ATWT, PISO, PPU, PPUER

IRFF = # of the peak in the following list to be used as reference.

PKS = # peaks in the following card.

ATWT = At. WT of Parent isotope

PISO = Percent natural abundance of Parent

PPU = PPM of Parent in sample (if = 0, set to 1)

PPUER = Percent error in ppm of isotope in sample

RESET

WHAT (1) = 1. Clear list of Peaks Found (NUMP = 0)

WHAT (2) = 1. Clear list of Peaks to be Fitted (NUMP = 0)

SAMPO

For batch Analysis - individual spectral data input by DATAIN

WHAT (1) = # Spectra to be searched for peaks if the number is less than 100 and NUMP is not reset.

WHAT (2) ≠ 0. PKFIT (Significance for peak fitting, initialized at 5 in MAIN)

WHAT (3) (IPG) determines the details of printout of peak fitting (See WHAT (3) of FITDO)

WHAT (4) IPCH = 1 + INT (WHAT (4)) determines punched output.

WHAT (5) = CW. Parameter for determining peak range. (see WHAT (5) of IOFILE)

WHAT (6) ≠ 0. ISET (RESET NUMP and NUMP after ISET SPECTRA.)

= 0. Reset results after each spectrum analysis.

TAPEIN

For batch analysis of spectra

Must be followed by tape description card (First 52 columns or less)

Used as spectral identification for all spectra when digital printout is NOT requested by WHAT (3)

WHAT (1) # spectra to be analyzed as a batch (20.)

WHAT (2) REF peak channel - (Same as WHAT (1) of RESULT)

WHAT (3) = 0. Digital printout NOT required
(WHAT (3) - 10) = WHAT (6) of DATAIN (magnetic tapes)

WHAT (4) = 0. Punched card output required
= 1. Punched card output NOT required

WHAT (5) = CCW (Average parameter for FWHM, not required if
SHAPEIN data are read in)

WHAT (6) = 0. Decay corrections NOT required
≠ 0. # Elements provided as input for Decay Corrections
(Same as WHAT (6) of RESULT)

CALDATA

Print data used for shape, energy, and efficiency calibration

WHAT	(1)	Specifies shape calibration requested
	= 0.	Print no data
	= 1.	Print arrays stored in program DATA statement
	= 2.	Print arrays read in or generated
WHAT	(2)	Specifies energy calibration requested
	= 0.	Print no data
	= 1.	Print arrays stored in DATA statement for linear interpolation
	= 2.	Print arrays read in or generated for linear interpolation
	= 3.	Print coefficients stored in DATA statement for polynomial curve
	= 4.	Print coefficients read in or generated
WHAT	(3)	Specifies efficiency calibration requested
	= 0.	Print no data
	= 1.	Print arrays stored in DATA statement for linear interpolation
	= 2.	Print arrays read in or generated for linear interpolation
	= 3.	Print parameters of the functional fit stored in DATA statement.
	= 4.	Print parameters read in or generated for functional fit.
STOP		Terminate computations and call exit.