A CODE TO UNFOLD Ge(Li) SPECTROMETER POLYENERGETIC GAMMA PHOTON EXPERIMENTAL DISTRIBUTIONS

July 1970

Prepared by

J. J. Steyn
and
U. Born

For

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, California

NUS CORPORATION
4 Research Place
Rockville, Maryland 20850
CODE CUGEL

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CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CALIFORNIA

NUS CORPORATION
4 Research Place
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Approved: E. A. Saltarelli
Vice President and Technical Director
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SUMMARY

A FORTRAN code has been developed for the UNIVAC-1108 digital computer to unfold lithium-drifted germanium semiconductor spectrometer polyenergetic gamma photon experimental distributions. It was specifically designed to analyze the combination continuous and monoenergetic gamma radiation field of radioisotope volumetric sources. The code generates the detector system response matrix function and applies it to the monoenergetic spectral components discretely and to the continuum iteratively. It corrects for system drift, source decay, background, and detection efficiency. Results are presented in digital form for differential and integrated photon number and energy distributions, and exposure dose.
1. INTRODUCTION

This report presents a description of and the user requirements for, code CUGEL—a digital computer code to unfold semiconductor spectrometer polyenergetic gamma photon experimental distributions developed for the JET PROPULSION LABORATORY under Contract No. 952706. Code CUGEL, written in the FORTRAN V language for the JPL UNIVAC-1108 digital computer, is a very much modified and redesigned version of code CUPED which was developed under contracts NAS5-10133 and NAS5-10337 for NASA-Goddard Space Flight Center (1-4). The experimental distributions which the code has been specifically developed to analyze, are those recorded by the germanium (lithium-drifted) Ge(Li) semiconductor detector coupled to a multichannel pulse-height analyzer and exposed to the continuous and line energy photons emitted by radioisotope volumetric sources.

The code can either read or generate the detector system response function matrix and apply it to unfold the pulse-height analyzer distributions to determine differential and integrated photon number and energy distributions, and exposure dose. The response matrix generation procedure relies on the spectra of standard radioisotopes such as Cd$^{109}$, Ce$^{139}$, Hg$^{203}$, Sr$^{85}$, Cs$^{137}$, Nb$^{95}$, Mn$^{54}$, Zn$^{65}$ and Co$^{60}$. The standard spectra are normalized with respect to photopeak pulse-height and area, and their photopeaks subtracted to obtain normalized Compton continua. The response matrix vectors are determined at each energy by interpolating the normalized continua and computing the associated Gaussian photopeaks. The thus interpolated vectors are redistributed in pulse-height to correspond to the detector system energy response and to satisfy the requirements of the spectra to be unfolded. Quadratic interpolation of the normalized continua is carried out by a specifically developed 'Method of Parts', described in this report.
Code CUGEL applies the response function either iteratively or discretely depending on whether the unknown is either a continuous spectrum, a complex spectrum consisting of a limited number of photopeaks or a spectrum consisting of a continuum-plus-photopeaks. The code determines the detector incident photon lines in the unknown spectra by photopeak analysis. The corresponding photopeak associated Compton continua are determined by an interpolation of the standard Compton continua. The thus determined photopeak-plus-continuum spectra are then subtracted to leave, ideally, either a continuous or zero residual spectrum. Continuous and residual spectra are iteratively unfolded according to the matrix inversion technique of Scofield $^{(5-8)}$, to determine detector-incident continuous photon spectra. The total incident gamma photon spectrum is determined as the sum of the line and continuous components.

The code corrects for partial photon energy deposition in the Ge(Li) detector through the application of the response function matrix. It corrects for the number of photon interactions in the detector crystal and for absorptions by the crystal cladding materials, interposed absorbers such as aluminum and the air medium between the source and the detector active region. In addition, it corrects for primary source decay, pulse-height drift and natural background.
2. CODE DESCRIPTION

2.1 INTRODUCTION

Code CUGEL is written in the FORTRAN V compiler language for the JPL UNIVAC-1108 digital computer. It was designed to run under the Executive 8 monitor system at the Jet Propulsion Laboratory. Input data are read from card-to-tape - - - TAPE 5, digital output is written on tape for print out - - - TAPE 6. The code calls only standard library subroutines, such as transcendental functions. Although CUGEL is designed for the UNIVAC-1108 it may be readily adapted to CDC and IBM machines. It has a total word size requirement of less ~ than 65000.

The code consists of a main control program and thirty subprograms. A subprogram glossary is given in Appendix I, in alphabetic name order, and a code FORTRAN punch card deck listing in Appendix II. Appendix III consists of a sample input card deck listing and Appendix IV of a program output listing corresponding to the input given in Appendix III: the execution time for the sample data was approximately 70 seconds with compile and loading time being approximately 45 seconds.

The logic and function of the main program, referred to as MAIN, and its subprograms are discussed in Section 2.2, in some detail. Those subprograms not discussed are considered as being adequately described in either Appendix I or references (1) through (4). The user is also referred to these same references for the theoretical bases of the precursor code, CUPED. The constants required by the code are explained in Section 2.3. Reference to this Section will allow the user to make changes as necessary, in for example, the relationship of such as the detector system photopeak resolution function. The general logic of code CUGEL is discussed
in Section 3.1. The code input is detailed in Section 3.2, and the output is
defined in Section 3.3. FORTRAN names and variables are shown capitalized
in what follows, with 'zero' and 'oh' thus: 0, Ø.

2.2 CODE LOGIC

2.2.1 MAIN PROGRAM

The main program was designed to execute data input and output opera-
tions, many of them under initially input option signals, and provide the
control connectivity for the hierarchy of thirty subprograms presented in
Figure 1. Figure 2 shows a simplified flow diagram of the main program;
the called subprograms are:

   RESFUN   GANE   DEC   DISCRT
   SØLN   DECAY   GEØMTR   DETECT

Subprogram RESFUN is called by MAIN to generate and return the detector
system response matrix and the associated vectors relating pulse-height
to photon energy; photopeak-area-to-total-spectrum-area ratios (experi-
mental photofractions, for code check purposes); and standard spectra
photopeak mean pulse-height and resolution. Under control of an input
option signal, the response matrix and its associated vectors may be read
as a card deck, instead of generated. For the analysis of many sets of
unknown spectra one response matrix may be applicable, and thus the main
program includes an option to bypass either the calling of RESFUN or the
input of a matrix card deck. For similar reasons an option is provided to
call RESFUN to generate a response matrix based on previously input stan-
dard spectra.
Input options allow either the execution of MAIN to continue, return to start or call EXIT, after the calling of RESFUN. Thus, for example, the code may be run only for the purpose of generating a response matrix.

Unknown spectra may be input to the code in uninterrupted blocks of up to 20 spectra through the calling of subprogram DEC by MAIN. If pulse-height analyzer background subtracted counts are recorded in a complement mode, i.e., as positive numbers, the code converts them to true negative numbers in subprogram DEC. A count greater than $9 \times 10^5$ is assumed to be in the complement mode.

MAIN is coded to subtract background spectra from source-plus-background spectra under an input option control signal. This allows the subtraction or addition, of a fraction or multiple of a background spectrum. It further allows the continued reuse, as desired, of a previously stored background spectrum, and of course the addition of similar spectra if this is the requirement of the user.

The energy correspondence of an unknown spectrum to the response function matrix is matched through MAIN calling subprogram GANE. Subprogram GANE returns the unknown spectrum to the main program after normalization to pulse-height analyzer true zero pulse-height and gain changing such that channel width corresponds to that of the response matrix.

Additional automated modification of an unknown spectrum may be optionally carried out by the code, namely:

(a) the counts in the first n 'dead' channels of the spectrum may be replaced with either the count stored in channel n + 1 or determined by a straight line function of specified slope; and/or
(b) the counts between specified limiting channels may be replaced by counts determined by a straight line function of specified slope.

Item (a) allows the user to make judgments with respect to the first few percent of the spectrum which is often either suspect or electronically distorted. Item (b) allows the removal of a known spurious peak, etc. in order to allow more meaningful subsequent analysis to be carried out.

At this point in the main program on both the first and subsequent loops, the response matrix is stored, and an unknown pulse-height analyzer spectrum is ready for analysis and conversion to a photon number spectrum. According to an input option signal the code is instructed that the unknown spectrum is either a pure continuum or a specified number of monoenergetic spectra "super-imposed" on a continuous spectrum. If the input option indicates the presence of superimposed monoenergetic spectra and if either their line energies and/or photopeak tail channel limits are input, MAIN calls subprogram DISCRT prior to calling subprogram SØLN to carry out iterative unfolding of the continuum. In the event that neither the energies or channel limits of the unknown spectrum peaks'are input they may optionally be 'searched-for' from channel MS to MX in subprogram FIND, which is called by DISCRT.

Subprogram DISCRT is called by MAIN to analyze the photopeaks indicated by the input options for the monoenergetic components of the unknown spectrum. Gaussian distributions may be fitted to each photopeak and the associated Compton continua determined by DISCRT calling subprogram RESFUN and the corresponding line photon numbers calculated. In this manner the monoenergetic spectral components may be calculated in turn and subtracted, i.e. stripped, from the unknown spectrum to leave a residual continuum spectrum. The residual spectrum is returned to MAIN
for subsequent analysis and unfolding. The monoenergetic photon numbers thus obtained are added to the residual photon number spectrum determined later by unfolding, to give the total photon number corresponding to the input pulse-height analyzer spectrum. If the photopeak is distributed over less than 6 channels a Gaussian function will not be fitted. In this last event the peak pulse-height and area will be obtained by moments and channel summation analysis, respectively.

Before calling subprogram SØLN the code tests certain input options, M(I), to determine specific requirements, e.g.

(a) is unknown spectrum to be corrected for detection efficiency by calling subprogram DETECT prior to gain changing, (eg. from 200 to 30 channels) and before unfolding or after?; or

(b) is unknown spectrum to be actually unfolded?

Item (a) allows the user to make decisions with respect to efficiency correction effects and accuracies. Item (b) allows the user to make decisions with respect to such as the significance of actually carrying out the unfolding procedure on a low energy spectrum such as that of Pm$^{147}$. The above options and all others, are defined in more detail in Section 3.2. The called subprograms RESFUN, DISCRT, DETECT, SØLN and GEØMTR are discussed further in Subsections 2.2.2 through 2.2.7.

At this point in the main program on both the first and subsequent loops, unknown spectra are considered as prepared for unfolding, and thus, they and the response matrix are communicated to subprogram SØLN. This subprogram is called by MAIN to control the iterative unfolding process according to the Scofield method$^{(2,5,6)}$ and to apply efficiency corrections. It returns the corrected photon number spectrum to the main program.
The main program calls subprogram DECAY to determine the primary source decay factor. Subprogram DECAY returns a correction factor by which the number spectrum is later multiplied. The calling of subprogram DECAY may be optionally bypassed, in which case a multiplying factor of unity is assumed.

Subprogram GEOMTR is called by the main program to apply the decay correction factor, carry out geometrical corrections, compute differential and integral photon number and energy distributions, and exposure dose.

Subprogram GEOMTR returns the final results to the main program for output, after which the code loops back along either paths 1, 2, or 3, as shown in Figure 2. The code loops back along path 1 primarily to read new data pertaining either to the response matrix or to the control options or both. The code loops back along path 2 to read new data pertaining either to the unknown source or if the maximum number (20) of allowable passes along path 3 have been equaled; the second reason is dictated by either code DIMENSION or computer finite capacity. The code loops back along path 3 to read a new unknown spectrum.
2.2.2 RESPONSE FUNCTION MATRIX

2.2.2.1 Response Matrix Generation

The detector system response function matrix is generated under the control of subprogram RESFUN. The subprograms called by RESFUN are namely:

```
SPNORM  POGELI  BS  XPL0T
ADPEAK  GANE  TE  TA  VECTMX
```

The main program supplies RESFUN with control parameters, and variables. RESFUN begins execution by input of a card deck of spectra of standard radioisotopes. The number of such spectra is equal to NSTAND, where NSTAND ≤ 9. This card deck is preceded by one parameter card containing information regarding the number of spectra in the deck (NSTAND) and the number of channels in the input standards (NXLIM). The single parameter card is followed by a card set of NSTAND spectra. Each spectrum is preceded by one parameter card and is input in order of energy ascendance. The parameter card for each spectrum contains the source identity, data regarding peak approximate locations and the deviation of the spectrum from true zero pulse-height, i.e. the normalizing spectrum shift required; further details are referred to Section 3.

The standard source spectra allowed by the code must be monoenergetic e.g.

\[
\begin{array}{cccc}
\text{Cd}^{109} & \text{Ce}^{139} & \text{Hg}^{203} & \text{Cr}^{51} \\
\text{Mn}^{54} & \text{Nb}^{95} & \text{Sr}^{85} & \text{Cs}^{137}
\end{array}
\]

Zn\textsuperscript{65} and Na\textsuperscript{22} are allowed if Sr\textsuperscript{85} has been input; Zn\textsuperscript{65} is preferred to Na\textsuperscript{22} because of the 0.51 MeV photopeak intensity relative to the high energy photopeak.
The code as presently designed also allows the inclusion of Co$^{60}$ and 'hand' prepared monoenergetic spectra of higher energies, e.g. the sample data in this report includes a hand modified spectrum of Th$^{228}$.

According to an input option and after the first call, calling of RESFUN by MAIN allows the by-passing of input of standard spectra. This allows the code to generate a response matrix based on already stored and normalized standard spectra. Similarly subprogram DISCRT calls RESFUN to determine Compton continua based on already stored current standard spectra.

After spectral data is input to RESFUN, counts in the complement mode are converted to their true negative value. The spectra are shifted to true-zero pulse-height by the calling of subprogram GANE. Their order of input is established prior to the calling of subprogram SPNORM for spectral normalization.

Subprogram SPNORM is called by subprogram RESFUN to normalize the single-photopeak and Zn$^{65}$ standard spectra with respect to photopeak area and pulse-height; photopeaks and source-characteristic X-ray peaks are subtracted. The multipeak spectrum of Co$^{60}$ is normalized in RESFUN after the return from SPNORM. The residual spectra determined by SPNORM (and RESFUN in the case of Co$^{60}$) consist of Compton continua characteristic of the primary photon energy. X-ray peaks are optionally subtracted where they are not representative of the primary photon energy but rather of the radioisotope source. The 0.51 MeV component photopeaks and their Compton continua are subtracted for the same reason. Figure 3 shows a typical set of spectral continua in the energy domain 0.166 MeV to 2.615 MeV, normalized by subprogram SPNORM as described in Section 2.2.2.2.
Subprogram SPNORM returns the normalized differential standard Compton distributions to subprogram RESFUN. The energy ordered normalized continua are interpolated quadratically with respect to the energy axis of the desired response function matrix through subprogram RESFUN calling subprogram POGELI. The result of this interpolation consists of \( N \) (corresponding to the required matrix size) Compton continuum vectors normalized to unit photopeak area and pulse-height. Subprogram DISCRT similarly calls RESFUN to obtain interpolated normalized Compton continua over a required number of channels and at the specific energies corresponding to photopeak analysis.

Unit area and mean pulse-height Gaussian photopeaks are added to the interpolated differential Compton continua to give \( N \) (matrix size) complete spectra (matrix vectors). The peaks are computed through RESFUN calling subprogram ADPEAK. The Gaussian photon energy dependent standard deviation \( \sigma(E) \), is determined by interpolation of those values obtained by the earlier photopeak fitting. Subprogram ADPEAK computes a Gaussian photopeak histogram in accord with the methods described for Equation (4) in Section 2.2.2.3 of this report. The \( N \) determined unit size differential spectra are redistributed linearly in pulse-height as a function of photon energy. The redistribution is obtained through RESFUN calling subprogram GANE.

At this point in the subprogram RESFUN execution, a response function matrix has been determined. This matrix and its corresponding vectors for pulse-height photon energy and photofraction are returned to the main program. Figure 4 compares the photofractions of the response matrix vectors as determined by RESFUN with actual values separately determined for the standard source experimental spectra.
Subprogram SPNORM normalizes the standard spectra input to RESFUN. It begins execution by carrying out necessary initializations. SPNORM calls subprogram PKFUN to carry out a Gaussian fit to the spectral photopeaks. Subprogram PKFUN estimates the necessary initial values of the peak function parameters: straight-line-base slope and intercept, Gaussian photopeak standard deviation, area and mean pulse-height. Subprogram PKFUN returns the parameters of the fitted and subtracted photopeaks and the residual spectra to subprogram SPNORM. Subprogram PKFUN calls subprogram STDFT3 to carry out the non-linear regression of the peak function. The peak function is obtained by STDFT3 calling subprogram FUNZ.

Subprogram SPNORM uses the determined photopeak pulse-height and area parameters to normalize the continua of the standard spectra. A subtraction of the characteristic X-ray peaks is carried out in the case of those spectra where they occur. The 0.51 MeV photopeak and continuum of Sr$^{85}$, if it has been input, is employed to subtract the 0.51 MeV spectrum contribution of Zn$^{65}$. This operation requires both count and pulse-height gain normalization, the gain normalization being carried out through the calling of subprogram GANE.

The residual Compton continua are gain normalized to a photopeak pulse-height of NORM (e.g. = 200) channels by the calling of subprogram GANE and count normalized to unit photopeak area by a division operation.
The resulting residual normalized continua are checked for negative count values, which are replaced by zero, and returned to the calling subprogram RESFUN. The fitted photopeak parameters are also returned to subprogram RESFUN.

The two-component spectrum of Co\(^{60}\) is normalized in RESFUN, although the photopeaks are subtracted under the control of SPNORM. The normalization is actually carried out on the 1.33 MeV contribution only, the 1.17 MeV contribution being discarded. The 1.33 MeV continuum is obtained as the residual remaining in the input Co\(^{60}\) continuum after subtraction of the 1.17 MeV continuum. The 1.17 MeV continuum is obtained by an extrapolation in subprogram POGELI based on the three highest energy standard normalized continua (e.g. Cs\(^{137}\), Mn\(^{54}\) and Zn\(^{65}\)). The 1.33 MeV residual continua so found is then normalized and included as a member of the previously determined set of standards. Figure 3 shows an example 1.33 MeV continuum and Figure 4 the photofraction determined by the code.

2.2.2.3 Photopeak Fitting

Subprogram SPNORM calls PKFUN, which in turn calls STDFT3, to fit the photopeaks of the standard source spectra with a 'Gaussian-plus-straight-line-base' function. Under options discussed in Section 2.2.4., subprogram DISCRT calls STDFT3 to fit the photopeaks in the unknown spectrum with the same function. As presently coded PKFUN requires that only the standard source energy and the approximate peak location be specified by SPNORM.

Initial estimates of the photopeak function parameters, which are regression fitted in STDFT3, are determined in PKFUN. The mean pulse-height parameter B (1) is estimated from the channel of maximum count in the vicinity
of the specified approximate channel location of the peak. The standard
deviation parameter $B(2)$, of the Gaussian, is obtained from the expression

$$B(2) = \sigma (B(1)/E), \text{ channels},$$  \hspace{1cm} (1)

where

$$\sigma = 0.001536 \exp (0.395 \times E), \text{ MeV},$$ \hspace{1cm} (2)

and

$$E = \text{photon energy corresponding to specific photopeak, MeV}.$$  

Figure 5 compares the above expression for $\sigma$ with the regression fitted
values obtained for the JPL standard spectra. The area parameter of the
Gaussian $B(3)$, is initially estimated from the expression

$$B(3) = H \times B(2) \times 2.35, \text{ counts},$$ \hspace{1cm} (3)

where

$$H = \text{count above straight-line-base in channel of maximum count i.e. in channel B(1)},$$

$$2.35 = \text{a Gaussian constant relating standard deviation to width at half of maximum peak height}.$$  

The photopeak base is taken as the straight line between the counts in the
channels defined by \[B(1) \pm 6.0 \times B(2), \text{ rounded up or down to integer}\].

Subprogram STDFT3 is called twice by PKFUN to fit the photopeaks of the
standard source spectra. On the first call the Gaussian is fitted over the
channel range defined by $B(1) \pm 6.0 \times B(2)$, but since Ge(Li) photopeaks
are quite assymetrical in comparison to those measured in NaI(Tl) spectro-
metry, the parameters determined on the first call are used as initial es-
timates for a second call. On the second call the photopeak is fitted with
the Gaussian function from channel $N_1$ to channel $B(1) + 6.0 \times B(2)$. $N_1$
is taken as the lowest count channel satisfying, $N(0.8H) \geq N_1 < B(1)$, where
N(0.8H) defines the channel < B (1) containing ≥ 80% of the count in channel B (1). In this manner the photopeak is systematically fitted with a Gaussian over the relatively symmetrically upper two-thirds of its extent. Appendix V shows sample residual counts for a number of the standard spectra after subtraction of the fitted Gaussian. The value of the count H, in the integer-B (1) channel is indicated. The residual can be seen to relatively consistent, especially in view of the limited number of photopeak channels over which the measurements were made.

Subprogram STDFT3 carries out the non-linear regression of the photopeak function. The logic of this subprogram is very similar to that of subprogram STDFIT, described in reference (4). The theoretical logic of STDFIT is given in Appendix VI; it is directly reproduced from reference (2) and is generally applicable to STDFT3. There are two major differences between the STDFIT and STDFT3 codes, the former is designed for a single Gaussian whereas STDFT3 is designed for n-Gaussians, although it is presently only 'DIMENSIONED' for two. The second major difference is that whereas STDFIT calls FUNUS to compute the photopeak function f(x_i) to be fitted to the photopeak counts y(x_i), STDFT3 calls FUNZ to determine F(x_i), a histogram, where x_i is the mid-channel pulse-height and

\[ P(x_i) = \int_{x_i - 0.5}^{x_i + 0.5} f(v) \, dv, \]  

(4)

\[ r \sum_{j=1}^{m} f(v_j) \Delta v, \]  

(5)
where

\[ v = \text{pulse-height variable of integration for channel } x_i; \]
\[ m = \text{number of subdivisions of channel } x_i. \]

The above approach is necessary for Ge(Li) photopeaks because of the superior resolution as compared to NaI(Tl). A comparison of experimental and fitted photopeak distributions are given in Appendix VI.

2.2.2.4 Compton Continuum Interpolation

Subprogram POGELI quadratically interpolates or extrapolates normalized Compton continua. It is called by RESFUN for response matrix vector generation purposes and multi-peak standard spectrum analysis. Actual quadratic interpolation is performed by function subprogram TE. For energies between zero and that of the lowest energy input standard, the interpolation is necessarily linear. The linear interpolation assumes, reasonably, that at zero energy the channel counts are also zero.

Although the interpolation is quadratic, the redistribution of the standards before and after interpolation is such that the method developed here is referred to as one of 'parts'. While code CUPED uses the 'method-of-three-parts' \(^{(1)}\), CUGEL uses the 'method-of-two-parts'. This method divides the continuum into two characteristic regions: A) zero energy to Compton edge, and B) Compton edge to photopeak mean pulse-height. The mutual boundary of each region is overlapped for continuity reasons. The dashed curves in Figure 3 indicates the regional boundaries.

The major difference between the CUGEL and CUPED methods is in the handling of the backscatter peak, which is smaller but sharper in Ge(Li) than its counterpart in NaI(Tl). In code CUGEL, the backscatter peaks
are subtracted from the main continuum, normalized and interpolated separately. The subtraction is done in subprogram FITLIN which is called by subprogram BS. The normalization is carried out in BS with respect to the standard of lowest energy; the interpolation is carried out in BBS. Where backscatter peaks are merged with the Compton edge, as in the case of Hg$^{203}$, a backscatter peak is interpolated and subtracted in subprogram BS to leave an unmasked Compton edge. Figure 6 shows the backscatter and Compton edge peak pulse-height as a function of photon energy. The merged-region is clearly seen in this figure to be defined as $0.24 < E < 0.34$, MeV.

Prior to interpolation (or extrapolation) the continuum regions A and B are aligned such that the regional boundaries on which the Compton edges lie are at the same pulse-height. Alignment is carried out with respect to the continuum of highest energy for the set of three standards in the quadratic, by the calling of subprogram GANE. The two interpolated components, A and B, are unaligned by gain changing to obtain the desired continuum. The pulse-height axis direction of region B is reversed for convenience during the whole operation, i.e. zero pulse-height is taken at the photopeak mean pulse-height. An empirically modified form of the Compton angular-energy relationship is used to aid in automatically locating the Compton edges and backscatter peaks.

POGELI returns the interpolated Compton continuum to the calling program, RESFUN. Figure 3 shows example Compton continua as determined by CUGEL; they can be seen to compare well with the normalized continua from which they were determined. The photofractions of Figure 4 also substantiate the interpolated continua.
2.2.3 Analysis of Monoenergetic Spectral Contributions

Subprogram DISCRT is called by MAIN according to an input option to analyze photopeaks and their associated Compton continua, in complex spectral distributions. Subprogram DISCRT will fit a 'single or double Gaussian-plus-straight-line' function to the photopeaks of a multipeak spectrum. It will subtract the fitted photopeaks and their associated continua to leave a residual continuous spectrum. In the case of no continuous component in the complex spectrum, the residual will, ideally, have zero intensity.

The code CUGEL user may optionally input either the energy of the photopeaks to be fitted in DISCRT, the photopeak fitting limits (channel numbers), request the code to search for peaks or alternately combine these three options. In the event that the energies of only certain peaks are known they may be input, while the remainder may be defined by fitting limits. The choice of energy order of monoenergetic peak analysis and spectral stripping is left to the user; the code permits a mixed order to be chosen.

In addition to fitting and subtracting the monoenergetic components of an unknown spectrum, DISCRT determines their corresponding efficiency-corrected detector-incident photon number. The thus determined photon number may be, optionally, either added to the continuous photon number determined by later unfolding or diverted for separate output. In this way the separated radiations can be studied, e.g. bremsstrahlung analyses may be carried out even though the subject source also emits monoenergetic photons.

Subprogram DISCRT begins execution by determining whether the photopeak fitting limits have been input to MAIN by the user or whether they are to be calculated. In the event that they are to be calculated, DISCRT begins execution by estimating their channel locations based on the peak input
energies. It first establishes the approximate channel region of the photo-peak. It then ascertains it more accurately for the approximated channel region by calling subprogram VECTMX to establish the channel of maximum count. The fitting limits are determined as a function of the photon energy dependent standard deviation. In the event that neither peak limits nor energies are input, DISCRT calls subprogram FIND to search for photopeaks. A check is made to ensure that all the limits determined are within the spectrum and that their domains do not overlap each other.

Subroutine FIND searches for peaks from channel MS to MX, excepting those channel regions where limits have been input. It will not examine spectral regions where the count is < $G$. The logic of FIND consists of testing the count $y_i$ in channel $i$ against the count in channels $i - 1$ and $i + 1$, between channels $N1$ and $N2$, where $N2 = N1 + II$; $II = 4$ was found to work satisfactorily for all spectra tested. A peak is assumed if

$$\frac{1}{2} \frac{y_{N1} + T * y_{N1}}{y_i} < \frac{1}{2} \frac{y_{N2} + T * y_{N2}}{y_i} \quad ; \quad N1 < i < N2,$$

where

$$T = 6$$

and $G = 100.0$, were found to work satisfactorily for all spectra tested.

With the fitting limits established a single or double Gaussian distribution is regression fitted to each photopeak in turn providing the number of channels in the peak is greater than six. Actual photopeak function fitting is carried out by the calling of subprogram PKFUN. In the case of double or merged peaks, subprogram GUESS3 is called to estimate initial values of the Gaussian parameters. GUESS3 estimating is carried out using the general logic described in Section 2.2.2.3 for PKFUN.

In the event that the photopeak is distributed over six or less channels, the area and mean pulse-height are determined from the counts in excess
of a straight line joining the counts in the limit channels and from the first moment of rotation, respectively.

The Compton continuum associated with each photopeak is determined by DISCRT calling subprogram RESFUN, which returns an interpolated continuum normalized with respect to a photopeak of unit area and pulse-height (NORM channels). The continuum is then scaled and gain changed according to the determined peak area and pulse-height.

Gain changing is carried out through DISCRT calling subprogram GANE. The photopeak and Compton continuum are then subtracted from the unknown spectrum for each monoenergetic spectral component in turn to finally leave a continuous residual spectrum. If no continuous contribution was present in the unknown, then ideally a zero spectrum will result.

Prior to returning the residual continua to MAIN for iterative unfolding, DISCRT determines the photon number corresponding to each monoenergetic spectral component. This is done by computing the photofraction, \( P(E) \), the detector interaction efficiency, \( \epsilon(E) \), and the attenuation term for air and other material interposed between the source and detector, \( k(E) \). The photon number is then determined from the relationship:

\[
N(E) = \frac{\text{Photopeak Area (or Counts)}}{P(E) \cdot \eta(E)}
\]

where

\[
\eta(E) = \epsilon(E) \cdot k(E).
\]
The corrections noted are carried out by subprogram DISCRT calling sub-
program DETECT. \( N(E) \) is returned to MAIN to be optionally either added
to the iteratively unfolded continuum number spectrum or to be output
separately.

2.2.4 Spectral Unfolding

The reduction of pulse-height analyzer continuous spectra to photon number
spectra and the application of efficiency corrections are carried out under
the control of subprogram SØLN called by the main program. Subprogram
SØLN begins execution by carrying out certain initializations after which
it calls subprogram RESMAT to unfold the pulse-height analyzer spectra
according to the Scofield method \((2,5,6)\). The number spectra returned
by subprogram RESMAT are corrected for efficiency by SØLN calling DETECT.
The thus corrected number spectra are returned to MAIN. The remainder of
this section describes the logic of the unfolding subprogram RESMAT and
of the efficiency vector subprogram DETECT, AIRABS and ALUM.

Subprogram RESMAT unfolds the pulse-height analyzer spectra by solving
the matrix equation (in matrix notation)

\[
\bar{P} = \bar{R} \bar{N}
\]  

(8)

where \( \bar{P} \) and \( \bar{N} \) are the \( m \)-dimensional vectors of the PHA spectrum and the
efficiency uncorrected photon number spectrum, respectively, and \( \bar{R} \) is
the \( m \times m \) square response function matrix. Equation (8) is formally solved
as

\[ \tilde{N}' = \tilde{R}^{-1}\tilde{N} \]  

where \( \tilde{R} \) is non-singular and \( \tilde{R}^{-1} \) is its inverse. Subprogram RESMAT executes equation (9) iteratively according to the Scofield method\(^{(5,6)}\). Figure 7 shows a flow diagram of the iterative algorithm coded in subprogram RESMAT. Further details are referred to references (1-8).

The efficiency corrected photon number spectrum \( N \), is determined from equation (9), as

\[ \tilde{N} = \tilde{\eta}^{-1}\tilde{N}' \]  

where \( \tilde{\eta} \) is a diagonal efficiency matrix accounting for interaction efficiency and photon attenuation by detector cladding, air and aluminum interposed between the source and the detector active region. Subprogram SOLN calls subprogram DETECT which in turn calls function subprograms EFFIC2, AIRABS and ALUM, to determine \( \tilde{\eta} \). SOLN then executes equation (10) and returns the determined photon number spectrum to MAIN. Figure 8 shows an example spectrum before (\( \tilde{P} \)) and after (\( \tilde{N} \)) unfolding.

Subprogram EFFIC2 determines the interaction efficiency for the right-cylindrical Ge(Li) detector exposed to an axially located source of photons of energy \( E \), as

\[ \epsilon (E,r) = \frac{1}{\Omega} \int_{\text{detector}} (1 - e^{-\mu(E)x}) \, dx \]  

where

\[ \mu(E) = \text{total linear attenuation coefficient of Ge(Li) for photons of energy } E \text{ (excluding coherent scattering).} \]
\( x \) = photon vector path length in the detector prior to interaction,

\( r \) = source-to-detector distance,

\( Q \) = the solid angle subtended at the source by the detector.

Equation (11) may be rewritten in a form more suitable for solution, as

\[
\epsilon(E, r) = \int_{0}^{\alpha_1} \left[ 1 - e^{-\mu(E) H \sec \alpha} \right] \sin \alpha \, d\alpha + \sqrt{\frac{\alpha_2}{\alpha_1}} \left[ 1 - e^{-\mu(E) (R_x \csc \alpha - r \sec \alpha)} \right] \sin \alpha \, d\alpha
\]

where

\[
\alpha_1 = \tan^{-1} \left( \frac{R_x}{r + H} \right)
\]

\[
\alpha_2 = \tan^{-1} \left( \frac{R_x}{r} \right)
\]

\( H \) = cylindrical length of Ge(Li) detector active region

\( R_x \) = cylindrical radius of Ge(Li) detector active region

The geometry for equation (12) is given in Figure 9.

In practice the source will have finite dimensions, but as long as they are relatively small, equation (12) is valid. The interaction efficiency
for small line and disc sources relative to a point source may be estimated from reference (17). Equation (12) is evaluated by a numerical integration, which is carried out by subprogram SIMPSN, which calls function FC to determine the integrand. The photon flux incident on the crystal is corrected for air and aluminum absorption. This correction, multiplied by Equation (12), yields the diagonal efficiency-matrix \( \eta \), as

\[
\eta_{ij} = \epsilon (E_i, r) \exp (-r \mu_{\text{air}} (E_i)) \cdot \exp (-\tau \cdot \mu_{\text{alum}} (E_i));
\]

\[
i = j = 1, 2, \ldots, m,
\]

where

\[
\mu (E) = \text{total linear attenuation coefficient of the material (air and aluminum per subscripts) interposed between source and detector for photons of energy } E_i, (13-17)
\]

\[
\tau = \text{thickness of the aluminum absorber material interposed between source and Ge(Li) detector, active region}
\]

\[
m = \text{matrix size}.
\]

In accord with input option signal \( m(19) \neq 0 \), the interactions efficiency given by Equations (12) and (13) may be bypassed and instead obtained from an empirical relationship as

\[
\epsilon (E) = 0.441 E^{-1.32} / P(E),
\]

The agreement between this equation and equation is seen in Figure 10.
2.2.5 Analysis of Unfolded Spectra

Subprogram GEØMTR is called by MAIN to carry out a final analysis on the unfolded photon number spectra. The spectra are corrected for primary source decay and converted by GEØMTR to differential photon number flux at the detector per unit time, \( N_x(E) \), (coded as PHI), as

\[
N_x(E) = \frac{N(E)}{\pi R_x^2}, \text{ } \gamma/\text{cm}^2\text{ sec}
\]

where

\( R_x = \text{Ge(Li) crystal radius, cm.} \)

The differential energy flux incident on the crystal per unit time, \( I_x(E) \), (codes as ENXTAL), is determined as

\[
I_x(E) = N_x(E) \cdot E, \text{ } \text{MeV/cm}^2\text{ sec}
\]

The energy integrated exposure dose rate at the crystal, \( D \), (coded as DOSDET), is determined as

\[
D = \int_{\text{energy}} N_x(E) E \mu_{\text{air}}(E) K dE, \text{ roentgens/hours}
\]

where

\( \mu_{\text{air}}(E) = \text{energy mass absorption coefficient of air, cm}^2/\text{gm} \)

\( K = \text{conversion constant} \)

\( = 3600/5.24 \times 10^7 \), (roentgens-second-gm air)/MeV-hour

The integration in equation (17) is carried out numerically by GEØMTR, as
The energy integrated photon number and photon energy flux at the crystal is determined by integrating \( N \cdot (E) \) and \( I \cdot (E) \) over \( E \), (coded as \( \text{SUMNUM} \) and \( \text{SUMENY} \)); the units are \( \gamma/\text{cm}^2\cdot\text{sec} \) and \( \text{MeV}/\text{cm}^2\cdot\text{sec} \). The following tabulated data are also determined by subprogram GEØMTR for output by the calling main program:

<table>
<thead>
<tr>
<th>FORTRAN NAME</th>
<th>EQUAL TO</th>
<th>DEFINITION &amp; UNITS</th>
</tr>
</thead>
<tbody>
<tr>
<td>(AT THE CRYSTAL)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AVENGY</td>
<td>( \frac{\sum N(E) \cdot E \cdot \Delta E}{\sum N(E) \cdot \Delta E} )</td>
<td>average energy, MeV</td>
</tr>
<tr>
<td>PHNUBE</td>
<td>( \frac{\sum N(E) \cdot \Delta E}{N \beta} )</td>
<td>integrated photon number flux per beta source strength, ( (\gamma/\text{cm}^2\cdot\text{sec})/(\beta/\text{sec})/\text{MeV} ); ( \beta ) defined below)*</td>
</tr>
<tr>
<td>ENBENY</td>
<td>( \frac{\sum N(E) \cdot E \cdot \Delta E}{E \beta_{\text{max}}} )</td>
<td>integrated energy flux per beta maximum energy, ( (\text{MeV}/\text{cm}^2\cdot\text{sec})/\text{MeV} ); ( E \beta_{\text{max}} ) defined below)*</td>
</tr>
<tr>
<td>PHENBE</td>
<td>( \frac{\sum N(E) \cdot \Delta E}{N \beta} )</td>
<td>integrated energy flux per beta source strength, ( (\text{MeV}/\text{cm}^2\cdot\text{sec})/(\beta/\text{sec}) )*</td>
</tr>
<tr>
<td>DOXBEX</td>
<td>( \frac{D}{N \beta} )</td>
<td>dose rate per beta source strength, ( (r/\text{hr})/(\beta/\text{sec}) ); ( D ) defined in equation 13)*</td>
</tr>
</tbody>
</table>

(AT THE SOURCE)

| DOSCYL            | \( \frac{\text{DOXBEX}}{G} \)                          | dose rate per beta source strength, \( (r/\text{hr})/(\beta/\text{sec}) \); \( G \) defined below)* |

*Beta, \( N \) and \( E \) are used in this section because of earlier bremsstrahlung analyses; gamma (\( \gamma \)) may be the substituted meaning where it applies.
where
\[ E_{\beta_{\text{max}}} = \text{maximum beta (or chosen } \gamma \text{) energy in MeV} \]
\[ = \text{EBMAX of card 6 of report section 3.2*} \]
\[ N_{\beta} = \text{number of source emitted betas or } \gamma \text{'s per unit time} \]
\[ = (\text{SBETA of card 6 of report section 3.2}) / (3.7 \times 10^{10}) \]

and
\[ G = \frac{\Omega_x}{\Omega} = 1/2(1 - r/(r^2 + R_x^2)^{1/2}) \]

where
\[ \Omega_x = \text{solid-angle subtended by the crystal at the source geometric center} \]
\[ \Omega = \text{total solid-angle at the source} = 4 \pi \text{ steradian} \]
\[ r = \text{source to crystal distance.} \]

Subprogram GEOMTR returns all of the above data to the main program for output.

* if not meaningful to code user, then input as, EBMAX = 1.0
** if not meaningful to code user, then input as, SBETA = 1.0/(3.7 \times 10^{10}).
2.3 Code Constants

In this section the origin and meaning of certain constants coded into CUGEL, are discussed. The discussion is carried through in alphabetic order of subprograms, except for General Discussion and MAIN which are presented first. Certain subprograms require no discussion.

**General Discussions:** Certain constant values appear periodically throughout CUGEL. The values $2.35482, 2354.82, 0.3989423$ and $1.065$ are Gaussian or normal distribution constants. The values $60$ (minutes/hr and seconds/min) and $1440$ (minutes/day) are clock time conversion constants. Other values are either obvious (e.g. $\pi = 3.14159265$) or constants unique to the code logic except as explained below.

**MAIN:** Certain constants required by CUGEL subprograms are coded in MAIN and communicated by `COMMON/CNSTNT/`. The constant $TKLUM$ is the thickness of aluminum absorber in front of the Ge(Li) detector; it is presently coded as $0.9$ cm for subprogram ALUM. The constants $T_{20} = 20.0, T_{50} = 50.0$ and $T_{01} = .0001$ are used by the code if input ($ON, HITMAX, EPS$) left blank; this is discussed in Section 3.2. The constant $T_{1293} = 0.001293$ is the density of air coded for subprogram AIRABS. The constants $T_{90} = 900000.$ and $T_{100} = 1000000.$ are used by subprograms DEC and RESFUN for checking for spectral counts in the complement mode. The constants associated with UT at statement numbers 40 to 47 are explained in Section 3.2. The constant $3.7 \times 10^{10}$ at statement number 128 + 1 is the conversion factor for Curies to disintegrations/second. $IFIFTY = 50,$ is the maximum number of photopeaks allowed in the unknown spectrum. $TEN$ and $IFOUR = 10,$ and $4$ are $T$ and $G$ of equation (6). $T06 = 10^{-6}$, is the integration criterion for function SIMPSN. $NORM = 200,$ is continuum pulse-height normalizing constant for RESFUN. $NLI = 800$ and $NLIMIT = 400$ are related to allowed vector dimensions.
EFFIC2: The total (less coherent scattering) linear attenuation coefficients for Ge(Li) in cm$^{-1}$ are stored in the R DATA Statement; the corresponding energies are stored in the X DATA Statement. Ge(Li) density was taken as 5.32 gm/cc.

ALUM: The total linear attenuation coefficients of aluminum in cm$^{-1}$, are stored in the R DATA Statement; the corresponding energies are stored in the X DATA Statement.

FITLIN: The constants 5, .5, and 12.0 are associated with the fitting of a straight line base under the backscatter peak based on the six channels on either side of the defined peak region.

AIRABS: The mass absorption coefficients of air are given in the A DATA statement in cm$^2$/gm. The coefficients include coherent scattering; the corresponding energies are stored in the X DATA statement. They are multiplied by the density of air (T 1293) in gm/cc to give output units in cm$^{-1}$.

DØSE: The energy mass absorption coefficients for air are given as R in the DATA statement in cm$^2$/gm. They are based at 20°C and a fractional weight composition of:

- Nitrogen: 0.755
- Oxygen: 0.232
- Argon: 0.013

The energies corresponding to R are given the X DATA statement.

GEØMRT: The constant defined as CONST has been already discussed for Equation (17).
STDFT3: The constant EPS = .00001 (at statement 100 - 3), is the fitting criterion for the photopeak non-linear regression. The constant NI = 10 is a stopping criterion for non-linear regression in the event of a non-convergence.

DISCRT: The product of the constants 1.2 and 0.00128 has been defined as 0.001536 in Equation (2); the constant 0.395 has also been defined in Equation (2).

DECAY: The constant 1440 = the number of minutes in 24 hours.

SIMPSN: TMAX = 2048 is the maximum allowable number of integration increments.

RESFUN: The constants 0.75, 0.85, 0.80, 0.85, 178./200. and 105./200 are general empirical values associated with analyzing of the JPL Co\textsuperscript{60} standard spectrum supplied; they may be interpreted as fraction of photopeak pulse-height.

BS: The equation expressed by Statement 61, is for smoothening the standard spectrum in the region below the backscatter peak, when E > 0.34 Mev; the constants were derived from the JPL standard spectra. The equation expressed by Statement 62 + 1 allows the backscatter peak to be normalized with respect to the lowest input standard even though the backscatter peak may be merged with the Compton edge; the constants were derived from the JPL standard spectra. The constants 0.875 and 1.16 at Statement 70 + 4 and 70 + 5 were derived from the JPL standard spectra to define the backscatter peak region for analysis in the Compton edge merging region, 0.24 to 0.34 Mev.
3. CODE OPERATING INFORMATION

3.1 GENERAL

Code CUGEL is written in a generalized FORTRAN-V for the UNIVAC-1108. It may be readily run on other computers with sufficient core size; i.e., the present version requires ~ 50K words. There are no Sense Switch or special tape requirements. Input formats are standard FORTRAN-IV or V, as given in any UNIVAC, IBM, or CDC FORTRAN manual; the code has been designed with a view to ease of translation for use on other computers. Input/output tapes are presently coded as LI and LØ equal to 5 and 6, respectively, at the beginning of MAIN (statement 2602 + 5 and + 6). A code listing is given in Appendix II.

Figure 11 shows a general arrangement for the data input cards. Input card details, order, formats, restrictions and location are given in Section 3.2. Card numbers are encircled and defined in the order in which they are read by the code. A sample input listing is presented in Appendix III.

The code CUGEL input data card deck consists of twelve (12) types of cards, referred to as Card 1, Card 2, etc. If the type requires more than a single card, the reference is made to Card Set. Card 1 is a single card, input only once. Cards 2, 3 and 4 are single cards input at least once. Card set 5 (5α or 5β) is input at least once in order to define the response matrix. If the user only wishes to generate a response matrix but not to apply it to any data, then no further input is required. If the matrix is to be applied to analyze unknown spectra, further input is required to define the spectral data and the required analysis.
Card set 6 consists of two cards which must be input to define parameters which are common to all PHA spectra in the PHA spectral data set (card set 12), e.g., source size, counting time, source strength, etc. Card set 7 must be input to define parameters unique to each PHA spectrum in the PHA spectral data set, e.g., zero shift required, subtract background or not, source-to-detector distance, energy calibration data, etc. Card 8 and card sets 9 through 11 are optional. Card set 12 consists of the unknown PHA-spectra to be analyzed and their PHA-background-spectra. The code will analyze spectra of up to 400 channels, although up to 1000 channels may be input and code gain-changed to 400 for analysis.

The optional cards are as follows: Card 8 is a single card to allow the user to study the iterative unfolding convergence, i.e., intermediate unfolding data is output. Card set 9 allows the user to replace undesirable peaks, prominences or spurious spectral counts with a straight-line shape. Card set 9 also allows the user to load initial spectral channels with a straight-line shape. Card set 10 allows the user to input the energy of photopeaks to be analyzed. Card set 11 allows the user to input the channel region of photopeaks to be analyzed. The input of both card set 10 and 11 allows the user to give the energy of certain peaks and the channel region of others. Card set 11 allows the user to input energy as well as channel domain for peaks, in which case the code will use the input energy as opposed to the code determined energy for such as efficiency calculations. This last is useful in applications where a prior knowledge indicates that the energy which the code would determine might not be precise.

The input of channel number values must be as recorded by the pulse-height analyzer. The code will change the input values in accord with requested shifts or gain changes. In Section 3.2, 'rounded-up' refers to the 'next highest integer value', i.e., 3.7 rounded-up is 4. The input order of card
sets 7, 9, 10, 11, and 12 must correspond to the spectra of card set 12.

The code output is reviewed in Section 3.3. Appendix IV is a sample output listing. It corresponds to sample input of Appendix III. Debug type output may be obtained by input of M(8) = 8 on card 3. The user is cautioned with respect to profusion of output under this option — a trial using sample data is recommended first.
3.2 Card Input Details

Card ① (one card; once only)

<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SET</td>
<td>1-10</td>
<td>F10.5</td>
<td>Total number of spectra to be unfolded by a code run (see index KK in Figure 2)</td>
</tr>
</tbody>
</table>

Card ② (single card)

<table>
<thead>
<tr>
<th>COLUMN</th>
<th>CASE</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-72</td>
<td>(column 1 for printer control)</td>
<td>A</td>
<td>User's problem description (alphanumeric)</td>
</tr>
</tbody>
</table>

Card ③ (single card) (See Figures 2 and 12 for additional M(I) details)

<table>
<thead>
<tr>
<th>M (1)</th>
<th>1-3</th>
<th>I3</th>
<th>Signal for routing after response matrix generation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>&gt; 0 CALL EXIT</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= 0 Continue</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>&lt; 0 Return to READ card ②</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= 0, use existing response matrix</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>≠ 0, generate new response matrix using existing standard spectra</td>
</tr>
<tr>
<td>M (2)</td>
<td>4-6</td>
<td>I3</td>
<td>If ≠ 0, read card ⑧ (iterative unfolding output signal)</td>
</tr>
<tr>
<td>M (3)</td>
<td>7-9</td>
<td>I3</td>
<td>If ≠ 0, read card set ⑨ (replace peak with straight line and/or &quot;fill-in&quot; initial NFILL channels)</td>
</tr>
<tr>
<td>M (4)</td>
<td>10-12</td>
<td>I3</td>
<td>If ≠ 0, by-pass RESMAT (unfolding) in subprogram SØLN (See Figure 12)</td>
</tr>
<tr>
<td>M (5)</td>
<td>13-15</td>
<td>I3</td>
<td>If ≠ 0, add photopeak contributions to iteratively unfolded continuous photon number spectrum</td>
</tr>
<tr>
<td>M (6)</td>
<td>16-18</td>
<td>I3</td>
<td>If ≠ 0, DISCRT called for monoenergetic contribution analysis.</td>
</tr>
<tr>
<td>M (7)</td>
<td>19-21</td>
<td>I3</td>
<td>Intermediate output (for debugging) if ≠ 0</td>
</tr>
<tr>
<td>M (8)</td>
<td>22-24</td>
<td>I3</td>
<td>If ≠ 0, the monoenergetic contributions determined by DISCRT are converted to photon flux, and output but they are not added to the unfolded flu</td>
</tr>
<tr>
<td>M (9)</td>
<td>25-27</td>
<td>I3</td>
<td></td>
</tr>
</tbody>
</table>

-34-
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>M (10)</td>
<td>28-30</td>
<td>I3</td>
<td>If ≠ 0, subprograms DETECT and SOLN are bypassed in MAIN. (See Figure 2)</td>
</tr>
<tr>
<td>M (11)</td>
<td>31-33</td>
<td>I3</td>
<td>If ≠ 0, the unknown spectrum is corrected for interaction efficiency before pulse-height gain change reduction (See Figure 2)</td>
</tr>
<tr>
<td>M (12)</td>
<td>34-36</td>
<td>I3</td>
<td>If = 0, call GANE before iterative unfolding (See Figure 2)</td>
</tr>
<tr>
<td>M (13)</td>
<td>37-39</td>
<td>I3</td>
<td>If 0, by-pass SOLN (See Figure 2)</td>
</tr>
<tr>
<td>M (14)</td>
<td>40-42</td>
<td>I3</td>
<td>If ≠ 0, by-pass DETECT (efficiency) in subprogram SOLN (See Figure 12)</td>
</tr>
<tr>
<td>M (15)</td>
<td>43-45</td>
<td>I3</td>
<td>If ≠ 0, assume efficiency vector elements = unity in subprogram SOLN (See Figure 12)</td>
</tr>
<tr>
<td>M (16)</td>
<td>46-48</td>
<td>I3</td>
<td>If ≠ 0, do not correct for source decay, i.e., assume decay factor = 1.0</td>
</tr>
<tr>
<td>M (17)</td>
<td>49-51</td>
<td>I3</td>
<td>If ≠ 0, output the PHA spectrum</td>
</tr>
<tr>
<td>M (18)</td>
<td>52-54</td>
<td>I3</td>
<td>If ≠ 0, bypass final result computations, i.e., bypass GEOMTR</td>
</tr>
<tr>
<td>M (19)</td>
<td>55-57</td>
<td>I3</td>
<td>If ≠0, Equation (14) used instead of equation (13).</td>
</tr>
</tbody>
</table>

NOTE: The choice of non-zero values required for M (I) is arbitrary, however, actual subscript index values will aid in identity, e.g., if M (7) ≠ 0 then input as = 7. Options M(19) to M(24) are spare.

Card (4) (single card; last 5 variables may be blank)

ELIMIT | 1-10 | F10.5 | The energy of the upper edge of the response matrix highest channel (MeV); should correspond to unknown spectra to be analyzed. e.g. if unknown 400 channel spectrum has 2.615 MeV calibrating peak in channel 380, then ELIMIT = (400/380)*2.615 = 2.753 MeV
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>ØJSØ</td>
<td>11-20</td>
<td>F10.5</td>
<td>Loop limit; number of sets of source data (card sets 7 through 8, except 8, before loopback to READ card 2).</td>
</tr>
<tr>
<td>ØMM</td>
<td>21-30</td>
<td>F10.5</td>
<td>If &lt; 0 READ a response matrix, (card set 5B), = 0 use already computed matrix. &gt; 0 generate new matrix; call RESFUN. Choice of values are arbitrary, e.g. -1. and +1.</td>
</tr>
<tr>
<td>ØN</td>
<td>31-40</td>
<td>F10.5</td>
<td>The size of the response matrix, i.e. number of channels; also the size of final flux spectra, ≤ 40.0.</td>
</tr>
<tr>
<td>HITMAX</td>
<td>41-50</td>
<td>F10.5</td>
<td>The maximum number of unfolding iterations; an even number such as 50.0 unless iterating output per M (3) required. ≤ 100.0.</td>
</tr>
<tr>
<td>EPS</td>
<td>51-60</td>
<td>F10.5</td>
<td>Convergence tolerance at which iteration will cease. e.g. .0001.</td>
</tr>
<tr>
<td>RX</td>
<td>61-66</td>
<td>F6.4</td>
<td>Radius of Ge(Li) active region (cm).</td>
</tr>
<tr>
<td>H</td>
<td>67-72</td>
<td>F6.4</td>
<td>Cylindrical length of Ge(Li) active region (cm).</td>
</tr>
</tbody>
</table>

NOTE: RX and H set equal to 1.63 and 3.1, respectively in two statements following read statement (in MAIN); if other values to be input, remove these statements.

Also,

Card 5

Card 5 refers to a deck of cards of which two kinds are allowable, namely: 5A or 5B. 

Card set 5A to be input, if ØMM > 0 (read by subprogram RESFUN to generate a response matrix).
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card Set 5B</td>
<td>to be input if $\phi M M &lt; 0$ (response matrix input to program MAIN).</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Neither set to be input if $\phi M M = 0$, i.e. a correct response matrix is assumed as existing in storage.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card Set 5A (Standard source spectra and associated parameters)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card 5A - 1 (single card) (See Figure 4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NSTAND</td>
<td>1-5</td>
<td>I5</td>
<td>The number of standard source spectra.</td>
</tr>
<tr>
<td>NXLIM</td>
<td>6-10</td>
<td>I5</td>
<td>Number of channels in each standard spectrum.</td>
</tr>
<tr>
<td>NADD</td>
<td>11-15</td>
<td>I5</td>
<td>The number of standard spectra with energy, STDEN (J, 1) 1.33 MeV</td>
</tr>
<tr>
<td>Card Set 5A - 2.1 (Single card preceding each spectrum) (See Appendix III)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ALABEL (I), BLABEL (I)</td>
<td>2-6</td>
<td>2A3</td>
<td>Standard source identity; user choice e.g. CS137.</td>
</tr>
<tr>
<td>STDEN (J, 1)</td>
<td>11-20</td>
<td>F10.5</td>
<td>Energy corresponding to standard source spectrum photopeak (MeV) (highest energy if two peaks, e.g. 1.33 for Co$^{60}$ and 1.114 for Zn$^{65}$).</td>
</tr>
<tr>
<td>STDEN (J, 2)</td>
<td>21-30</td>
<td>F10.5</td>
<td>Energy corresponding to standard source spectrum photopeak (MeV) (lowest energy if two peaks, e.g. 1.17 for Co$^{60}$ and 0.511 for Zn$^{65}$).</td>
</tr>
<tr>
<td>SHIFT (I)</td>
<td>31-40</td>
<td>F10.5</td>
<td>The channel location ($\Delta$) of the standard spectrum true zero pulse-height. The code carries out a shift correction.</td>
</tr>
<tr>
<td>MENSJ</td>
<td>41-45</td>
<td>I5</td>
<td>Approximate mean pulse-height of standard source spectrum photopeak corresponding to STDEN (J, 1) (channel)</td>
</tr>
<tr>
<td>MSØ</td>
<td>46-50</td>
<td>I5</td>
<td>Atomic number corresponding to standard source spectrum (e.g. 60 for Co$^{60}$ and 203 for Hg$^{203}$).</td>
</tr>
<tr>
<td>NAME</td>
<td>COLUMN</td>
<td>FORMAT</td>
<td>DESCRIPTION, PURPOSE OR USE</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>---------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>MSXJ</td>
<td>51-55</td>
<td>I5</td>
<td>Replace region from channel MSXJ to MFXJ with straight line, e.g. use for removal of 0.073 MeV Hg\textsuperscript{203} X-ray (channel).</td>
</tr>
<tr>
<td>MFXJ</td>
<td>56-60</td>
<td>I5</td>
<td>Replace region from channel MSXJ to MFXJ with straight line, e.g. use for removal of 0.073 MeV Hg\textsuperscript{203} X-ray (channel).</td>
</tr>
<tr>
<td>MENCS</td>
<td>61-65</td>
<td>I5</td>
<td>Replace initial ENCS + 1 (channel).</td>
</tr>
</tbody>
</table>

Card Set 5A - 2.2 (NXLIM/10 (rounded-up) cards); (See Appendix III)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R (1, 1)</td>
<td>1-7</td>
</tr>
<tr>
<td>R (2, 1)</td>
<td>8-14</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>R (10, 1)</td>
<td>63-70</td>
</tr>
<tr>
<td>R (11, 1)</td>
<td>1-7</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>R (NXLIM, 1)</td>
<td>-</td>
</tr>
</tbody>
</table>

NOTE: Repeat Card 5A - 2.1 and Card Set 5A - 2.2 for each standard source spectrum i.e. NSTAND times; the lowest energy standard must be input first and the remainder must be in energy ascending order (with respect to STDEN (J, 1)).

Card Set 5B (Response matrix)

Card Set 5B - 1 ((\(\text{\(\Omega\)} N \times \text{\(\text{\(\Omega\)} N/5\) Cards}); ((R(J, I), I = 1, \(\text{\(\Omega\)} N\), J = 1, \(\text{\(\Omega\)} N\))

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R (1, 1)</td>
<td>1-11</td>
</tr>
<tr>
<td>R (1, 2)</td>
<td>12-22</td>
</tr>
<tr>
<td>NAME</td>
<td>COLUMN</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>R (1, 3)</td>
<td>23-33</td>
</tr>
<tr>
<td>R (1, 4)</td>
<td>34-44</td>
</tr>
<tr>
<td>R (1, 5)</td>
<td>45-55</td>
</tr>
<tr>
<td>R (1, 6)</td>
<td>1-11</td>
</tr>
</tbody>
</table>

(second card)

R (F, 0N) 45-55 E11.4 " " " " 0N, 0N

NOTE: The first 0N elements input represent the lowest energy matrix vector spectrum (analogous to a PHA spectrum); similarly, the second 0N elements, etc. The sum over each vector must = unity.

Card 6P -2 (single card)

NSTAND 1-10 I10 Number of cards in 5B -3.

K 11-20 I10 Index of first non-zero increment in response matrix.

Card Set 6P -3 (NSTAND cards)

(Photopake calibration energies, pulse-heights and standard deviations e.g. from a previous RESFUN output.)

STDEN (1,1) 1-10 F10.5 First calibration energy (MeV).

PARAV (1,1) 11-20 F10.5 First calibration photopeak pulse-height (channels).

PARAS (1,1) 21-30 F10.5 First calibration photopeak Gaussian standard deviation (channels).

...

STDEN (NSTAND,1) 1-10 F10.5 NSTAND calibration energy (MeV).

PARAV (NSTAND, 1) 11-20 F10.5 NSTAND calibration photopeak pulse-height (channels).

PARAS (NSTAND, 1) 21-30 F10.5 NSTAND calibration photopeak Gaussian standard deviation (channels).
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card 6 (two cards)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>First Card:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BTAG, BTAGA</td>
<td>2-6</td>
<td>A4, A2</td>
<td>Unknown source identity (alphanumeric)</td>
</tr>
<tr>
<td>SBETA</td>
<td>11-20</td>
<td>F10.5</td>
<td>Unknown source strength (Curies); see page 27 footnote.</td>
</tr>
<tr>
<td>EBMAX</td>
<td>21-30</td>
<td>F10.5</td>
<td>Unknown source maximum or reference energy (MeV) (see page 27 footnote).</td>
</tr>
<tr>
<td>CYLDIA</td>
<td>31-40</td>
<td>F10.5</td>
<td>Unknown source cylindrical diameter (cm).</td>
</tr>
<tr>
<td>TH</td>
<td>41-50</td>
<td>F10.5</td>
<td>Unknown source half-life (optional units; see UT this card).</td>
</tr>
<tr>
<td>RUNS</td>
<td>51-60</td>
<td>F10.5</td>
<td>Number of spectra per unknown source data set, ≤ 20.0.</td>
</tr>
<tr>
<td>CHANLS</td>
<td>61-66</td>
<td>F6.0</td>
<td>Number of channels in unknown spectrum ≤ 400. If &gt; 400, use CHANLS = 400 and refer to MNX (See next card)</td>
</tr>
<tr>
<td>UT</td>
<td>67-72</td>
<td>F6.0</td>
<td>Multiplier for TH:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>UT = 0.0; TH in years</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= 1.0; TH in seconds</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= .60.0; TH in minutes</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= 24.0; TH in hours</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= 365.0; TH in days</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(Values other than these will cause output of error flag followed by CALL EXIT)</td>
</tr>
<tr>
<td><strong>Second Card:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M222</td>
<td>1-5</td>
<td>I5</td>
<td>The number of peaks to be fitted with a Gaussian for which channel limits must be input (per card set 13) ≥ 20-M66; See card set 10 note.</td>
</tr>
</tbody>
</table>
| M66     | 6-10   | I5     | The number of peaks to be fitted with a Gaussian for which only the energy is to be input (per card set 10); ≥ 20-M22.
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>MZ</td>
<td>11-15</td>
<td>I5</td>
<td>The number of channels, in each unknown spectrum, which are to be loaded with zero counts (beginning at channel 1).</td>
</tr>
<tr>
<td>MNX</td>
<td>16-20</td>
<td>I5</td>
<td>Unknown spectra of MNX channels may be input to code</td>
</tr>
<tr>
<td>MBX</td>
<td>21-25</td>
<td>I5</td>
<td>Same as MNX, except that it refers to background spectra.</td>
</tr>
<tr>
<td>MSM</td>
<td>26-30</td>
<td>I5</td>
<td>If ≠ 0, smooth spectra before analysis; use 1.0 or 2.0 for single or double smoothing pass by subprogram GANE.</td>
</tr>
<tr>
<td>MS</td>
<td>31-35</td>
<td>I5</td>
<td>Subroutine FIND will &quot;search&quot; for peaks from channel MS to MX.</td>
</tr>
<tr>
<td>MX</td>
<td>35-40</td>
<td>I5</td>
<td>Subroutine FIND will &quot;search&quot; for peaks from channel MS to MX.</td>
</tr>
</tbody>
</table>

**NOTE:** BTAG/BTAGA, SBETA and EBMAX may be 'blank', 1.0 and 1.0 respectively, if not known prior to analysis. Actual values are used only for normalizing in subprogram GEOMTR prior to output of analysis results; see page 27 footnote.

**Card Set 7**

"Number of cards in set (7)" = RUNS. Input of card I = 1 detailed below, cards 2 to RUNS similar. Card order must correspond to related pulse-height analyzer unknown spectra, I ≥ 20.0.

If number of channels in the unknown spectrum is > 400 then specify the value as MNX and input CHANLS = 400 (see last card).

**DOST (I)**

<table>
<thead>
<tr>
<th>DOST (I)</th>
<th>1-10</th>
<th>F10.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance from unknown source to front face of Ge(Li) active region (cm).</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**DELT (I)**

<table>
<thead>
<tr>
<th>DELT (I)</th>
<th>11-20</th>
<th>F10.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Live time counting duration for unknown spectrum (minutes).</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NAME</td>
<td>COLUMN</td>
<td>FORMAT</td>
</tr>
<tr>
<td>-------------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>TM1 (I)</td>
<td>21-30</td>
<td>F10.5</td>
</tr>
<tr>
<td>TTZ (I)</td>
<td>31-40</td>
<td>F10.5</td>
</tr>
<tr>
<td>BK (I)</td>
<td>41-50</td>
<td>F10.5</td>
</tr>
<tr>
<td>BNBK (I)</td>
<td>51-60</td>
<td>F10.5</td>
</tr>
</tbody>
</table>

**Card (8)** (one card input if M (3) ≠ 0)

This card may contain up to 18 integer numbers to define the iterating or unfolding loop at which intermediate output is desired. ≥ eighteen indices may be input. The card format is 18I4.

Example:

- **MN (1)**: 1-4, Iterating loop index e.g. 3
- **MN (2)**: 5-8, Iterating loop index e.g. 5
- **MN (3)**: 9-12, Iterating loop index e.g. 9

will cause subprogram RESMAT to output on iterating loops 3, 5 and 9.

**Card Set (9)** (RUNS cards (rounded-up) to be input if M (4) ≠ 0)

- **NIX (1)**: 1-5, Replace a peak (or other prominence in spectrum 1 of card set (12) with a straight line from channel NIX (1) to N2X (1); the count rate in M1X (1) and N2X (1) are used to determine the slope and intercept of a straight line replacement.
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2X (1)</td>
<td>6-10</td>
<td>I5</td>
<td>See above.</td>
</tr>
<tr>
<td>NFILL (1)</td>
<td>11-15</td>
<td>I5</td>
<td>Replace in unknown spectrum 1 of card set (12), channels 1 to (NFILL (1) -1) with a straight</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>line of slope VAL (1) based on the count in channel NFILL (1).</td>
</tr>
<tr>
<td>VAL (1)</td>
<td>16-25</td>
<td>F10.5</td>
<td>Same as above.</td>
</tr>
<tr>
<td>N1X (2)</td>
<td>26-30</td>
<td>I5</td>
<td>Same as N1X (1) only for second spectrum.</td>
</tr>
<tr>
<td>N2X (2)</td>
<td>31-35</td>
<td>I5</td>
<td>Same as N2X (1) only for second spectrum.</td>
</tr>
<tr>
<td>NFILL (2)</td>
<td>36-40</td>
<td>I5</td>
<td>Same as NFILL (1) only for second spectrum.</td>
</tr>
<tr>
<td>VAL (2)</td>
<td>41-50</td>
<td>F10.5</td>
<td>Same as VAL (1) only for second spectrum.</td>
</tr>
</tbody>
</table>

**NOTE:** VAL (9) would be the fourth and last field of fifth card for RUNS = 9; the number of cards (≥ 10) depends on RUNS.

**Card Set 10 (1 to 4 cards input if M6 ≠ 0)**

This card set is input only when M6 ≠ 0. It must consist of M6/5 (rounded-up) cards corresponding to the number of unknown energy-specified peaks in the card set (12) spectra. Each card contains ≥ 5 photopeak photon energies corresponding to the unknown complex-plus-continuous spectrum to be analyzed. From one to 20 (= M222) photopeaks may be energy specified per spectrum i.e. a maximum of 4 cards per spectrum.

| EU (1)      | 1-10    | F10.5  | Energy of the first energy specified photopeak in card set 12 spectra (MeV).              |
## NAME

| EU (2) | 11-20 | F10.5 | Energy of the second energy-specified photopeak in card set 12 spectra (MeV). |
| EU (3) | 21-30 | F10.5 | Similar to above. |

NOTE: The first photopeak in each spectrum is that of lowest energy with the remainder being in energy ascending order. The user is cautioned that peak channels may also be input instead or in addition, per card set if M22 ≤ 0; M22 + M6 ≥ 20.

**Card Set (1) (1*RUNS to 7*RUNS cards input if M22 ≠ 0) (See Figure 12)**

This card set is input only when M22 ≠ 0. It must consist of (M22/3 (rounded-up) cards corresponding to the number of unknown channel-limit specified spectral photopeaks in card set 12. Each card contains information for ≥ 3 photopeaks. The information advises the code of whether peak is a single peak or is instead one of a pair, of the upper and lower fitting limits (channels) and of the energy if it is not known.

| NJ (1) | 1-4 | I4 | Signal for first channel-limit-specified peak of set 12 spectra: |
| NSS (1) | 5-8 | I4 | Channel number defining fitting limit on low energy side of first channel-limit-specified peak, i.e. fit peak from channel NSS (1) to NFNN (1). |
| NFNN (1) | 9-12 | I4 | Channel number defining fitting limit on high energy side of first channel-limit-specified peak, i.e. fit peak from channel NSS (1) to NFNN (1). |
| EU (1) | 13-20 | F8.4 | Energy of first specified peak (MeV). |
NAME | COLUMN | FORMAT | DESCRIPTION, PURPOSE OR USE
---|---|---|---
NJ (2) | 21-24 | I4 | Similar to NJ (1).

EU (3) | 53-60 | F8.4 | Similar to EU (1).
NJ (4) | 1-4 | I4 | Similar to NJ (1).
EU (M22) | - | F8.4 | Similar to EU (1).

NOTE: The user is cautioned that peak energy data may also be input instead or in addition, per card set (10) if M66 = 0; M222 + M66 >= 20. If M66 = 0 and M222 = 0 then photopeaks data may be input in any energy order; if M66 = 0 and M222 = 0 then input is expected in energy ascending order. Where data is input for double peaks NJ (I) and NJ (I + 1) = 2 and 0, respectively, then energy ascending order is expected if (I and I + 1) = 2 and 3, is given:

<table>
<thead>
<tr>
<th>NJ (2)</th>
<th>NSS (2)</th>
<th>NFNN (2)</th>
<th>EU (2)</th>
<th>NJ (3)</th>
<th>NSS (3)</th>
<th>NFNN (3)</th>
<th>EU (3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>46</td>
<td>-</td>
<td>0.501</td>
<td>0</td>
<td>7</td>
<td>66</td>
<td>0.575</td>
</tr>
</tbody>
</table>

This specifies that the code shall carry out a double peak analysis between channels 46 and 66, that peak energies are 0.501 and 0.575 MeV and that the peaks are approximately 7 channels apart. The code analysis will determine the actual separation distance and thus 7 is given only as an estimate.

Card Set (12)
The number of cards in this set = (CHANLS * RUNS/10.0 + the number of background cards if any)*. The cards will contain the unknown source spectra to be unfolded. The number of spectra which may be input is limited by the DIMENSION (20) = RUNS. The spectra, corresponding to card sets 6 and 7, may be stacked together. A background spectrum, if input, must directly follow the unknown spectrum from which it is to be subtracted. Twenty unknown spectra, each followed by a background spectrum, are regarded as twenty spectra from the standpoint of 20 being the maximum number. Each spectrum contains CHANLS (or MNX) channels and background spectra must correspond*. Each card contains 10 channels of information. Thus, the following is typical of card set (12) as read by subprogram DEC:

-45-
<table>
<thead>
<tr>
<th>NAME</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>DESCRIPTION, PURPOSE OR USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>S (1)</td>
<td>1-7</td>
<td>F7.1</td>
<td>Pulse-height analyzer count in channel 1.</td>
</tr>
<tr>
<td>S (2)</td>
<td>8-13</td>
<td>F7.1</td>
<td>Pulse-height analyzer count in channel 2.</td>
</tr>
<tr>
<td>S (3)</td>
<td>15-20</td>
<td>F7.1</td>
<td>Pulse-height analyzer count in channel 3.</td>
</tr>
<tr>
<td>S (10)</td>
<td>64-70</td>
<td>F7.1</td>
<td>Pulse-height analyzer count in channel 10.</td>
</tr>
<tr>
<td>S (11)</td>
<td>1-7</td>
<td>F7.1</td>
<td>Pulse-height analyzer count in channel 11.</td>
</tr>
<tr>
<td>S (CHANLS)*</td>
<td>-</td>
<td>F7.1</td>
<td>Pulse-height analyzer count in channel CHANLS.*</td>
</tr>
</tbody>
</table>

(last card in spectrum)

*For input purposes, if MNX > CHANLS then replace CHANLS above with MNX for unknown and MBX for backgrounds, i.e. CUGEL will read spectra up to 1024 channels in size (per MNX and MBX) but will immediately reduce them to CHANLS = 400, by DEC calling GANE.
3.3 CODE OUTPUT

Throughout the discussion in this section, reference to Appendix IV, Sample Code Output Listing, is necessary and understood. Those outputs which are clearly defined by format headings are either not discussed or are mentioned only briefly. Output pages are referred to through the encircled letters A, B, C, etc.

A. The values on this page are output by MAIN, and are as input on card sets 1 to 4, with the exception of EM(=EN/ELIMIT).

B. The values on this page are output by RESFUN, and correspond to those standard source spectral parameters input on card sets 5A -1 and -2. Indicated channel numbers are those values after shifting with respect to true zero channel has been carried out.

C. The values on this and following similar pages are the standard source spectral counts corrected for input in the complement mode and true zero channel. This output by RESFUN corresponds to card set 5A -3 input.

D. The results of the Gaussian function regression analysis by STDFT3 for the standard spectra photopeaks are output on these two pages by SPNORM. The output is for the two photopeak energies STDEN (1,1) and STDEN (1,2) and is otherwise self-explanatory.

E. The output on this and the following similar pages, by RESFUN, consists of the Compton continua of the standard source spectra normalized with respect to unit photopeak area and pulse-height. The integral normalized count for the continuum and photofraction are also output.

-47-
F. This page presents the response matrix generated by RESFUN and output by MAIN. It corresponds to that input which would be required for card set 5B -1.

G. This page presents the energies (MeV), pulse-heights (channels) and photofractions corresponding to the generated response matrix, at increment midpoints, as determined by RESFUN and output by MAIN. The photofractions correspond to the solid curve in Figure 4. Standard spectra photopeak standard deviations in channels for unit pulse-height are also output.

H. The output on this page, by MAIN, corresponds to the input specified for card sets 6 and 7, excepting that the units in some cases are modified before output and are as indicated.

I. Optional output by MAIN giving the indices for which unfolding iteration output has been requested by input of card 8.

K. The output on this page by MAIN corresponds to the (first) spectrum to be analyzed and as input on card set 12. Background spectrum subtraction and complement mode correction is carried out before output.

L. Output of spectrum before entry to DISCRT.

M. The output on this page by DISCRT is self-explanatory and refers to the fitting of an monoenergetic spectral component of the unknown spectrum.
N. The output gives the PHA spectrum after stripping of photopeaks and associated continua by SINGLE; gain parameters for subsequent unfolding are also output. The optionally subtracted discrete peak photon number flux at the detector is also given.

O. The output on this page by MAIN corresponds to the unknown spectrum after gain changing and before unfolding analysis.

P. The output on this page by RESMAT is that requested by input of card 8. It consists of the gain changed unknown spectrum normalized to unit integral count; output at loop IT, corresponding to that requested (per MN), of the determined photon number spectrum (PHI) and the iterated input spectrum (PP); the iterated spectrum and the iteration convergence loop (IT), the normalizing integral count (SU); the final value of the iteration arresting criterion term (TERM = $\chi^2$, Pearson's Chi Square); and the rate of convergence or fitting differences, during unfolding ($\Delta\chi^2$).

Q. The output on this page by DETECT is self-explanatory and consists of the components of the diagonal efficiency matrix, $n$, defined by Equation (13) of Section 2.2.4.

R. The optional output on this page by MAIN, consists of the efficiency corrected and unfolded spectrum after post-normalization.

S. The optional output on this page, by MAIN, is self-explanatory and consists of $N_x(E)$ and $I_x(E)$, as already discussed in Section 2.2.5.

T. The output on this page, by MAIN, is self-explanatory and consists of SUMNUM, SUMENY, D (Equation 14), AVENGY, etc., in order of, and as already discussed in, Section 2.2.5.
4. SUMMARY AND CONCLUSIONS

A FORTRAN-V, UNIVAC 1108 package code --- CUGEL, has been developed for the rapid analysis of complex gamma photon spectra. The code is readily applicable to the analysis of Ge(Li) semiconductor detector complex-continuous spectra. The response matrix generating portion of the code is suitable for use as a separate entity for problems in spectral analysis such as are frequently encountered in the various fields of gamma spectrometry.

The code employs an iterative unfolding method which has been used successfully by its authors: N. E. Scofield and R. Gold, by the present author and others. While this method is necessarily approximate because of the iterative technique used, it is most suitable where continuous spectra are involved. It is suggested that degree of accuracy be the subject of future work, wherein the iterative method results would be compared with results obtained by other methods. The best value of the matrix size consistent with non-oscillatory good results and computer efficiency would be of interest here. The present contract did not allow for detail studies during the development of code CUGEL.

It is proposed that the response matrix generating portion of the code be made more versatile by studying the use of additional standard sources. A detailed debugging of the code in energy range 1.4 to 3.0 MeV was not possible because of the lack of standard spectra in this range.

It is proposed that standard spectra generated by the Monte Carlo technique be considered for energies in the range 3.0 to 10.0 MeV. NUS has developed such an NaI(Tl) scintillation detector code --- NUGAM-3 --- for NASA/GSFC under contract NAS5-11781. NUGAM-3 considers the crystal cladding and associated photomultiplier. A Ge(Li) code version may be efficiently adapted from NUGAM-3.
It is concluded that the developed code CUGEL is an operable and useful addition to the field of gamma photon spectrometry. It allows the semi-automatic generation of Ge(Li) detector system response function matrices, spectral unfolding process and final analysis of unknown complex-continuous spectra to be carried out in a single computer run; i.e., without human interfacing. It is very suited for modification to on-line applications.
REFERENCES


12. Lazar, N. H., Davis, R. C., and Bell, P. R., "Peak Efficiency of NaI", Nucleonics, p. 52 (April 1956).


19. Rieir, M., Jet Propulsion Laboratory, Private Communication (July 1970)


Figure 1
CODE CU GEL SUBPROGRAM CONNECTIVITY
Figure 2
CODE CUGEL MAIN PROGRAM SIMPLIFIED FLOW DIAGRAM
Figure 3
COMPARISON OF STANDARD SOURCE AND CODE GENERATED COMPTON CONTINUUM, PULSE-HEIGHT NORMALIZED TO UNIT AREA PHOTOPAKE
Figure 5
PHOTOPEAK STANDARD DEVIATION
FOR FITTED GAUSSIAN AS A FUNCTION OF ENERGY
Figure 6
VARIATION OF COMPTON EDGE AND BACKSCATTER PEAK PULSE HEIGHTS (Vc and Vb) AS A FUNCTION OF PHOTON ENERGY.
FIGURE 7

FLOW DIAGRAM SHOWING THE GENERAL LOGIC OF SUBPROGRAM RESMAT

P = INPUT SPECTRUM
R = RESPONSE MATRIX
N = OUTPUT PHOTON SPECTRUM
k = ITERATION INDEX
k_{max} = MAX. ALLOWED ITERATIONS
P' = ITERATED SPECTRUM \Rightarrow P
FIG. 9
GEOMETRY FOR EQUATION (12)
Figure 10
PHOTOPEAK EFFICIENCY ($P \cdot C$) AS A FUNCTION OF PHOTON ENERGY

Equation (12)

Equation (14)
Figure 11
GENERAL ARRANGEMENT FOR INPUT CARD DATA DECK
SUBPROGRAM SOLN SIMPLIFIED FLOW DIAGRAM

Figure 12
APPENDIX I

GLOSSARY OF SUBPROGRAMS
APPENDIX I

GLOSSARY OF PROGRAMS FOR CODE CUGEL
(In alphabetical order, except for MAIN)

<table>
<thead>
<tr>
<th>NUMBER</th>
<th>NAME</th>
<th>FUNCTION or USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>MAIN</td>
<td>Input, output and linking of subprograms.</td>
</tr>
<tr>
<td>2</td>
<td>ADPEAK</td>
<td>Adds photopeaks to interpolated Compton continua.</td>
</tr>
<tr>
<td>3</td>
<td>AIRABS</td>
<td>Computes air attenuation factor.</td>
</tr>
<tr>
<td>4</td>
<td>ALUM</td>
<td>Computes Ge(Li) detector aluminum absorber attenuation factors.</td>
</tr>
<tr>
<td>5</td>
<td>BBS</td>
<td>Interpolates normalized backscatter peaks.</td>
</tr>
<tr>
<td>6</td>
<td>BS</td>
<td>Normalizes and subtracts backscatter peaks.</td>
</tr>
<tr>
<td>7</td>
<td>DEC</td>
<td>Reads pulse-height analyzer spectra; checks for PHA-complemented counts.</td>
</tr>
<tr>
<td>8</td>
<td>DECAY</td>
<td>Computes source decay correction factor.</td>
</tr>
<tr>
<td>9</td>
<td>DETECT</td>
<td>Controls computation of Detector total efficiency.</td>
</tr>
<tr>
<td>10</td>
<td>DISCRT</td>
<td>Determines monoenergetic spectral contribution in unknown spectra.</td>
</tr>
<tr>
<td>11</td>
<td>DØSE</td>
<td>Converts gamma photon flux to exposure dose.</td>
</tr>
</tbody>
</table>

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<table>
<thead>
<tr>
<th>NUMBER</th>
<th>NAME</th>
<th>FUNCTION or USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>EFFIC2</td>
<td>Computes elements of detector interaction efficiency vector. (F)</td>
</tr>
<tr>
<td>13</td>
<td>FC</td>
<td>Ge(Li) interaction efficiency function. (F)</td>
</tr>
<tr>
<td>14</td>
<td>FIND</td>
<td>Determines location of photopeaks in unknown spectra.</td>
</tr>
<tr>
<td>15</td>
<td>FITLIN</td>
<td>Determines continuum base for backscatter and photopeaks.</td>
</tr>
<tr>
<td>16</td>
<td>FUNZ</td>
<td>Photopeak fitting function, partial derivatives and Chi-square term for STDFT3.</td>
</tr>
<tr>
<td>17</td>
<td>GANE</td>
<td>Gain changing program; also spectral shifting and smoothing.</td>
</tr>
<tr>
<td>18</td>
<td>GEØMTR</td>
<td>Computes geometry factors, integrates number and energy spectra and calculates normalized dose data for final code results.</td>
</tr>
<tr>
<td>19</td>
<td>GUESS3</td>
<td>Provides initial estimates of the photopeak function parameter for non-linear regression analysis in subprogram STDFT3, for double peaks.</td>
</tr>
<tr>
<td>20</td>
<td>PKFUN</td>
<td>Control program for photopeak fitting and subtraction.</td>
</tr>
<tr>
<td>21</td>
<td>POGELI</td>
<td>Interpolates normalized Compton continua by the method of parts.</td>
</tr>
<tr>
<td>22</td>
<td>RESFUN</td>
<td>Control program for response matrix generation.</td>
</tr>
<tr>
<td>NUMBER</td>
<td>NAME</td>
<td>FUNCTION or USE</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>-------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>23</td>
<td>RESMAT</td>
<td>Pulse-height analyzer spectrum unfolding according to the Scofield algorithm.</td>
</tr>
<tr>
<td>24</td>
<td>SIMPSN</td>
<td>Simpson's rule integrating program for function FC.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(F)</td>
</tr>
<tr>
<td>25</td>
<td>SØLN</td>
<td>Control program for unfolding and detector efficiency correction.</td>
</tr>
<tr>
<td>26</td>
<td>SPNØRM</td>
<td>Orders and normalizes standard spectra for response matrix interpolation.</td>
</tr>
<tr>
<td>27</td>
<td>STDFT3</td>
<td>Non-linear regression analysis of standard spectra photopeaks.</td>
</tr>
<tr>
<td>28</td>
<td>TA</td>
<td>Binary table searching program.</td>
</tr>
<tr>
<td>29</td>
<td>TE</td>
<td>n-degree Lagrangian interpolation program.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(F)</td>
</tr>
<tr>
<td>30</td>
<td>VECTMX</td>
<td>Determines the index and value of the maximum valued element in a vector of elements.</td>
</tr>
<tr>
<td>31</td>
<td>XPLØT</td>
<td>Plots spectral distributions.</td>
</tr>
</tbody>
</table>
APPENDIX II

FORTRAN CARD DECK LISTING
CLAMDA=ALOG((2+0)/TH
C
C CALL DEC (NX*FM+MNX)
C IF(NNX=1+1)22222+11
C 11 CALL DEC (NX+BNX)
C 6 DO 3 J=1+NX
3 FM(1+FM(1+FMGM=1+1)
22222 CONTINUE
WRITE(LO+32+2,1) J=1+JTAG+UTAGA+(FM(1)+1+NX)
25123 FORMAT('I17H SPECTRUM NUMBER ,13+5H FOR A A source //
13+5H (AFTER BACKGROUND SUBTRACTION) // (1X+10F8.0)
T2=T2(J)
N2=N2
GAIN=N2=T2
SLOPE=ELIMIT/GAIN
SNR=0.0
IF(N2=1+J) 3230,3234,3230
3230 NX1=NX(J)
NX2=NX2(J)
NX1+iNX1
NX2+iNX2
SLP=(FM(NX2)-FM(NX1))/(NX2-NX1)
NX1=NX1+1
NX2=NX2+1
DO 3231 I=NX1+NX2
X=X+NX1
3231 FM(1)=FM(NX1)+SLP*X
WRITE(LO,NX2391NX1+NA2
3234 IF(NFILL(1)) 3232,3233,3232
3232 IF((VAL(J))=3235,3236,3235
3235 NX2+NFILL(J)
NX1=1
FILL = NX2
SLP = (FM(NX2)-FM(NX1))/FILL
NX1=NX1+1
NX2=NX2+1
DO 3237 I=1+NX1+NX2
X=X+NX1
3237 FM(1)=VAL(J)+SLP*X
WRITE(LO+7232+1NX22+SLP+VAL(J)
7242 FORMAT (AM FIRST 1+4+2+4+4+4H DEAD CHANNELS FILLED PER FM(1)*MNX+C WH
ERE M = E14.7+9H AND C = E14.7.
GO TO 3233
3236 NX2 = NFILL(J)+1
NX1 = NFILL(J)
DO 3238 I=1+NX2
SLP=S0.0
WRITE(LO+72+1NX1+2+SLP+FM(NX1)
3233 CONTINUE
WRITE(LO+7232+1NX2+SLP+FM(NX1)
7878 CALL GANE(TZ+M+NAX+GAIN+ROGAIN+5+FM)
WRITE(LO+8552+NZ)+GAIN+ROGAIN+(FM(1)+1+1N)
8552 FORMAT (0H INPUT SPECTRUM GAIN CHANGED TO
1/2M GAIN CHANGE RATIO = +F10.5+1M/ +F10.5 // (1X+5E14.7))
C
C CALL DISCRT. (FM*ETA+NX+RX+TLKLM+M19)
C
C CALL DISCRT. (FM*ETA+NX+HOGAIN+SM)+(FM(1)+1+1N)
22332 FORMAT(1H+4+3H GAIN PARAMETERS AFTER CAL SING IN MAIN
1/1X+1F8.3+15,3F10.4/(1X+10F8.0))
15493 IF(M(9)) 300,306,300
300 WRITE(LO,202)
302 FORMAT(0H+AM TRACTED DISCRETE PEAK PHOTON NUMBER Flux //
13X+5H INDEX+4+8+10ENERGY+17X+I11 NUMBER FLUX /
25X+5H(VEV)+4+10+11H(PHOTONS/CN+2-SEC) //)
DEF=DECAY(IT,TH+IN,CLAMDA)
DO 301 I=1+IN
PHOT((1)=DEFPHOT(1)/UT+60.3+4.14159265+RX+RX)
WRITE(LO+303)(EI+1+I)+PHOT(1)
303 FORMAT(1H+34+X+12+Z+3+2.5)
301 CONTINUE
C
C CALL DISCRT. (FM*ETA+NX+HOGAIN+SM)+(FM(1)+1+1N)
32330 FORMAT(1H+15+5+I+6E14.7)
305 DO 305 I=1+IN
306 CONTINUE
IF(M(10)) 121,124+21
121 IF(M(11)) 110,113,110
110 ELENM
ELN=ELN11/GAIN
DELN=ELN2
DO 116 I=1+IN
116格式为5E14.7
C
C CALL DETECT (NS,NQ,N*ETA+DIST,入口,TLKLM+PFRAC+0)
C
C IF(M(17)) 132,202+11
202 DO 502 I=NS,N
502 FORMAT(1H+FM(1)=FM(1)+ETA(1)
M(14)=14
MF=1
113 IF(M(12)) 209,778,209
209 IF(M(13)) 120+112+206
C
C MAKE SPECTRUM COMPARABLE IN GAIN WITH RESP MATRIX
C
C 778 CALL GANE(TZ+M+NAX+GAIN+ROGAIN+5+FM)
WRITE(LO+8852+NZ)+GAIN+ROGAIN+(FM(1)+1+IN)
8852 FORMAT (0H INPUT SPECTRUM GAIN CHANGED TO
1/2M GAIN CHANGE RATIO = +F10.5+1M/ +F10.5 // (1X+5E14.7))
C
C 112 DO 213 N=NS,N
213 FORMAT(1H+N(1)
NPP=N+1
DO 205 N=NPP,N,LIM1
205 IF(1+1)=0
C
C CALL SOLN (NS*PHI+FM*ETA+DIST+入口,TLKLM+PFRAC+M19)
C
C WRITE(LO+2094)
8891 FORMAT 125H AT THE SOURCE CYLINDER //
1 7TH PHOTON DOSE / SOURCE EMITTED BETA NUMBER (R/HR)/(BETA/SEC)
2 = E14.7/92PH PHOTON DOSE / SOURCE EMITTED BETA NUM
3 NEW PEK SOURCE VOLUME ((R/HR)/(BETA/SEC))/(CM+3) = E14.7
500 CONTINUE
IF (JS=JS0) 1=1111.61
61 JS=JS+1
GO TO 2
111 IF (KK,LT,NSET) GO TO 1
STOP
END
IFOR15 ADPEAK
SUBROUTINE ADPEAK(FM+NAM+BL+82+B3+PH+NF)
************ PROGRAM NUMBER - 2 CUGEL ************

C ADDS PHOTON NUMBER TO INTERPOLATED COMPTON CONTINUA
C COMMON/L10/L10/L0LP+NLIMIT+NUMX+MOUT
DIMENSION FM(800)
SUM=0.0
NS=01=7.**B2 -1,
NF=81=1.***B2 +1.
IF (NS,LE,0.1NS=1.
IF (NF,GT,NS1=1
NDF=NG-NF)
52 IF (NSDIF=50,51,50,50)
51 ND=2*ND
NSDIF=NSDIF+NSDFID
GO TO 52
50 DNN=ND
D=0.6/(12.0*ONN)
DE=ON+DN
CONS=3.99943939/ON
C WRITE (LO,9918) B2,B3+DNN,DE,CNS,NS,ND,NSDFID
C 99 FORMAT (15H BS,BS, NS /1A7E15.4/15A4(1S))
DO 800 I=NS,1
X=1
X=X+1
C WRITE (LO,98) 1X+DN
C 98 FORMAT (3M 1+14+5A3) X=0.84+5A4MD= =14+4)
SAM=0.0
DO 900 I=1,ND
X=X+DE
PON=X B1/B2
PON2=PON+PON
ARH=0.5/PON2
IF (ARH,LT,2.0) 2=1,3
2=P=CONS*EXPI-AH*DE
FM(1)=FM(1)+P
SAM=SAM+P
C WRITE (LO,97) 1X+X+PO+PON2+AR+P+FM(1)
C 97 FORMAT (1M INODA+15+S16.E3)
3 CONTINUE
900 CONTINUE
SUM=SUM+SAM
800 CONTINUE
SUMP=0.
SUMP=SUM+SAM
555 SUMP=SUMP+FM(1)
DO 5555 I=1,1
5555 FM(1)=FM(1)+SUMP
PHI=1./SUMP
C WRITE (LO,96) NS,NS=1M+SMPF+B2+B3+SUMP(1+FM(1)+1=NS1
C 96 FORMAT (1H NS,NS=1M+SUMP+B2+B3+SUMP(1+FM(1))=113.61
RETURN

MK1IP=0
206 IF (MP,LT,122) 122
122 WRITE (LO,126) (PHI(1)1=1=1,1)
126 FORMAT (1H1+10PH PHOTON SPECTRUM CORRECTED FOR EFFICIENCY /15(2.xx1E12.
15))
M=0
GO TO 21
79 IF (MP10) 179,125,179
179 DO 79 JN=1,1N
D=0.16(1JN)*EM
1=0Y
1=1Y
71 IF (IY,LT,71) 71
71 N=K
GO TO 78
76 I=1+1
D=1Y
GO TO 74
73 N=1+1
73 N=1+1
78 PHI(NJ,K)=PHI(NJ,K)+PHI(JN)
GO TO 75
74 QY=QY+QY+0.5
TW=0.1-0.1Y
PHI(1)=PHI(1)+PHI(JN)*QY
PHI(1)=PHI(1)+PHI(JN)*QY
75 CONTINUE
70 CONTINUE
125 CONTINUE
20 WRITE (LO,20) IT
1 (PHI(I) 1=NS1
2020 FORMAT (1H DIFFERENTIAL FLUX AT ITERATION NUMBER = \+15/
1 (5XX1E12.51))
21 IF (MP10) 800,801,800
800 DE=1.0
GO TO 802
801 DE=DECAYTI,DT,TH,CM,CLMADL
802 CONTINUE
C WRITE (LO,2025) NS,FNM11,1NS1
C 2025 FORMAT (1H17 SINGLE SPECTRUM *1S+10CHANNELS \+11(1X10F9.0))
99 IF (MP10) 15+10+500
C 24 CALL GEOM1R (EXTNAT+XPHI+NS+XN+XDE+DIVOL+RA+DIST
C WRITE (LO,8890) 1+Q11PHI(1)1+EXTNAT+1+1NS1

8890 FORMAT (44HNUMER AND ENERGY SPECTRUM AT THE CRYSTAL //
1 19H INCREASE ENERGY+13X1+11+NUMBER FLUX+13X1+11ENERGY FLUX//
2 13X5+MEV)+10X1+1PHONI+CM+2SEC=/13X1+1MIN+CM+2SEC//
3 (1X,16+3+X+10.5+10.4+10+1E4.7+1E1.4+7.1)
WHITE (LO,8992)
8892 FORMAT (41H INTEGRATED RESULTS AT SOURCE AND CRYSTAL //
1 SUM ENERGY INTEGRATED PHOTON (BREMSS) VALUES AT THE CRYSTAL //)
C WRITE (LO,8895) SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM
900 FORMAT (85H SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM+SUM)
8895 FORMAT (37HPHOTON NUMBER (PHOTON/CM+2SEC) = E14.7/7.3TH PHOTON
1 ENERGY (MEV/CM+2SEC) = E14.7/7.3TH PHOTON DOSE (ROENTGENS/N)
20UKH) = E14.7/7.23H AVERAGE ENERGY (MEV) = E14.7/7.7TH PHOTON NUM
3MHER + 500 IM Emitted BETA NUMBER (PHOTON/CM+2SEC)/(BETA/SEC) =
4E14.7/7.7TH PHOTON ENERGY / SOURCE EMITTED BETA ENERGY (MEV/CM+2
SEC/MEV) = E14.7/7.7TH PHOTON ENERGY SOURCE EMITTED BETA ONE
61A NUMER (MEV/CM+2SEC)/(BETA/SEC) = E14.7/7.7TH PHOTON DOSE
7 SOURCE EMITTED BETA NUMBER (R/HR)/(BETA/SEC) = E14.7/7.7TH PHOTON DOSE
8 LINE ((5HHR)/(BETA/SEC))/(CM+3) = E14.7//)
WHITE (LO,8995) DOSCYL/DOSYOL
Bb(1)=BB(2)
CALL GUESS3(NS+NFN+SLINE+BB+V1+V2)
NPARA(1)=1
NPARA(2)=3
NPARA(3)=4
NPARA(4)=6
CALL STDF1(SLINE+BB+NFN+NS3+2,NPARA+NS3,FA+TITLE+1)
CALL STDF1(SLINE+HD+NFN+NS3+2,NPARA+NS3,FA+TITLE+0)
NS=NS3
DO 1351 1=1,NS+NFIN
IF(EU(J)+1)=1516,S18,518
518 AT=EU(J).
EU(J)=EU(J-1)+EU(J) 1
JP(J)+1=JP(J)+1
EU(J))=AT
519 CONTINUE
B(1)=BB(1)
B(2)=BB(2)
B(3)=BB(3)
B(4)=BB(4)
B(5)=BB(5)
EU(J)=BB(1) ELIMIT/UG
VENY=BB(1)
ENY=EU(J)
nhs=1
GO TO 8020
8013 BB(1)=EUG(J)
BB(2)=1.20.00128*EXP(0.395*EU(J))1*EUG(J)/EU(J)
NS=NS3
IF(NF=NFN(J))=1
C CALL VECTMAX(SLINE+NS+NFN+NXMAX+YMAX)
C BB(3)=BB(2)*2.35*YMAX-((SLINE+NFN+SLINE+NSM2))/2+1)
NX=NFN+NS3
BB(3)=SLINE(NS3)-SLINE+(NFN/(1-NF)
BB(5)=SLINE(NS)
NPARA(1)=1
NPARA(2)=2
NPARA(3)=3
NS=NS3
ENY=BB(1)+1 SLOP
C CALL STDF1(SLINE+BB+NFN+NS3+1,NPARA+NS3,FA+TITLE+1)
C CALL STDF1(SLINE+BB+NFN+NS3+1,NPARA+NS3,FA+TITLE+0)
DO 1350 1=NS+NFIN
1350 FM(J)=FA(J)
1350 1=1,NS3
8020 DO 99 P=1.1,NLIMIT
99 PP(1)=0.0
MRPE=MRPEAT
MENY=MEN
MNF=MNP
C CALL NESPUN
C N=MNP
MRPEAT=MRPE
MEN=MENY
DO 850 1=1,HLIMIT
IF(PP(1))=1851.851.852
851 INDEX=1
GO TO 853
852 CONTINUE
850 CONTINUE
853 DO 999 = INDEX+NLIMIT
999 PP(1)=0.0
SUM=0.0
DO 999 I=1,NLIM
999 SUM=SUM+PP(I)
PX=0.1+SUM
NX=NLF+1
GAIN=iev(1)
PNH=PHT(J)
C WRITE (LO=1888) K,*+NS+NFN+MRPEAT,NS+MENYM+NS+MOUT+NS+NFN+
C 1 NLIN+ELIMINT+ENY+AINBL1+PHO+VETY+EEB1(2)
C 9888 FORMAT (0H TEST +1219/1X+BEI3+6)
C WRITE (LO=1977+NP+EM+BB))=BB(3)+PHT(J)+FM(J)+1,NSNFN)
C 977 FORMAT (0H SINGLE J +1X+110+14.71+1X+51.7+7)
C CALL GANEL(0.0+NX+000N+GAIN+0.0+PP)
C IF(NX=NLIMITER+1800.0+1801.0+1801
1801 NX=NLIMITER-1
1800 ON 1100 T=NX
FM(J)=FM(J)+PP(1)+H(J)
IF(FM(J))=1873.0+1874.0+1874
1873 FM(J)=0.0
1874 CONTINUE
1100 CONTINUE
C WRITE (LO=800+NX+GAIN)+FM(J)+1,NSLIMITER)+PP(J)+1,NSLIMITER)
C 800 FORMAT (0H SINGLE J +1X+110.4+71+1X+51.4+7)
C PHOT(J)=8(3)+PHT(J)
PHOT(J)=PHT(J)
ETAT=ETAJ(J)
J=J
SLINE(J)=ENY
P=PHO
C CALL DETECT(J)+J=J+SLINE+H+ETA+DIST+RX+TAML+PM+M19
C PHT(J)=PHT(J)+ETAJ(J)
ETAJ(J)=ETAT
WRITE (LO=555)+PHT(J)+PHO
555 FORMAT (1HM/694+25+PHOTON NUMBER =+E29.7+/)
1 694+25+PHOTON
WRITE (LO=1500)
1500 FORMAT (1HM/643+31+DISCRETE PHOTOPEAK FITTING DATA('/',)
1 6X+MLOCATION+15A+MENERGY+16X+12PULSE+HEIGHT+10X+18MSTANDAR
2 DEVIATION+14X+MAREARE+19X CHANNEL TO CHANNEL+10X+SM+MVEI+16X+3
10X CHANNELS+15A+10X CHANNELS+14X+MCCOUNTS+15X)/
WRITE (LO=1000)+NS+NFN+ENY+8(1)+8(2)+8(3)
1000 FORMAT (1HM/2X+13B+13+32+B+32+E25.7+/)
100 IF(J=IN)+9020.0+9030.9+920
9020 J=J
IF(NS(N)=8040.0+8015.8+8040
8040 NBS=0
DO 8041 I=1,NLIMITER
8041 SLINE(J)=0.0
DO 8042 J=NS+NFN
8042 SLINE(J)=FM(J)
EUG(J)=BB(1)
VENY=EUG(J)
B(3)=BB(6)
B(2)=BB(5)
B(1)=BB(4)
IF(EU(J))=32.5+32.5+32
32 ENY=EU(J)
GO TO 833
532 ENV=BU(44)*SLOP
533 GO TO 8020
8030 NGE=1
N.X=IX
B40 RETURN
END
(FOR=1 IS DOSE
FUNCTION DOSE(E)
C****** PROGRAM NUMBER = 11 CUGEL ***********
C
C COMPUTES GAMMA PHOTON DOSE.
C
C DIMENSION X(20),R(20),Z(3),Y(3)
C
C DATA X,0.015,0.02,0.03,0.04,0.05,0.06,0.08,0.1,0.15,0.2,0.4
1
C DATA R,0.06,0.07,0.08,0.09,0.1,0.15,0.2,0.25,0.3,0.35,0.4
2
C DATA Z,0.0,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,1.0
C CALL TA(E,X+201,MOX=MUN+Z*Y+R+2*L+0)
C
DOSE=TE (3,2,3)*E
RETURN
END
(FOR=1 IS EFF2C
FUNCTION EFF2C(E,DAST+ROX+HH)
C****** PROGRAM NUMBER = 12 CUGEL ***********
C
C COMPUTES ELEMENTS OF DETECTION EFFICIENCY VECTOR.
C
C COMMON/CSINT/T01,T02,150,1192,T00,T100,T06
C COMMON /LIO/LI+LO+LP+LIMIT+NORMAL+MOUT
C COMMON /KL/UEGAM*RX*DIST+H
C DIMENSION X(29),R(29),Z(3),Y(3)
C DIST=DAST
C
C HHMH
C RX=RX
C ARG=RX/(DIST+H)
C EPS=T06
C WRITELO(IO,101010,DIST,H,RX,ARG)
C 100 FORMAT(I4,4E14.7)
C
C DATA X,0.01103,0.015,0.02,0.03,0.04,0.05,0.06,0.08,0.09,1
C 1,0.125,0.25,0.4,0.6,0.8,1,0.125,0.25,0.4,0.6,0.8,1
C 2,0,0.075,3.09,3.15,3.21,3.27,3.33,3.36,3.42,3.48,3.54,3.6,3.72,3.88,3.94,3.10,3.16,3.22,3.28,3.34,3.4,3.46,3.52,3.58,3.64,3.7,3.76,3.82,3.88,3.94,4
C DATA R,0.0,0.072,0.145,0.218,0.291,0.364,0.437,0.51,0.583,0.656,0.729,0.8,0.873,0.946,1.019,1.092,1.165,1.2,1.273,1.346,1.419,1.492,1.565,1.638,1.711,1.784,1.857,1.93,1.97,2.02,2.07,2.12,2.17,2.22,2.27,2.32,2.37,2.42,2.47,2.52,2.57,2.62,2.67,2.72,2.77,2.82,2.87,2.92,2.97,3.02,3.07,3.12,3.17,3.22,3.27,3.32,3.37,3.42,3.47,3.52,3.57,3.62,3.67,3.72,3.77,3.82,3.87,3.92,3.97,4
C DATA Z,0.0,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,1.0
C WRITELO(IO,101010,DIST,H,RX,ARG)
C 110 FORMAT(I4,4E14.7)
C
C CALL TA (E,X+291,MOX=MUN+Z*Y+R+2*L+0)
C
UEGAM*TE (3,2,3)*E
C WRITELO(IO,120) MOX=MUN+L*UEGAM*E
C 120 FORMAT(I4,3E14.7)
C IF(ARG=0.01246)X=5
C S=0.0
C A=ATAN(ARG)
C KL=0
C CASE=SIMPSN(A+B,EPS)
C A=H
C B=ATAN(RA/DIST)
C KL=1
C UNUM=CASE + SIMPSN(A+B,EPS)
C DENT=1.0-DIST/SORT(DIST+DIST+RX+RA)
C WRITELO(IO,130) A+B,CASE,UNUM,DENT
C 130 FORMAT(I4,3E14.7)
C EFF2C=UNUM/DENT
C RETURN
C 6 EFF2C=1.0 - EXP(-UEGAM*H)
C RETURN
C END
(FOR=1 IS FC
FUNCTION FC(X)
C****** PROGRAM NUMBER = 13 CUGEL ***********
C
C CRYSTAL INTERACTION EFFICIENCY FUNCTION.
C
C COMMON /KL/UEGAM+R+DIST+H
C IF(KL=1)IF=2.1
C IF(A)=3.4...3
C 3*UEGAM+(R/SIN(X)+DIST+COS(X))
C IF(A)=GT(100)+GO TO B
C FC=(1.0-EXP(-A1)*SIN(X))
C RETURN
C 4 FC=0.0
C RETURN
C 2 AA=UEGAM*M/COS(X)
C IF(AA=GT(100)+GO TO S
C FC=(1.0-EXP(-A1))*SIN(X)
C RETURN
C 5 FC=SIN(X)
C RETURN
C END
(FOR=1 IS FIND
SUBROUTINE FIND(Y,M5,MX,M10,M7,M27,P15,NS,NF)
1 SLOP+E,U+NJ)
C****** PROGRAM NUMBER = 14 CUGEL ***********
C
C SEARCHES SPECTRUM FOR PEAKS
C
C DIMENSION Y(400),P(50),MNS(50),NF(50),NS(50),EU(50)
C COMMON/LIO/LI+LO+LP+LIMIT+NORMAL+MOUT
C K=1
C SLOP=0
C E=IN
C M7=IN+1
C M5=M7
C 501 IF (IN) 105,105,105
C 105 GO 107,K=IN+1
C IF(I=IN,AND,11=NF(K)) GO TO 108
C GO TO 109
C 108 ISTNF(K)
C GO TO 106
C 109 CONTINUE
C 107 CONTINUE
C 106 IF(Y(I)=100,12,12,21)
C 21 N1=1
C N2=IF(FOUR
C IF(N2=MX)2,1,18
C 2 CALL VECTM(Y,N1,N2=5,MAX)
C IF(BIG=GT(101,AND,116,L1T=N2)GO TO 4
C GO TO 5
C 4 IF(Y(N1)+1EN=SORT(Y(N1)))=11=112,8,8
C 7 IF(Y(N2)+1EN=SORT(Y(N2)))=11=119,10,10
C 10 N2=N2+1
C GO TO 11
C 8 N1=N1+1
C 11 IF(N1=NT)=4,12,4
9 IF(INIG-NOP)=35+36+36
35 NOP=1816
JL=1
IF(I-IFIFTY)=37+37+10
37 P(I)=1816
E(J)=F(J)*SLOP
NS(J)=N1
NF(J)=N2
NJ(J)=3
GO TO 5
36 NF(J)=N2
5 CONTINUE
12 CONTINUE
IF(M=N1)=7+18+18
17 I=I+1
50 TO 51
10 M2=7
IF(M2+IN)=118+118+118
119 IN=M2
118 CONTINUE
C WRITE (LO,100) M2+1,N+NS,M1,M1+MF
100 FORMAT (6M9,15S,15S,15S,15S,15S,15S)
RETURN
END
FOR,15 FUNZ
SUBROUTINE FUNZ(NP,K,B+FA)
C*********** PROGRAM NUMBER = 15 CUGEL ***********
C
C STRAIGHT-LINE BASE FITTING
C COMMON/LID/L1,LI,LP+NM1+NM2+NM3+NM4,DU
C COMMON/BS/ABS+DS+VOUN(I)
C DIMENSION FM(1000),RUS(60+12)
M2=M1+1
N1+1=5
N2+2=5
SUMX=0.0
SUMZ=0.0
SUM0=0.0
SUMXY=0.0
DO 1 I=1,N1
SUMX=SUMX+FM(I)
SUMZ=SUMZ+FM(I)
1 SUM=SUMX+SUMZ
DO 2 I=2,N2
SUMX=SUMX+FM(I)
SUMZ=SUMZ+FM(I)
2 SUMX=SUMX+FM(I)
SUMZ=SUMZ+FM(I)
A=SUMX+SUMZ+SUMM2+B=SUMM2+2.12*SUMZ
5 BE=0.0
SUMX=SUMX+BE
SUMZ=SUMZ+BE
SUMN=SUMN+BE
SUMN=SUMN+BE
C WRITE(LO,101)M+NP,EM,SN,SLNX,SLNUI
C 101 FORMAT(15S,15S,15S,15S,15S)
IF(M=I+1),LO=110+110+10
110 FORMAT(INCH,+44.1)BS PEAK IN RBS
10 ND=NYX=30
DO 7 I=1,10
J=I
7 RSH(I-M2)=FMI-I-EM+BE
FM(I)=EM+BE
1 IF(RBS(J+MX1)+5+6
5 RMS(J+MX1)=0.0
6 CONTINUE
7 CONTINUE
11 RETURN
END
RETURN
END

IF FOR IS GANE
SUBROUTINE GANE (TZ, NX, GAIN, ROGAIN, SMOOTH, CT)

************** PROGRAM NUMBER - 17 CUGEL **************

C
C REF. JR. NUC. SCI. AND ENG, VOL 35, MAR, 1969 STEYN AND ANDREWS
C MARCH 1968 VERSION, I.E. DIMENSION CAPACITY CHECK
C GAIN CHANGING PROGRAM, ALSO SPECTRAL SHIFTING.

COMMON /GAIN/NLI
DIMENSION C(600), FM(600)
NLI=NL
WONX=NX
ONX=(ROGAIN/GAIN)*WONX
NONX=ONX
IF(NNX-NLIMT)'620, 620+621
621 NX=NX-NLIMT, NX=NX-1
620 IF(TZ)'600, 601
600 JTZ=ABS(TZ)
NX=NX/JTZ
IF(NNX-NLIMT)'601, 601+603
603 NX=NLIMT
601 IF(TZ)'1000, 275+1000
1000 NZC=MT
NXO=NX-NZC
C
C INTEGER SHIFT IF *NZC* NOT EQUAL TO ZERO.
C
IF(TZ)'1913, 910+911
913 NZC=NZC-1
NSNZC=-1, 1
NSX=NX-1
NXO=NX-1
NXO=NSX+NX
955 DO 956 I=NS, NXO
956 FM(I)=C(I)
DO 956 I=NS, NXO
957 C(I)=FM(I)
GO TO 93
911 NS=1
NXO=NXO+1
945 DO 911 I=NS, NXO
911 C(I)=C(K)
93 DO 921 I=NS, NXO
92 C(I)=0.0
910 NX=NXO
C
C DECIMAL SHIFT.
C
274 TNZC=NZC
DIF=TZ-TNZC
IF(DIF)'271, 272+271
271 NXO=NX-2
DIF=1, 0-DIF
DO 270 I=2, NXON
C(I)=C(I)-DIF
270 C(I)=C(I)+DIF
C(I)=C(NXON-1)+DIF
GO TO 273
272 IF(NZC)'273, 275+275
273 NX=NX-1
275 NZ=0.

L=1
G=GAIN
DO 50 I=1, NLIMT
50 FM(I)'1, 0
FMUL'=GAIN/RQGAIN
C
C DEL=0.5 WHEN GAIN=ROGAIN OR 0.1, I.E. DOUBLING REQUIRED.
C DEL=2.0 WHEN GAIN=ROGAIN OR 0.1, I.E. HALVING REQUIRED.
C
1 DEL=GAIN/ROGAIN
IF(DEL)'2, 0, 402
402 IF(DEL)'0.5, 1, 3
3 L=1
GAIN=GAIN/2.0
GO TO 1

C
C INITIALIZE FOR REDUCING ALGORITHM.
C
4 I=1
K=1
X=0.0
XNP=1
DEL=0.0
60 DEL=DE
IF(DEL)'1.0, 499, 499
499 IF(L)'497, 497
497 DEL=DEGAIN/2.0
L=1
496 DO 498 I=1, NX
498 FM(I)'C(I)
GO TO 201

C
C INCREASE. ..... LOAD EVEN CHANNELS WITH QUADRATICALLY
C INTERPOLATED COUNT. "SHIF_ EVERY SPIRUM UPWARD ONE, HALF CHANNEL.
C
5 DELT=ROGAIN/2.0
DEL=GAIN/DELT
GO TO 60
303 NXO=J-4
DO 305 J=4, NXA+2
J=J+1
305 C(I)'J, 0.08*C(J-2)+6.0*C(J-2)-C(J-4)))*1.25
C(I-2)'J, 0.08*C(J-2)+6.0*C(J-1)-C(J-1)))*1.25
NXO=I
DO 305 I=4, NX
303 C(I)'FM(I)
GO TO 304

C
C REDUCTION ALGORITHM.
C
105 X=DEL
DEL=XN

KC=K
106 FM(K)'FM(X)+DEL*C(I)
IF(I)'I, 1, 107
112 X=X+DEL
IF(X)'XNP+1.0E-9108, 107+107
107 K=I
XNP=K
D=X+X
KC=K
GO TO 106

108 ANF/K
DEL=NX\*X
100 IF(DEL=1)goto1101
110 IF(DEL=1)goto1
DEL=DEL/DIF
GO TO 109
111 I=I+1
GO TO 106
202 DO 1999 I=1+NLIMIT
1999 C(I+N)=0.0
X=NX
NX=NX*NY/N
MX=NX
C LOAD ODD CHANNELS IF *DELT* EQUAL TO ZERO.
C
201 IF(DELT)300+301,300
300 NC=1
NO=3
301 NC=1
NO=3
302 DO 200 I=1,NX
J=NC*1-NO
200 C(I,J)=FMI
IF(DELT)303+304,303
304 IF(L-1)404,500,404
404 L=L-1
GO TO 496
C HALVING.
C
204 I=1
CNCHECK=NX
NX=NX/2
NC=NCHECK-(NX+NX)
219 IF(NK)555,564,555
555 NX=NX-1
594 K=2-1
C(I)=C(K)+C(K+1)
IF(N-I)502,503,503
502 I=I+1
GO TO 504
503 IF(L-1)525,525,205
C SMOOTHING IF *SMOOTH* NOT EQUAL TO ZERO.
C
525 IF(NSMOOTH)526,500,526
526 DEL=DEL
SMOOTH=SMOOTH - 1.0
FMULT=FMULT/5
GO TO 204
205 L=L-1
GO TO 204
C COUNTS SCALED IN ACCORD WITH *FMULT* FOR INCREASED SPECTRA.
C
500 KK=0
915 CONTINUE
916 KK=KK+1
GO TO 915
917 GO TO 920
920 C(I)=C(I)*FMULT
925 IF(NSMOOTH)204,527,204
527 GAINING
RETURN
END
FOR IS GEOMTR
SUBROUTINE GEOMTR (ENXTAL=E+PHI*NX+DE+DT+VOL+RX+RO)
C******** PROGRAM NUMBER = 19 CUGEL *********
C
C COMPUTES GEOMETRY FACTORS, INTEGRATES NUMBER AND ENERGY SPECTRA.
C CALCulates NORMALIZED Dose DATA FOR FINAL CODE RESULTS.
C
COMMON /C/ SUMNUM,SUMENY,DOSDET,AVERAGE,FNUME,ENERGY,PHENBE
DOSREX=DOSCYL+DBAVOL+DXY+CYLIA
DIMENSION PHI(400)+E(400)+ENXTAL(400)
PI=3.14159265
VOL=(PI*CYLIA**3)/4.0
TIME=DT+60.0
AREAX=PI*RX**RX
CONST=2600.0/5.24E+07
SUNNUM=0.0
SUNENY=0.0
SODDET=0.0
SODCYL=0.511.0-RO/SORT(R0+RO+RX+RX)
SODDET=0.0
C INTEGRATE.
DO 2 I=NS,NX
PHI(I)*DE*PHI(I)/(AREAX*TIME)
ENXTAL(I)=PHI(I)*RI(I)
EC=E(I)
DOSXTL = PHI(I)*CONST*DOSE (EC)
SUMNUM=SUMNUM+PHI(I)
SUMENY=SUMENY+ENXTAL(I)
2 DOSDET=DOSDET+DOSXTL
C
AVERAGE=SUMENY/SUMNUM
PHNUM=SUMNUM/BETNUM
EnB=SUMENY/BETENY
PHENBE=SUMENY/BETNUM
DOSREX=DOSDET+BETNUM
DOSCYL=DOSREX/SODGEM
DBAVOL=DOSREX/VOL
DCYVOL=DOSREX/SODCYL
VOL
C RETURN
END
FOR IS GUESS3
SUBROUTINE GUESS3 (NS,NF,NB,VB,V2)
C******** PROGRAM NUMBER = 19 CUGEL *********
C
C DOUBLE PHOTOPACK INITIAL PARAMETER ESTIMATES
C
COMMON/L10/L1+L0+LP+NLIMIT,NORM,OUT
DIMENSION B(18)+Y(400)+VT(50)
AREA=0.0
II=0
NX=NS
NX=NF
B(I)=(Y(NF)-Y(NB))/(NX-NS)
NI=NS
IF(Y2)n25+26+25
25 N1=1
VB1
VB2
DO 100 I=NV1+NB
I=I+1
100 VT(I)=1.0/VT(I)

JMIN=MIN
NO2
GO TO 7
C GO TO 4 FOR GENERAL INTERPOLATION
4 M1=M1N
M2=M1N+1
M3=M1N+2
N=3
EX=EXB/E1.0*(E/0.511)+2.0
EXC=EXB
7 DO 44 I=1,NORM
44 FM(I)=FM(I+MIN3)
C WRITE(L0=502) MINI+MIN2+MIN3+JMIN+NSIG+NSIG+NY+NSTAND+EXB+EXC+EX
C DO 40 J=1,3
J(I)=MIN1-1
EC(I)=STADN(JJ=1)+EBS(JJ)
C WRITE(L0=2500) JJ+STADN(JJ=1)
40 VCE(J)=EC(J)+NORM/STADN(JJ=1)
C WRITE(L0=104) (EBS(I)=MINI+MIN3)
C WRITE(L0=104) (VCE(I)=I=1,3)
N1=VCE(I)-0.05*VCE(J)
N2=VCE(I)+0.05*VCE(J)
CALL VECTRX(FM(N1),N2,JMAX+YMAX)
NCE(I)=JMAX
FMCE=FMCE+1
FMCE=FMCE/VCE(J)
DO 45 J=1,2
45 VCE(J)=VCE(J)+FMCE
VCE(J)=NCE(J)
DO 81 I=1,NORM
81 FM(I)=0.0
C WRITE(L0=503) (VCE(I)=I=1,3)+N1+N2+JMAX+EXC
C CHANGE FIRST HALF OF STANDARD CONTINUA
C DO 46 J=1,3
46 RC(I)=RTO=0.0
NX(I)=NCE(I)+20
DO 48 J=1,2
GAIN=VCE(J)
RGAIN=NCE(J)
NX=NCE(J)
J(I)=MINI-1
DO 49 I=1,NX
49 FM(I)=FM(I)+JJ
M=NX
C WRITE(L0=1000) NVX(I)=NX+GAIN+RGAIN
CALL GAME(TAZ,MX,GAIN,ROGAIN,SM+FM)
NVX=NVX
DO 50 J=1,NX
50 "I"=FM(I)
51 "I"=NORM
52 DO 50 J=1,NX
51 DO 50 J=1,NX
C IF(N=1)5252+5253+5252
5253 Z(1)=Z(2)
Z(2)=Z(3)
DO 5254 J=1,NX
Y(1)=H(J+1)
Y(1)=H(J+1)+MIN3
5254 FOUT(I)=FZ-T/E+Y
GO TO 5255
5252 DO 52 J=1,NX
Y(1)=H(J+1)
Y(2)=H(J+1)+2
Y(3)=H(J+1)+3
52 FOUT(I)=FZ-T/E+Y
5255 Z(1)=ECE(I)
Z(2)=ECE(I)
Z(3)=ECE(I)
C WRITE(L0=5194)ECEA+ECEC+ECE(1)+ECE(2)+ECE(3)+FOUT(I)+I=1
C NORM
Cbloo FORMAT/(10H FIRST/12 I5,6E14.7/1X,10F11.41)
951 DO 952 I=1,NLIM
952 FM(I)=RI(NY)
GAIN=PARAV(NY,1)
RGAIN=NORM
KH=NLH
CALL GAME(TAZ,KH,GAIN,ROGAIN,SM+FM)
SM=1.0
N=NRM
CALL GAME(TAZ,NS+1.0+1.0+SM1+FM)
NS=CEA-S-0.0
NF=CEA+10.0
CALL VECTRM(FM,N+S+JMAX+YMAX)
DEJ=MAX-CEA
C WRITE(L0=1003) NY,NS,NF,NSG+NG+DEA+GAIN
C CONTINUE
C WRITE(L0=1002) CEH=Z(1)+Z(2)+Z(3),VCEC1)+VCE(2)+VCE(3)
GAIN=VCEC(3)
NG=VCEC(3)
MX=NX
C WRITE(L0=1000) NVX(I)+GAIN+RGAIN
DO 9000 I=1,NRM
9000 FOUT(I)=FOUT(I)
CALL GAME(TAZ,MX,GAIN,ROGAIN,SM+FM)
DO 9050 I=1,NRM
9050 FOUT(I)=FM(I)
NX=NX+1
DO 53 I=NX,NORM
53 FOUT(I)=0.0
C WRITE(L0=105) (FOUT(I)+I=1,NX)
C RELOCATE 2ND HALF OF STANDARD CONTINUA
C DO 71 I=1,NRM
71 FM(I)=0.0
NX=NORM+VCEC+VCEC1)+20
GSA=ROGAIN
DO 56 J=1,2
NCE(J)=VCEC(J)+0.5
GAIN=NORM+VCEC(J)+1
J=J+MINI-1
DO 57 J=1,NX
57 FM(I)=FM(I)+1
J=J+2
COMMON/NRES=N+EMDUM(2)+NDEG+OMU1(160)+K+MP+UUM2(2)
COMMON/SOLRES/EPS=1.111*ITMAX/MN+DUM3(2)+IF*SIGMA(2)
COMMON/LII=LO+L+LP+NLIMIT+NONLIM
DIMENSION PP(50),P(1800),KL(40),40,PHI(400),FIT(100),DIF(100)

1

C INITIALIZE

C NCHECK=1*ITMAX/Z
NCHECK=1*ITMAX-2*NCHECK
SUM=0.0
DO 1999 I=K,N
1999 SUM=SUM+P(I)
DO 1999 I=K,N
1800 P(I)=P(I)/SU
YAX=0.0
CALL VECTMX (P,K,N,MAX,MAX)
C
C YLW=MAXX*(1.0E-13)
DO 1 I=1,N
P(I)=0.0
1 PH1(I)=P(I)
C WRITE IF ITMAX IS AN ODD NUMBER.
IF (NCHECK*999+8000.0:0999
8999 WRITE (LO=8999) (P(I),I),N)
8999 FORMAT (30M) NORMALIZED INPUT SPECTRUM
INDEX=1
8000 CONTINUE

C MATRIX MULTIPLICATION P=PHI
10 DO 2 I=K,N
2 PH=PHI(I)
30 DO 2 J=1,N
2001 PP(I)=PP(I)+K(1,J)*PH(I,J)
2000 CONTINUE
2 CONTINUE
TERM=0.0
C
C ARRESTING CHECK WHEN IF(SUM(P-P)=2/P) FOR LOOP(IT) AND LOOP(IT-1)
C ARE LESS THAN EPS.... OR IT=ITMAX.
C
DO 5 I=K,N
5 IF(P(I))=0.0
4 TFH=-(PP(I)-PP(I)**2)/(P(I)+TERM
6 CONTINUE
5 CONTINUE
IF (NCHECK*16000.0:15000.0:16000
16000 INPUT(I)=1715000.0:17000.0:15000
17000 WRITE(LO=17000) IT,MIN(INDEX)+(PP(I),I),K+N
WRITE(L0=17000) IT,MIN(INDEX)+(PP(I),I),K+N
INDEX=INDEX+1
15000 CONTINUE
19000 FORMAT (5I5) INTERMEDIATE ITERATING OUTPUT (IT, MN. AND PH(I)) 215
1/ (1x10E11+4)
19005 FORMAT (5I5) INTERMEDIATE ITERATING OUTPUT (IT, MN. AND PP(I)) 215
1/ (1x10E11+4)
20 IT=IT+1
FIT=FIT+TFH
DIFF=ABS(FIT(IT)-FIT(IT-1))
IF (DIFF(I)) 29
29 IF(IT=ITMAX)224:7,7

C SUBROUTINE RESMAT (PHI,P)
C************************** PROGRAM NUMBER = 23 CUCEL **************
C
C PULSE-HEIGHT ANALYZER SPECTRUM UNFOLDING ACCORDING TO THE SCOFIELD ALGORITHM.
DETERMINES AND APPLIES DETECTOR EFFICIENCY VECTOR.

```
COMMON /A/ DI=M-MF
COMMON/RES/N+Ndum(2)+Nump=E+Dum2(0)+K+Mrdum+Dum3(2)
COMMON/SOLRES/EPs+IT+ITMAX+ Mn+Hs+M+DIF + SIGMA(12)
COMMON/L0/L1/L0+L1+LIMIT+NUM=M+MOUT
DIMENSION PI(100),ETA(100),E1(100),DIF(100),N(240)
1 N(1A)+PFRACT(160)
MP=0
IF (K1)=30+50
30=1
50 Km=K-1
IF (K1)=601.602.602
602 Do Do (I)=1.MK
600 P(I)=0.0
601 CONTINUE
IF (M(5)=12)+1.12
C
11 CALL RESMAT (PHI+P)
WHITE (L0+1424) (DIF(I)=1.I+1)IT
1424 FORMAT (30M FITTING DIFFERENCES /(1X,SE14.7))
C
12 IF (DIST=DI)+3.4.3
40 IF (MSKIP)+3.4
3 IF (M(1))=0.0
13 CALL DETECT (NS,N+M+ETA+DIST,RX,TKLM,PFRACT,M19)
2 DIST=DI
4 IF (M(1))=50.4.4.4
44 Do Do INS=N
22 PHI(I)=PHI(I)+ETA(I)
MF=0
C
WRITE DIF (I) IF (I)+ITMAX
IF (I)+ITMAX (B)+1.00.100
100 WRITE (L0+105) (DIF(I)=1.I+1)IT
105 FORMAT (1H1,3H FLUX FITTING DIFFERENCES (I+ITMAX)/(1X,SE14.7))
BY RETURN
54 IF (MP)+0.0
98 Do Do INS=N
96 ETA(I)=1.0
99 Do Do INS=N
999 PHI(I)=PHI(I)+ETA(I)
MF=1
NEIGHTH END
IFON+IS SPNORM
C
*************** PROGRAM NUMBER = 26 CUGEL ***************
C
CALLS BY SPNORM TO NORMALIZE STANDARD SPECTRA
FITS GE(I) PHOTOPEAKS. NORMALIZES COMPTON CONTINU
C
DIMENSION M(400+12),ALABEL(12),AHELAE(12)+SUIEN(12)+12*12+12+12
PARAS(12)+PARA+12,1+12,1+12,1+12,1+12,1+12,1+12,1+12,1+12
SNUJNFJN+1STAND
COMMON/L0/L1/L0+L1+LIMIT+NUM=M+MOUT
COMMON/SN/N+V+S/DEN+P+P+P+P+P+A+ALABEL+ALABEL
COMMON/N0+NL1
```
APPENDIX III

SAMPLE INPUT CARD DECK LISTING
APPENDIX IV

SAMPLE OUTPUT LISTING
**BRIEF DESCRIPTION OF PHA RUNS**

**TEST RUN WITH RESFUN GROUP**

**CONTROL NUMBERS**

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**EM = 14.51066 CHANNELS/MEV**

**ELIMIT = 2.7500**

**ITERATIVE ERROR TOLERANCE, EPS = 0.00001**

**NUMBER OF BETA SOURCE SETS, OJ5O = 1**

**MAX NUMBER OF ITERATIONS, ITMAX = 51**

**NUMBER OF CHANNELS INPUT, N = 40**

**GELLI CRYSTAL SIZE = 2.26 X 3.10 (CM)**

---

**STANDARD SOURCE SPECTRAL PARAMETERS**

8 SPECTRA IN STANDARD SOURCE DECK

CHANNELS ONE TO 2 ASSUMED AS REDUNDANT

**REFERENCE COARSE GAIN = 0.0**

<table>
<thead>
<tr>
<th>STANDARD SOURCE</th>
<th>PHOTOPENK FROM</th>
<th>PHOTOPENK TO</th>
<th>X-RAY OR 5 PEAK FROM</th>
<th>X-RAY OR 5 PEAK TO</th>
<th>SHIFT SPECTRUM CHANNELS</th>
<th>PHOTOPEAK ENERGIES MEV</th>
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<td>HG203</td>
<td>391</td>
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<td>0</td>
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<td>SH253</td>
<td>396</td>
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<td>108</td>
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### RESULTS OF PHOTOPAK FITTING

<table>
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<th>INDEX</th>
<th>STANDARD SOURCE</th>
<th>PULSE-HEIGHT (CHANNELS)</th>
<th>STANDARD DEVIATION (CHANNELS)</th>
<th>AREA (COUNTS/TIME)</th>
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<td>0.3066857E 01</td>
<td>0.3102433E 00</td>
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<tr>
<td>2</td>
<td>HG203</td>
<td>0.3805890E 03</td>
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### RESULTS OF PHOTOPAK FITTING

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### Normalized Continuum of Standard Spectra

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<th>Energy (keV)</th>
<th>0.1060 MeV</th>
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### Integral

\[ I = 0.212025 \times 10^2 \]

### Photofraction

\[ P = \frac{I}{\text{Energy}} \]
### Normalized Continuum of Standard Spectra

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### Normalized Continuum of Standard Spectra

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**Integral**

**Photofraction**
### NORMALIZED CONTINUUM OF STANDARD SPECTRA

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**Integral**

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(After Background Subtraction)

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### Sheet 11-16
## Efficiency Factors

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- Photon Number = 0.419274E+02
- Photon Fraction = 0.335509E+01

### Discrete Photopeak Fitting Data

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<th>Pulse-Height (Channels)</th>
<th>Standard Deviation (Channels)</th>
<th>Area (Counts/Time)</th>
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## Efficiency Factors

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- Photon Number = 0.335509E+02
- Photon Fraction = 0.133411E+07

### Discrete Photopeak Fitting Data

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- Photon Number = 9.398811E 04
- Photon Fraction = 0.120054E 04

### Discrete Photopeak Fitting Data

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### Efficiency Factors

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<th>ENERGY (NEV)</th>
<th>AIR ATTENUATION</th>
<th>ABSORBER ATTENUATION</th>
<th>CRYSTAL EFFICIENCY</th>
<th>TOTAL EFFICIENCY</th>
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</thead>
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<tr>
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<td>6.1483E-06</td>
<td>0.99902E 02</td>
<td>9.8248E-06</td>
<td>0.06462E 00</td>
<td>0.65343E 00</td>
</tr>
</tbody>
</table>

- Photon Number = 9.398811E 04
- Photon Fraction = 0.120054E 04

### Discrete Photopeak Fitting Data

<table>
<thead>
<tr>
<th>LOCATION (CHANNEL TO CHANNEL)</th>
<th>ENERGY (NEV)</th>
<th>PULSE-HEIGHT (CHANNELS)</th>
<th>STANDARD DEVIATION (CHANNELS)</th>
<th>AREA (COUNTS/TIME)</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
<td>Index</td>
<td>Energy (MeV)</td>
<td>Number Flux (Photons/cm²•sec)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>--------------</td>
<td>-------------------------------</td>
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<td></td>
</tr>
<tr>
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GAIN PARAMETERS AFTER CALL DISCRET IN MAIN

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<tr>
<th>CAIN</th>
<th>PARAMETERS</th>
<th>AFTER</th>
<th>CALL</th>
<th>DISCRET</th>
<th>IN</th>
<th>MAIN</th>
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<tr>
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<td>0.6</td>
<td>0.6</td>
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<td>0.6</td>
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</tbody>
</table>

INPUT SPECTRUM GAIN CHANGED TO 47 CHANNELS

GAIN CHANGE RATIO = GAIN Before Change/GAIN After Change

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<th>Channel</th>
<th>Gain Change Ratio</th>
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<td>0.5090282E 00</td>
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<tr>
<td>0.6649596E 01</td>
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<td>0.8866612E 01</td>
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-119-
### Energy and Number Spectrum at the Crystal

<table>
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<tr>
<th>INCREMENT</th>
<th>ENERGY (MeV)</th>
<th>NUMBER FLUX (PHOTONS/CM²-SEC)</th>
<th>ENERGY FLUX (REV/CM²-SEC)</th>
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<td>0.0</td>
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<td>0.11688×10⁴ E 01</td>
<td>0.2109797E 00</td>
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<td>0.3399449E 01</td>
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</tbody>
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### Integrated Results at Source and Crystal

**Energy Integrated Photon (PHCMS1) Values at the Crystal**

| PHOTON NUMBER (PHOTONS/CM²-SEC) | 3.5952485E 02 |
| PHOTON ENERGY (REV/CM²-SEC) | 0.7773551E-04 |
| PHOTON DOSE (PHOTONS/H/CM²-SEC) | 0.4137635E-01 |

**Average Energy (MeV)** = 0.7134254E 00

**Photon Number / Source Emitted Beta Number (PHOTONS/CM²-SEC) (BETA/SEC) = 3.1839285E-08**

**Photon Energy / Source Emitted Beta Energy (REV/CM²-SEC) (MEV) = 0.1372125E 02**

**Photon Doise / Source Emitted Beta Number (Mev/CM²-SEC) (BETAS/SEC) = 3.2127225E-14**

**Photon Dose / Source Emitted Beta Number per Source Volume (E/PHOTONS/CM²-SEC) (BETA/SEC) = 0.2673769E-11**

**At the Source Cylinder**

**Photon Dose / Source Emitted Beta Number per Source Volume (E/PHOTONS/CM²-SEC) (BETA/SEC) = 0.4413446E-11**
APPENDIX V

PHOTOPEAK AND BACKSCATTER PEAK DISTRIBUTIONS
APPENDIX V

Photopeak and Backscatter Peak Distributions

Figures V-1 through V-8 give the residual spectral count distributions in the photopeak region after systematic fitting and subtraction of the Gaussian function. The residuals are approximately zero at channels greater than the Gaussian mean pulse height. For $^{139}$Ce and $^{203}$Hg the residuals below mean pulse height are as expected, i.e., the Compton tail appears regular in shape. The Compton tail of the other standards exhibits peak asymmetry, perhaps associated with Ge(Li) electron-hole trapping. A more detailed analysis was not possible within the economic constraints of the present work.

Figures V-9 through V-17 (generated by subroutine XPLOT) give the generally very good agreement between the fitted Gaussian function (zeros' i.e., 0) and the experimental photopeaks (ex's i.e., x); the asterisks indicate x and o superimposed. In these figures the true photopeak channel is obtained by adding the figure specified-number to plot channels (at bottom of figure).

Figure V-18 shows the normalized backscatter peak distributions, with respect to unit pulse height (200 channels) and photopeak area. These peaks were obtained after fitting a straight line base through counts on both sides of the peak region (see FITLIN description in Section 2.2.2.4). All peaks exhibit a regular shape pattern with the exception of $^{139}$Ce; $^{139}$Ce continuum counts were statistically poor and thus this may account in part for spurious region between channels 10 and 20 in Figure V-18. Figure V-19 presents the backscatter peak height as a function of energy. The behaviour is seen to be satisfactorily regular.

-124-
Ce$^{139}$, $E = 0.166$ MeV
Maximum Count = 40,357

Figure V-1
Hg^{203}, E = 0.279 MeV
Maximum Count = 7.493

Figure V.2
Cs$^+$, $E = 0.6616$ MeV
Maximum Count = 79,962

Figure V-4

Counts

Channel

-128-
Mn$^{54}$, $E = 0.835$ MeV
Maximum Counts = 46,336

Zn$^{65}$, $E = 1.114$ MeV
Maximum Count = 16,691

Figure V-5

Figure V-6
Na\textsuperscript{22}, $E = 1.28$ MeV
Maximum Count = 50,548

Co\textsuperscript{60}, $E = 1.333$ MeV
Maximum Count = 57,738
Add 335 to Channel 1
Figure V-9
Ce$^{139}$, E = .166 MeV

Add 354 to Channel 1
Figure V-10
Hg$^{203}$, E = .279 MeV
Add 378 to Channel 1
Figure V-11
Sr$^{85}$, $E = 0.514$ MeV

Add 366 to Channel 1
Figure V-12
Cs$^{137}$, $E = 0.6616$ MeV
Add 368 to Channel 1
Figure V-13
Mn$^{54}$, $E = 0.835$ MeV

Add 378 to Channel 1
Figure V-14
Zn$^{65}$, $E = 1.114$ MeV

Add 379 to Channel 1
Figure V-15
Co$^{60}$, $E = 1.333$ MeV
Add 171 to Channel 1
Figure V-16
Zn\textsuperscript{65}, E = 0.51 MeV

Add 334 to Channel 1
Figure V-17
Co\textsuperscript{60}, E = 1.173 MeV
Note: Backscatter peaks shown are normalized to photopeak unit area and pulse-height.

Source Energy (MeV)
- 1.333
- 1.114
- 0.835
- 0.662
- 0.514
- 0.166

Normalized Counts Per Channel

Normalized Channels

Figure V-18

Normalized Backscatter Peaks

0.004952 counts
Note: $H_B$ defined in inset to Figure 6.

**Figure V-19**

Backscatter Peak Height as a Function of Photon Energy
APPENDIX VI

REPRODUCTION OF APPENDIX II OF REFERENCE (2):

PHOTOPEAK FUNCTION FITTING

Note: The Following Are Approximately Equivalent in This Appendix:

- CUBED, read as CUGEL
- STDFIT, read as STDFT3
- GUESS, read as PKFUN
- PHOFRA, read as RESFUN
APPENDIX II
PHOTOPEAK FUNCTION FITTING

The pulse-height analyzer spectral photopeak counts, \( y(x_i) \), are fitted to the Gaussian-plus-straight-line non-linear function

\[
f(x) = f(x; p) = \frac{G p_3 e^{-\frac{(x-p_1)^2}{2p_2^2}}}{p_2} + p_4 x + p_5
\]  

(1)

where

- \( p_1 \) = photopeak mean pulse-height.
- \( p_2 \) = photopeak standard deviation.
- \( p_3 \) = photopeak area.
- \( p_4 \) = slope of photopeak assumed straight-line base.
- \( p_5 \) = intercept of photopeak assumed straight-line base.
- \( G = 0.3989423 \), a Gaussian constant.
- \( i = 1, 2, \ldots, n; \ell \) and \( n \) are input to code CUBED.
- \( j = 1, 2, \ldots, m; \) m=5 in equation (1) and in code CUBED.

The partial derivatives of equation (1), with respect to the parameters, \( p_j \), are determined as

\[
f_{p_1} = \left( \frac{\partial f}{\partial p_1} \right)_{x_i} = f(x_i^*) \left( \frac{x_i - p_1}{p_2^2} \right) 
\]

\[
f_{p_2} = \left( \frac{\partial f}{\partial p_2} \right)_{x_i} = \frac{f(x_i^*)}{p_2} \left( \left( \frac{x_i - p_1}{p_2} \right)^2 - 1 \right) 
\]

(2)
Equations (1) and (2) are coded in subprogram FUNUS. Equation (1) is fitted to the experimental data, \((x_i, y_i)\), according to the iterative least-squares method of differential correction; it is coded in subprogram STDFIT. This method, as it is applied in code CUBED, is outlined as follows:

A set of non-linear residual equations are defined and after some manipulation expressed as first linear approximations. An initial estimate of values of the fitting function parameters is employed for the first approximation (iteration). The linearized approximation residual equations are minimized by the method of least-squares such as to generate a set of normal equations which are in turn solved to determine the coefficients. These differential correction coefficients are applied additively to the current (initial on first iteration) parameter values to obtain the values for the next (second, third, etc.) iteration. This is repeated until the sum of the squares of the residuals (between function and experimental values) differ by less then some preassigned value, as determined for consecutive iterations.

The set of non-linear residual equations are defined as:

\[
\begin{align*}
\frac{df}{dp_3} &= \left(\frac{df}{dp_3}\right)_i = -f(x_i)^*/p_3 \\
\frac{df}{dp_4} &= \left(\frac{df}{dp_4}\right)_i = x_i \\
\frac{df}{dp_5} &= \left(\frac{df}{dp_5}\right)_i = 1
\end{align*}
\]
The set of non-linear residual equations are defined as:

\[ R_i = f(x_i; p_j^{(k)}) - y(x_i) \]  \hspace{1cm} (3)

which may be rewritten as

\[ R_i = f(x_i; p_j^{(k)} + q_j^{(k)}) - y(x_i) \]  \hspace{1cm} (4)

where

- \[ p_j^{(0)} \] = initially estimated value of j\textsuperscript{th} parameter.
- \[ p_j^{(k)} \] = value of j\textsuperscript{th} parameter for iteration k.
- \[ k \] = iteration index
- \[ q_j^{(k)} = p_j^{(k)} - p_j \], differential correction coefficient (ideally equal to zero).

Expanding equation (4) by means of Taylor's theorem for a function of several variables, it may be seen that

\[ R_i = f(x_i; p_j^{(k)}) - y(x_i) + \sum_{j=1}^{m} q_j^{(k)} \left( \frac{\partial f}{\partial p_j^{(k)}} \right)_i + \delta \]  \hspace{1cm} (5)

where

\[ \delta = \text{neglected higher order terms in } p_j. \]

Thus equation (5) can be expressed as:

\[ R_i = r_i + \sum_{j=1}^{m} q_j^{(k)} \left( \frac{\partial f}{\partial p_j^{(k)}} \right)_i \]  \hspace{1cm} (6)

a set of residual equations, linear in \( p_j \).

Minimizing as

\[ \sum_{i=1}^{n} R_i^2 = u(p_j^{(k)}) \]  \hspace{1cm} (7)
The normal equations may be written as:

\[
\begin{align*}
\left( \sum_{p_1 p_1} f_{p_1 p_1} \right) q_1 + \left( \sum_{p_1 p_2} f_{p_1 p_2} \right) q_2 + \ldots + \left( \sum_{p_1 p_m} f_{p_1 p_m} \right) q_m + \sum_{p_1} f_{p_1 r_1} &= 0 \\
\left( \sum_{p_2 p_1} f_{p_2 p_1} \right) q_1 + \left( \sum_{p_2 p_2} f_{p_2 p_2} \right) q_2 + \ldots + \left( \sum_{p_2 p_m} f_{p_2 p_m} \right) q_m + \sum_{p_2} f_{p_2 r_1} &= 0 \\
\left( \sum_{p_m p_1} f_{p_m p_1} \right) q_1 + \left( \sum_{p_m p_2} f_{p_m p_2} \right) q_2 + \ldots + \left( \sum_{p_m p_m} f_{p_m p_m} \right) q_m + \sum_{p_m} f_{p_m r_1} &= 0
\end{align*}
\] (8)

and solved for the differential correction coefficients \( q_j^{(k)} \).

Iterating is continued with the iteration parameter values determined as

\[
p_j^{(k+1)} = p_j^{(k)} + q_j^{(k)}
\] (9)

until the arresting criterion employed is satisfied. Iterating is arrested when

\[
\left| \frac{S^{(k-1)} - S^{(k)}}{S^{(k)}} \right| \leq e'
\]

where

\[
e' = \text{an assigned tolerance value; } e' = 10^{-5} \text{ in code CUBED subprogram STDFIT.}
\]

\[
S^{(k)} = \sum_{i=1}^{n} \left( y(x_i) - f(x_i; p_j^{(k)}) \right)^2 \cdot W(x_i)
\]

\[
W(x_i) = \text{set of statistical weights; } = \left( \frac{(y(x_i))^b}{L} \right)^2 \text{ in code CUBED subprogram STDFIT.}
\]
In general, subprogram STDFIT ceased fitting equation (1) at \( k=5 \). Subprogram GUESS communicates the \( p_j^{(0)} \) to subprogram STDFIT semi-automatically, i.e., it requires \( l \) and \( n \), the lower and upper fitting indices to be input to subprogram PHOFRA (encoded as NSJ and NFNJ). Equation (8) is solved according to the conventional Gauss-Jordan pivoting method\(^{35}\).