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Mollenauer, James F.

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Laboratory*

A COMPUTER ANALYSIS FOR COMPLEX
SODIUM IODIDE GAMMA SPECTRA

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James F. Mollenauer

August, 1961

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A COMPUTER ANALYSIS
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James F. Mollenauer

Lawrence Radiation Laboratory
University of California
Berkeley, California

August 1961

ABSTRACT

A method of analysis for complex or continuous gamma spectra obtained from a 3-in. NaI(Tl) crystal detector is presented. The crystal response was calibrated with a number of sources. A method of interpolation for intermediate energies was then devised. An IBM 704 computer program was written to perform this interpolation and to obtain the incident gamma-ray spectrum by applying a matrix method. An option is provided in the program to allow correction for small gain-drift effects on the spectrum. Though written for a particular crystal and shield configuration, the program can easily be modified to accommodate other shielding arrangements and crystal sizes.

A. Introduction

For the detection of gamma radiation, a single NaI(Tl) crystal has advantages of high efficiency and simplicity; yet its response to radiation is complicated by the presence of the Compton tail on the spectrum and by other nonlinear effects. Discrete gamma lines can be resolved fairly quantitatively by inspection, if they are not too numerous; but more formal analysis is required for spectra containing large numbers of lines or for continuous spectra. This report describes a simple and flexible method of analysis in which the IBM 704 computer is used.

The Fortran listing of the program written for the spectrum analysis (or unfolding) is reproduced at the end of this report. The program can be modified quite easily to accommodate varying experimental conditions. A change in shield configuration from that used here may produce a different response in the detector, especially as the radiation scattered into the crystal is affected. Also, the accuracy of the program may be improved if necessary by fitting more complex functions to the parameters describing the detector response.

The method described here was developed for an experiment measuring gamma-ray yields in nuclear reactions. It was felt that a separate and slightly more extensive description of the spectrum analysis would be useful.

B. Calibration of the Crystal Response

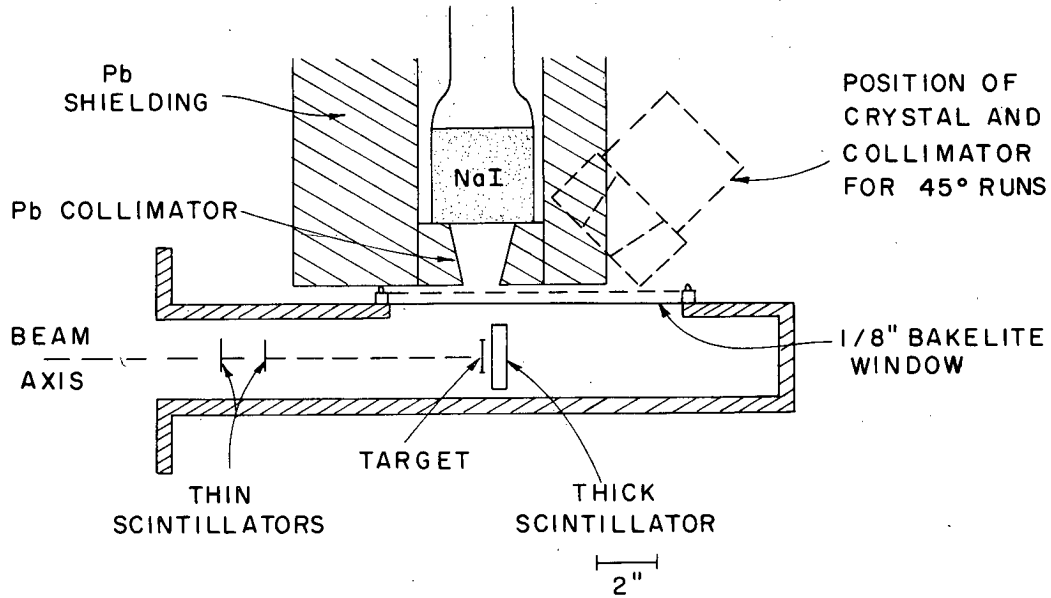
In order to correct for the non-unique response of the NaI(Tl) crystal to gamma radiation, its output pulse-height distribution for radiation of any energy must be known. Not only the photopeak efficiency but also the whole spectrum from a monoenergetic gamma line must be obtained. For arbitrary energies, the response may be found by interpolation between known responses

of standard sources. The over-all response is a function of the shield configuration. Our arrangement is illustrated in Fig. 1. To reduce the large backscattering peak resulting from the close proximity of shield and crystal, a 2-in.-thick collimator was placed in front of the crystal. The collimator also served to position the crystal at a reproducible distance from the source holder. A conical hole, tapering from a 2-in. diameter at the face of the crystal to a 1 1/4-in. diameter at the side near the source, minimized scattering at the inner edges of the collimator. To duplicate the conditions under which the bombardment spectra were obtained, the sources were located in the target holder, which was kept at the same position relative to the shield for each source.

The electronic equipment used in the calibration was relatively simple. The NaI(Tl) pulses were amplified in a DD2 linear amplifier and recorded on a Penco 100-channel pulse-height analyzer. Background spectra were taken after each source run. The sources used for calibration are listed in Table I.

The components into which the spectra were resolved included the photopeak, two escape peaks, the Compton distribution, the scattering peak, and the annihilation peak. The position, height (or area), and width of these components were fitted with functions of the gamma energy.

While the response of the crystal may be calculated theoretically, a strictly empirical approach was preferred because of possible effects of the shield and target block on the spectrum. The predicted proportionality of the half-width of the photopeak to the square root of the gamma energy was found to be a good approximation and was retained. The functional dependences were otherwise derived empirically. The components of the spectra and the dependence of their parameters on the gamma energy E are found in Table II.



MU - 24507

1. Shield configuration: (a) perspective view of shield blocks; and (b) relation of shield to target block, shown from above.

Table I

Sources used in crystal calibration	
Source	E_{γ} (Mev)
Am ²⁴¹	0.060
Co ⁵⁷	0.122
Na ²²	0.51 (1.28 Mev not used)
Rb ⁸⁶	1.08
Na ²⁴	1.38
	2.75
Po - Be	4.45

Table II

Dependence of spectrum components on gamma energy E and pulse height x: E and x in Mev

Component	Condition	Height of component	Half-width
Photopeak height $P_1(E)$	$E < 0.65$	$P_1 = 4.59 \times 10^{-3} E^{-0.033}$	$0.0815 \sqrt{E}$
	$E > 0.65$	$P_1 = 2.53 \times 10^{-3} E^{-1.46}$	(10% of E at $E=0.66$)
1st escape peak height $P_2(E)$	$E < 1.75$	$P_2 = 0$	Same as photopeak
	$E > 1.75$	$P_2 = 0.623 P_1 \ln(E/1.75)$	
2nd escape peak height $P_3(E)$	$E < 1.75$	$P_3 = 0$	Same as photopeak
	$E > 1.75$	$P_3 = 0.247 P_1 \ln(E/1.75)$	
Annihilation peak height $A(E)$	$E < 1.75$	$A = 0$	
	$E > 1.75$	$A = 1.2 [P_2(E) + P_3(E)]$	
Position of Compton edge $c(E)$	$E < 0.5$	$c = 0.6E$	
	$0.5 < E < 1.0$	$c = 0.9E - 0.15$	
	$E > 1.0$	$c = E - 0.25$	
Basic Compton height $H(E)$		$H = \frac{7.7 \times 10^{-3} (E + 0.235) - 1.806 \times 10^{-3}}{10(E+c) (E+0.235)}$	
Compton distribution height $D(E, x)$	$E < 1.75$	$D = H$	
	$x < c$	$D = H(E-x) / (E-c)$	
	$c < x < E$		
	$x > E$	$D = 0$	

Table II (continued)

Dependence of spectrum components on gamma energy E and pulse height x: E and x in Mev

Component	Condition	Height of component	Half-width
Compton distribution height $D(E,x)$	$E > 1.75$; $1.22 < E-x$	$D=x$	
	$0.87 < E-x < 1.22$; $P_2 < H$	$D=x$	
	$P_2 > H$	$D=H+(P_2-H)(x-E+1.22)/0.35$	
	$0.51 < E-x < 0.87$	$D=P_2$	
	$E-c < E-x < 0.51$	$D=P_2+0.1H(x-E+0.51)/(c-E+0.51)$	
	$0 < E-x < E-c$	$D=(P_2+0.1H)(E-x)/(E-c)$	
	$E-x < 0$	$D=0$	

Since accuracy of the response functions on the order of 10% was adequate for purposes of the calculation, no effort was made to derive more accurate parameters. It should be relatively easy to modify the program to incorporate more accurate functional dependences, should greater accuracy be desired, since this step of the calculation is handled separately in function subroutine CURVE.

C. Method of Analysis

The non-unique response of the NaI(TL) crystal complicates the analysis of a complex spectrum. An efficiency correction cannot be applied separately to each interval of the spectrum because each contains Compton events from higher-energy gamma rays. It is necessary in any method of analysis to have a spectrum going nearly to zero at the high-energy end. Otherwise there will be contributions of uncertain magnitude from higher-energy photons to the portion of the spectrum being analyzed. Extrapolating the spectrum to one additional channel can provide an approximate correction for a small number of counts above the upper energy limit. The number of counts in this channel is then subtracted from all the channels being analyzed.

A stripping technique is the simplest method for unfolding a complex spectrum. Pulses in the highest energy interval are assumed to constitute a photopeak. Then the remainder of the pulse-height distribution associated with a photopeak of that size and energy is calculated. This distribution is subtracted from the initial spectrum and the process is repeated with the remainder until all the channels have been treated. A disadvantage of this method is that errors accumulate in the lower-energy channels.

Accordingly, matrix methods have been developed to unfold, or correct, NaI(TL) gamma spectra.^{2,3} In such procedures, the crystal response to gamma

radiation is represented by a matrix. One dimension provides the energy intervals and the other the pulse-height intervals. The rows then denote pulse-height distributions corresponding to the incident energies. This response matrix is inverted and multiplied by the vector representing the observed pulse-height distribution, to obtain the incident-energy distribution. Such a method was found satisfactory by Hubbell and Scofield in analyzing continuous brehmsstrahlung spectra.³

The matrix may be derived from the response functions as follows:⁴ We denote the response of the counter in counts per photon by $R(V,E)$, a function of both gamma energy E and pulse-height voltage V ; if the incident spectrum of the photons is $N(E)$, the observed pulse-height distribution is

$$C(V) = \int_0^{\infty} R(V,E) N(E) dE.$$

In the matrix formulation, this equation appears as

$$\bar{C} = \bar{R} \times \bar{N}$$

where

$$R_{ij} = \int_{v_{i-1}}^{v_i} R(V, \bar{E}_j) dV,$$

$$R(V, \bar{E}_j) \approx \int_{E_{j-1}}^{E_j} R(V,E) dE / E_j - E_{j-1},$$

$$C_i = \int_{v_{i-1}}^{v_i} C(V) dV,$$

and

$$N_j = \int_{E_{j-1}}^{E_j} N(E) dE.$$

In theory, inversion of the matrix R leads to the initial spectrum:

$$\bar{N} = \bar{R}^{-1} \times \bar{C}.$$

While mathematically exact, this method is unsuitable where there are statistical fluctuations in the data and inaccuracy in the response function. It was found to fail completely with the experimental spectra. Presumably because of poor statistics at the high-energy end of the spectrum and the presence of discrete peaks there, large fluctuations between positive and negative values were seen in the unfolded spectrum.

In order to avoid such difficulties, an iterative method had been developed by Scofield, who replaced the matrix inversion by an iterative procedure.⁴ Even in the face of the unfavorable conditions mentioned above, it was found to work well on experimental spectra.

In the iterative method, the vector representing the observed spectrum is multiplied by the response matrix to obtain a doubly folded spectrum. Each channel or element of the observed spectrum is individually corrected by a factor equal to the ratio of the original to the doubly folded value of that element. The corrected spectrum vector is multiplied by the response matrix and the ratios are again found, element by element. These ratios are applied as corrections to the originally observed spectrum (not to the first corrected spectrum). The process is repeated, applying correction factors each time to the original spectrum, until the desired degree of convergence is obtained.

If we denote the original observed spectrum by \bar{C}_0 , the corrected observed spectra by \bar{C}_1 , and the approximations to the incident gamma spectrum by \bar{N}_1 , then

$$\bar{N}_1 = \bar{C}_0.$$

$$\bar{C}_1 = \bar{R} \times \bar{N}_1$$

$$\left(\bar{N}_2\right)_i = \frac{\left(\bar{N}_1\right)_i}{\left(\bar{C}_1\right)_i} \times \left(\bar{C}_0\right)_i$$

$$\bar{C}_2 = \bar{R} \times \bar{N}_2$$

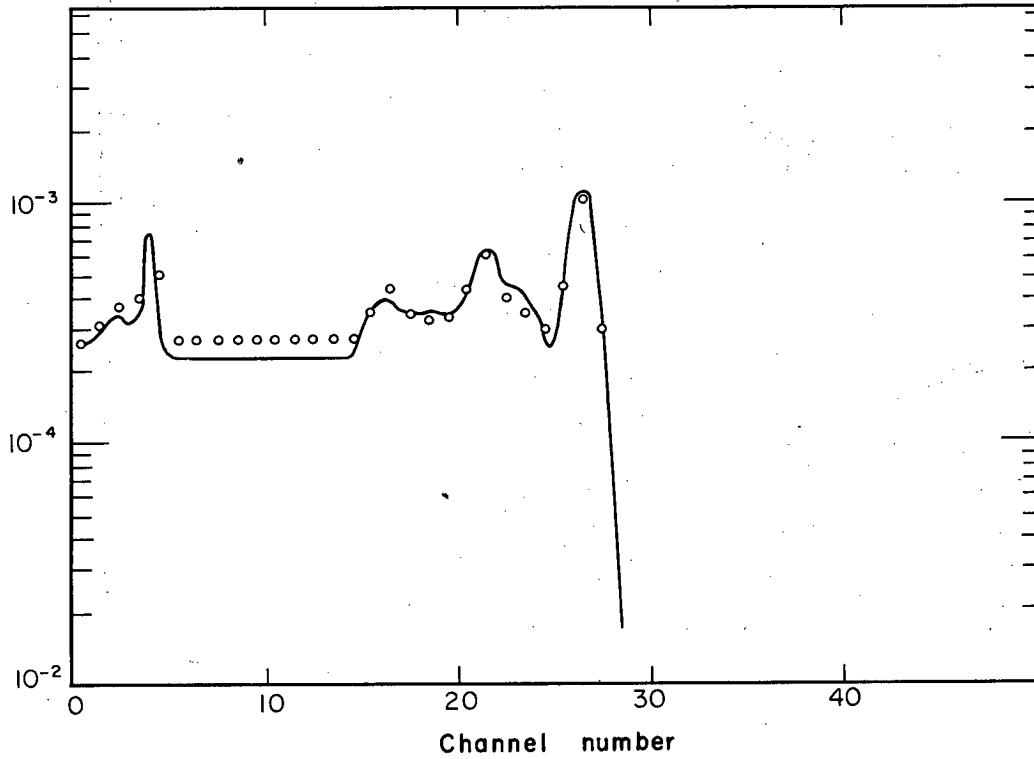
$$\left(\bar{N}_3\right)_i = \frac{\left(N_2\right)_i}{\left(C_2\right)_i} \times \left(\bar{C}_0\right)_i$$

In practice, 50 iterations give convergence within one part in 10^4 .

A comparison of the spectrum of the 2.75-Mev gamma ray of Na^{24} with the corresponding row of the generated response matrix is provided in Fig. 2. The lower-energy gamma ray of Na^{24} at 1.38 Mev is subtracted from the experimental spectrum for purposes of the comparison. The peaks visible are, in order of increasing energy or channel number, the scattering peak, annihilation peak, two escape peaks, and the photopeak.

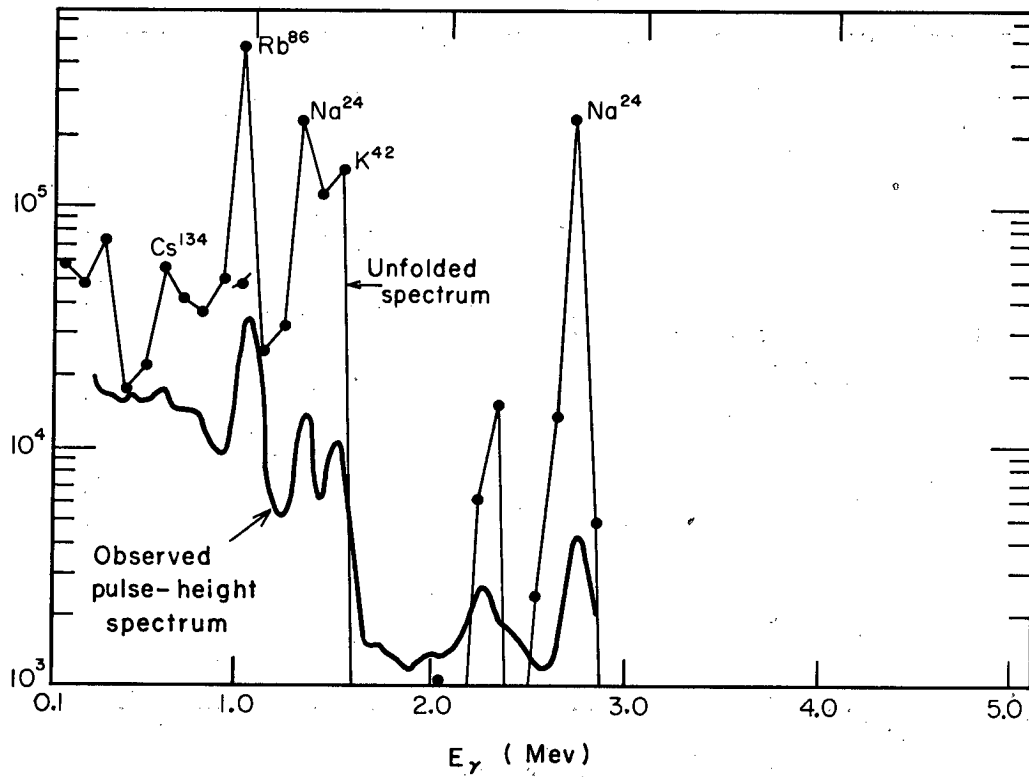
The analysis of a complex spectrum by the program is demonstrated in Fig. 3. A spectrum of several sources is shown before and after unfolding. All the lines except those at 1.38 and 1.55 Mev are well resolved with 50 channels. The accuracy of the matrix is fair; the areas of all the unfolded peaks are 10% higher than the source strengths as measured individually with a standardized crystal. The matrix fails to allow sufficiently for the first escape peak of Na^{24} , with a remainder of 5% of the unfolded photopeak. Also, the valley between the Cs^{134} and Rb^{86} peaks does not fall as low as would be desirable. The peak at 0.35 Mev may result from contamination originating in the reactor production of the Rb^{86} and Na^{24} .

Another check on the validity of the unfolding procedures was made by unfolding a known spectrum. A spectrum of gamma rays in fast coincidence with the fission of Cf^{252} was unfolded, and the results compared with those of Smith, Fields, and Friedman;⁵ the average gamma energy was found to be



MU-24116

2. Comparison of the spectrum of the 2.75-Mev gamma ray of Na^{24} with the appropriate row of the 50-channel response matrix. The spectrum of the 1.38-Mev gamma ray has been subtracted from the experimental spectrum shown.



MU-24118

3. Comparison of observed and unfolded spectra for a mixture of sources.

0.78 Mev, in excellent agreement with the published value of 0.80 Mev. Both spectra showed a peak at about 0.3 Mev, with the main difference being a greater yield in the published spectrum at higher energies. The two are compared in Fig. 4.

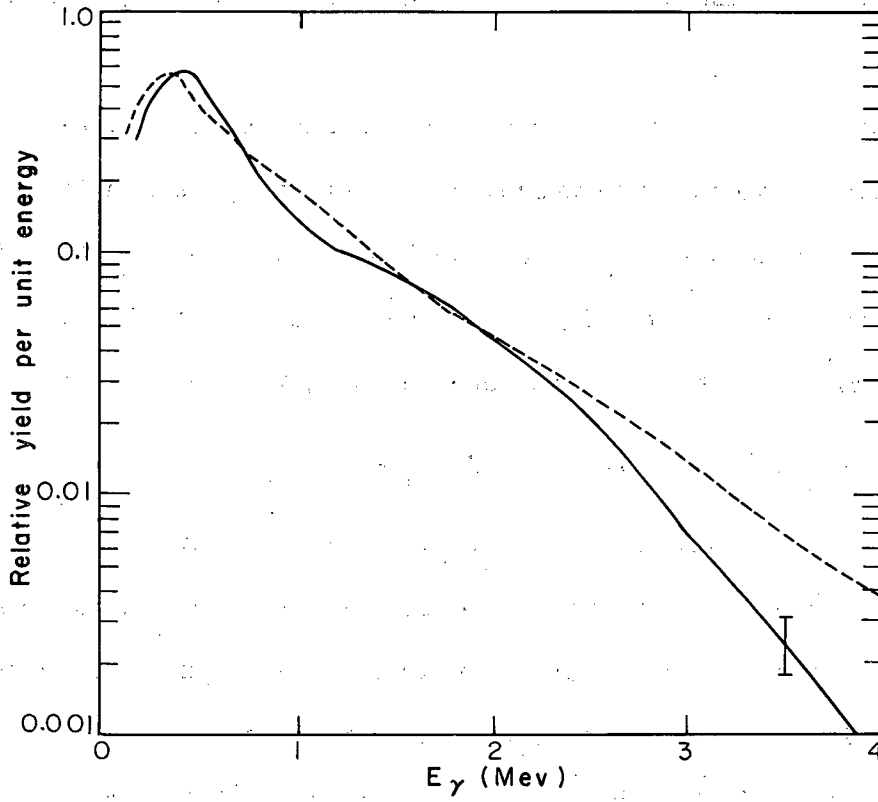
Another possible source of error in the analysis of spectra lies in the statistical fluctuations. The procedure of unfolding is similar to differentiation, and fluctuations in the input spectrum are magnified in the product. To reduce such random effects, various types of smoothing were employed. One was smoothing by the computer according to the formula

$$Y_i' = 1/4 Y_{i-1} + 1/2 Y_i + 1/4 Y_{i+1}$$

either before or after unfolding, or both. Since this formula does not take the better statistics at the low-energy end of the spectrum into account, hand smoothing was tried on all input channels with fewer than 100 counts. All combinations of the three types of smoothing were tried on a test spectrum from the bombardment of Co⁵⁹ with α particles, for both fifty and twenty channels. The results from certain of the smoothing combinations are shown in Figs. 5 and 6. In all cases the average energies were within 3% of each other. Statistical fluctuations caused the unsmoothed 50-channel analysis to generate spurious peaks, whereas a smoothed spectrum appeared to be handled adequately by 20 channels. Hand smoothing alone was selected for use in our experiment, because it did not eliminate structure in the spectrum where the statistics were good. Options remain in the program to cover all combinations of smoothing and number of channels.

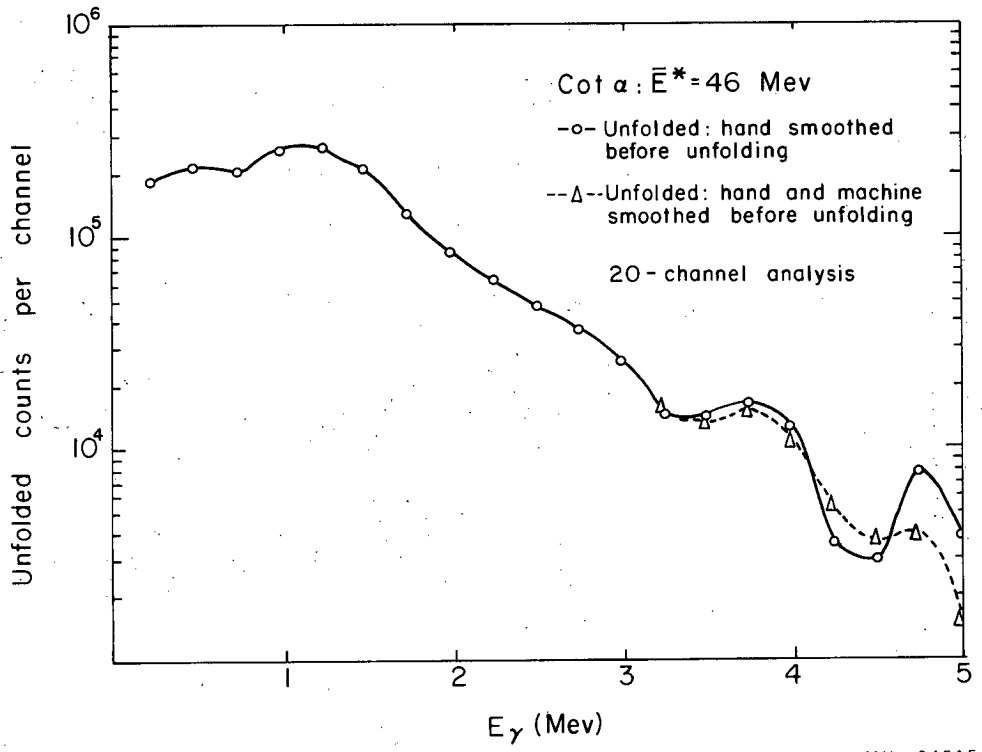
D. Computer Program GAMSPEC

The IBM program that performs the gamma spectral analysis is written in Fortran as a main program and three subprograms. The computation

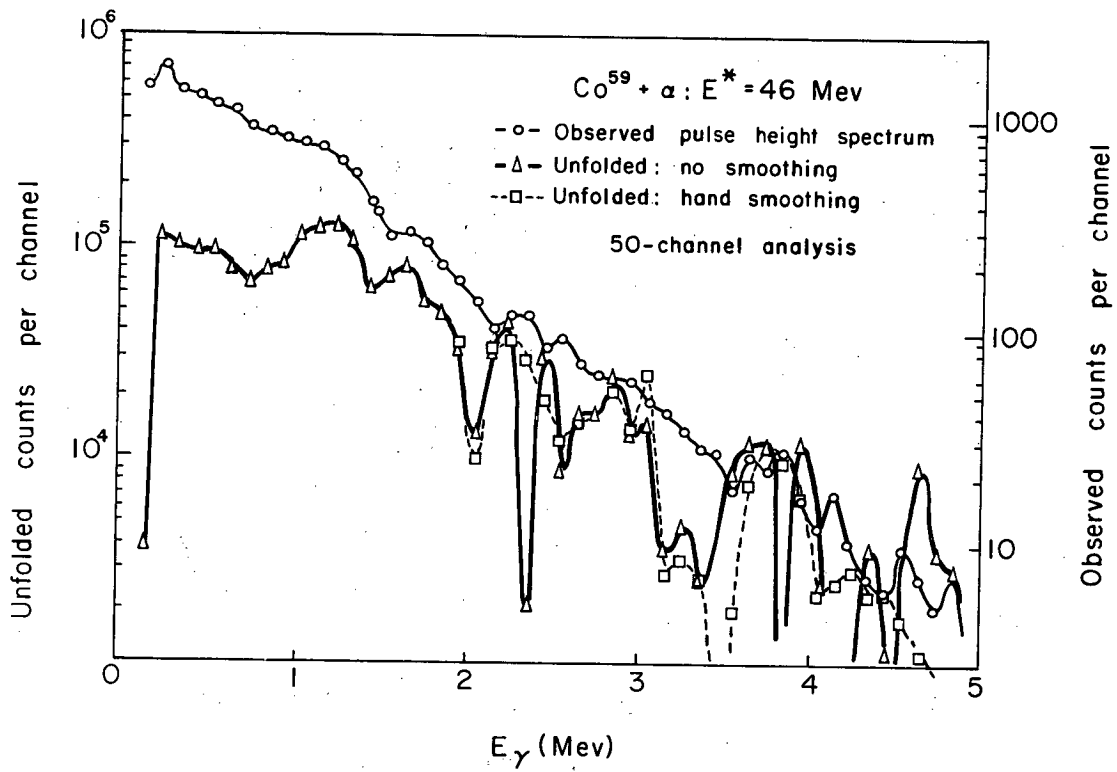


MU-24105

4. Comparison of unfolded fission gamma-ray spectrum of Cf^{252} with that obtained by Smith, Fields, and Friedman (Ref. 5).



5. Spectrum unfolded with various smoothing options; 20 channels.



MU-24516

6. Spectrum unfolded with various smoothing options; 50 channels.

proceeds as follows:

To correct for gain drift observed in a spectrum, subroutine GAINAJ may be called in to apply a correction. The response matrix may then be read from a tape or generated for the required energy range by subroutine RESPON, using the values of the response function $R(V,E)$ generated in function subroutine CURVE.

Spectra may be processed by the program in batches having the same energy limits and number of pulse-height intervals or channels. A gain adjustment factor is specified for each spectrum individually. The data cards for the spectrum are preceded by a card specifying the following constants:

- (a) MESH — the number of channels in the spectrum and the dimension of the response matrix;
- (b) NRUNS — the number of spectra in the batch;
- (c) THRES — the lower gamma-energy limit; and
- (d) EMAX — the upper gamma-energy limit.

The data cards then follow, with each spectrum preceded by the factor GAIN by which the energy scale is to be multiplied. For example, to move a peak from 25 volts to 26 volts pulse height, GAIN is set equal to 1.04. Formats for the cards are given in the listing reproduced in the appendix.

If the value of GAIN is not unity, the program initially calls in subroutine GAINAJ to apply the correction. This subroutine finds the corrected spectrum by interpolating linearly between the points of the input spectrum and correcting for changed channel width. In extrapolating at either end when necessary, it assumes an exponential dependence on pulse height. This approximation was reasonable for the spectra studied. The corrected input spectrum is written on tape 3.

The response matrix may be generated in subroutine RESPON or read from tape 5. The use of the sense switches in exercising the various options is summarized in Table III. After the response matrix has been delivered to the main program, the gain-adjusted input spectrum is smoothed if required; then the spectrum is unfolded according to the iterative scheme. The successive approximations are optionally listed on tape 3. The spectrum may be smoothed after unfolding, if desired.

As a check after the analysis has been completed, the resultant incident spectrum vector is multiplied by the response matrix, and the product written on tape 3. If the number of iterations is sufficient, the product is equal to the input spectrum corrected for gain. The unfolded spectra are written, smoothed and unsmoothed, on tape 3.

In the unfolding, 50 iterations are specified, but the successive approximations to the incident spectrum are checked for divergence after each iteration. However, in our calculation, no early exits from the iteration loop because of divergence were observed.

In writing the response matrix, subroutine RESPON selects the energy and pulse-height intervals according to the specified values of MESH, THRES, and EMAX. The pulse-height intervals are divided into 10 subintervals, the response of the crystal calculated in function subroutine CURVE, and an average taken over the 10 values.

The running time for the evaluation of the response matrix is about 3 minutes for 20 channels and 18 minutes for 50 channels. After generation of the matrix, or if it is already on the tape, the running time per spectrum is less than 30 seconds for 20 channels and slightly over 1 minute for 50 channels.

Table III.

Sense-switch options.

<u>Switch</u>	<u>Position</u>	<u>Result</u>
1	Up Down	No smoothing before unfolding. Machine smoothing applied before unfolding.
2	Up Down	No smoothing after unfolding. Machine smoothing applied after unfolding.
3	Up Down	Successive approximations are not listed. Successive approximations listed on tape 3.
4	Up Down	No correction to geometry. Correction factor of 2.25 applied to product spectrum for second experimental source position.
5	Up Down	Response matrix read from tape 5. Response matrix generated and written on tape 5.

ACKNOWLEDGMENTS

The author would like to express his gratitude to Dr. Bernard G. Harvey for his advice and encouragement. This work was greatly facilitated by discussions with Dr. N.E. Scofield, Mr. Harry Bowman, and Dr. Lloyd Mann.

Thanks are due to Mr. Douglas Brainard for assistance with the coding in times of difficulty.

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APPENDIX

Fortran Listings of GAMSPEC and Subroutines

C PROGRAM BLOB FOR ENERGIES OF DEFORMED ROTATING LIQUID DROP

```

1 DIMENSION BSTEP(40),INTGAM(40), SURFE(40,40), ECOUL(40,40),
  XEROT(40,40),ETOTAL(40,40),W(6), Z(6), PSI(6)
5 READ 10, XSTART, XSTOP, RSTART, RSTOP, ISTEPS, JSTEPS, KSTEPS,
  XLSTEPS, XFIXED, RFIXED
10 FORMAT (4F8.4, 4I4, 2F8.4)
12 READ 13, (W(I),I=1,6), (Z(J),J=1,6)
13 FORMAT (6F12.9 )
30 DO 200 I=1,ISTEPS
  B = I
  BSTEPS = ISTEPS
  BETA = (B*1.0)/BSTEPS
  BSTEP(I) = BETA
35 DO 200 J=1,JSTEPS
  G=J
  GSTEPS=JSTEPS
  GAMMA = 120.0+((G-1.0)*60.0)/(GSTEPS-1.0)
  INTGAM(J) = GAMMA
  PI= 3.14159265
  GAMMA = GAMMA/57.2957795
50 CANG=COSF(GAMMA)
  BANG=COSF(GAMMA+(2.0*PI)/3.0)
  AANG=COSF(GAMMA -(2.0*PI)/3.0)
60 ASQ= EXPF ((2.0*BETA)*AANG)
  BSQ= EXPF ((2.0*BETA)*BANG)
  CSQ= EXPF ((2.0*BETA)*CANG)
70 ALPASQ= (ASQ-CSQ)/ASQ
  DLTASQ= (BSQ-CSQ)/BSQ
  TSQ= DLTASQ/ALPASQ
  T= SQRTF(TSQ)
  ALPHA= SQRTF(ALPASQ)
  CHI= SQRTF(1.0-ALPASQ)
  PHI = ATANF(ALPHA/CHI)
80 RHO=SQRTF(1.0-DLTASQ)
  CINVER= EXPF(-BETA*CANG)

83 CALL ELLIP (PHI, T, W, Z, E, F)
85 BSURF= 0.5*CINVER*(RHO*CHI+(1.0/ALPHA-ALPHA)*F+ (ALPHA*E))

```

C NOW CALCULATE BCOUL AND BROT

```

100 EPSLON = SQRTF(1.0/(ASQ-CSQ))
  TAU = EPSLON * SQRTF(ASQ-BSQ)
  CALL ELLIP(PHI, TAU, W, Z, E, F)
120 BCOUL = EPSLON*F
  BROT = 2.0/(ASQ+BSQ)
  SURFE(I,J) = BSURF-1.0
  ECOUL(I,J) = BCOUL-1.0
200 EROT(I,J) = BROT

```

C WRITE TABLES OF SURFACE AND COULOMB ENERGY AND BROT

```

WRITE OUTPUT TAPE 1,210
210 FORMAT(22H1SURFACE ENERGY CHANGE)
211 WRITE OUTPUT TAPE 1,212, (INTGAM(J),J=1,JSTEPS)
212 FORMAT (7HOGAMMA= 14I8)
213 WRITE OUTPUT TAPE 1,214
214 FORMAT(5H BETA)
  DO 215 I=1, ISTEPS
215 WRITE OUTPUT TAPE 1,216, BSTEP(I), (SURFE(I,J), J=1, JSTEPS)
216 FORMAT (1H F5.3, F10.5, 13F8.5)
  WRITE OUTPUT TAPE 1,230

```

```
230 FORMAT(22H1COULOMB ENERGY CHANGE)
231 WRITE OUTPUT TAPE 1,212, (INTGAM(J),J=1,JSTEPS)
232 WRITE OUTPUT TAPE 1,214
234 DO 236 I=1,ISTEPS
236 WRITE OUTPUT TAPE 1,216, BSTEP(I), (ECOUL(I,J), J=1, JSWEPS)
    WRITE OUTPUT TAPE 1,240
240 FORMAT(27H1ROTATIONAL PARAMETER BROT )
241 WRITE OUTPUT TAPE 1,212, (INTGAM(J),J=1,JSTEPS)
242 WRITE OUTPUT TAPE 1,214
244 DO 246 I=1,ISTEPS
246 WRITE OUTPUT TAPE 1,216, BSTEP(I), (EROT (I,J), J=1, JSTEPS)

C    OPTION FOR SINGLE X AND R VALUE

247 IF (SENSE SWITCH 3) 248,255
248 DO 250 I=1, ISTEPS
    DO 250 J=1, JSTEPS
250 ETOTAL(I,J)=SURFE(I,J)+2.0*XFIXED*ECOUL(I,J)+RFIXED*EROT(I,J)
252 GO TO 287

C    COMPUTE ENERGY TABLES FOR MESH OF X AND R VALUES

255 DO 285 K=1,KSTEPS
    XSTEP = K-1
    XSTEPS = KSTEPS-1
    X = XSTART + XSTEP*(XSTOP-XSTART)/XSTEPS
260 DO 285 L=1,LSTEPS
    RSTEP = L-1
    RSTEPS = LSTEPS-1
    R = RSTART + RSTEP*(RSTOP-RSTART)/RSTEPS
270 DO 275 I=1,ISTEPS
    DO 275 J=1,JSTEPS
275 ETOTAL(I,J)=SURFE(I,J)+2.0*X *ECOUL(I,J)+R *EROT(I,J)
278 WRITE OUTPUT TAPE 1, 280
279 WRITE OUTPUT TAPE 1, 277, X, R
277 FORMAT (28H0FISSIONABILITY PARAMETER X= F5.3,
    X16HLAMBDA SQUARED = F5.3)
280 FORMAT (51H1TOTAL ENERGY CHANGE AS FRACTION OF SURFACE ENERGY )
281 WRITE OUTPUT TAPE 1,212, (INTGAM(J),J=1,JSTEPS)
282 WRITE OUTPUT TAPE 1,214
284 DO 285 I=1,ISTEPS
285 WRITE OUTPUT TAPE 1,216, BSTEP(I),(ETOTAL(I,J), J=1, JSTEPS)
286 GO TO 299
287 CONTINUE
288 WRITE OUTPUT TAPE 1, 280
290 FORMAT (51H1TOTAL ENERGY CHANGE AS FRACTION OF SURFACE ENERGY )
291 WRITE OUTPUT TAPE 1,212, (INTGAM(J),J=1,JSTEPS)
292 WRITE OUTPUT TAPE 1,214
294 DO 295 I=1,ISTEPS
295 WRITE OUTPUT TAPE 1,216, BSTEP(I),(ETOTAL(I,J), J=1, JSTEPS)
299 CONTINUE
300 END (0,1,0,0,1)
```

SUBROUTINE ELLIP (PHI, T, W, Z, E, F)
DIMENSION W(6), Z(6), PSI(6)

C DETERMINE THE NUMBER OF ITERATIONS

```
5 IF(T-0.55) 10,10,15
10 N=1
11 GO TO 30
15 IF(T-0.85) 17,17,20
17 N=2
18 GO TO 30
20 IF(T-0.95) 22,22,25
22 N=3
23 GO TO 30
25 IF (T-0.99) 27 ,27,29
27 N = 5
28 GO TO 30
29 E = SIN (PHI)
   DIFFE = (1.0+E)/(1.0-E)
   F = 0.5*LOGF (DIFFE)
   GO TO 91
30 PSI(1) = 0.0
```

C DO SUMMATIONS TO FIND E AND F

```
DO 35 I=1,N
  FLI = I
  FLN = N
35 PSI(I+1) = FLI*PHI/FLN
   F = 0.0
   E = 0.0
40 DO 90 I=1,N
  FSUMJ = 0.0
  ESUMJ = 0.0
50 DO 75 J = 1,6
  OMEGA = (PSI(I+1) - PSI(I))*W(J) + PSI(I)
  SINOM = SIN(OMEGA)
60 CN = SQRTF(1.0-T*T*SINOM*SINOM)
  FTERMJ = Z(J)/CN
70 ETERMJ = Z(J)*CN
  FSUMJ = FSUMJ + FTERMJ
  ESUMJ = ESUMJ + ETERMJ
75 CONTINUE
  FTERMI =FSUMJ*(PSI(I+1) - PSI(I))
  ETERMI =ESUMJ*(PSI(I+1) - PSI(I))
  F = FTERMI + F
  E = ETERMI + E
90 CONTINUE
98 RETURN
100 END(0,1,0,0,1)
```

C GAMMA SPECTRUM ANALYSIS - PROGRAM GAMSPEC

DIMENSION R(50,50), F(50),H(50), B(50,50), X(50,50),D(50,50),
XW(50,50), SUM(50), ESUM(50), E(50), RESID(50), DIF(50,50),
X Y(50,50)

READ 5, MESH, NRUNS, THRES, EMAX
5 FORMAT (2I5, 2F10.3)
WRITE OUTPUT TAPE 3,13
13 FORMAT (14H1INPUT SPECTRA)
10 DO 35 JS=1, NRUNS
READ 12, GAIN, (F(I), I=1,MESH)
12 FORMAT (7F10.3)
WRITE OUTPUT TAPE 3, 93, JS, (F(J), J=1,MESH)
CALL EFM (0,0)

C ADJUST GAIN IF REQUIRED

IF (GAIN-1.0) 20,30,20
20 CALL GAINAJ (F, H, MESH, GAIN, THRES, EMAX)
DO 25 I=1, MESH
25 B(I,JS) = H(I)
GO TO 35
30 DO 34 K=1, MESH
34 B(K,JS) = F(K)
35 CONTINUE
FLMESH = MESH
DO 36 J=1, MESH
EINDEX = J
36 E(J) = ((EMAX-THRES)/FLMESH) * (EINDEX-0.5) + THRES

C GENERATE RESPONSE MATRIX OR READ IT FROM TAPE

IF (SENSE SWITCH 5) 40,47
40 CALL RESPON (MESH, EMAX, THRES, R)
WRITE OUTPUT TAPE 5, 45, ((R(I,J), I=1,MESH), J=1, MESH)
45 FORMAT (1P5E18.9)
END FILE 5
REWIND 5
GO TO 48
47 READ INPUT TAPE 5, 45, ((R(I,J), I=1,MESH), J=1, MESH)
REWIND 5
48 CONTINUE

C OPTIONAL SMOOTHING BEFORE UNFOLDING

IF (SENSE SWITCH 1) 50,58
50 DO 55 N=1,NRUNS
MINUS = MESH - 1
DO 53 L=2, MINUS
53 X(L,N) = 0.25*B(L-1,N) + 0.5*B(L,N) + 0.25*B(L+1,N)
X(MESH,N) = 0.25* B(MINUS,N) + 0.75* B(MESH,N)
X(1,N) = 0.75*B(1,N) + 0.25* B(2,N)
DO 55 L=1, MESH
55 B(L,N) = X(L,N)

C UNFOLD BY SUCCESSIVE APPROXIMATIONS

58 DO 140 N=1,NRUNS
DO 110 I=1, MESH
DO 110 J=1,50
DIF (I,J) = 0.0
D(I,J) = 0.0
110 W(I,J) = 0.0


```

DO 115 I=1,MESH
115 W(I,1) = B(I,N)
DO 120 I = 1, MESH
DO 120 J = 1, MESH
120 D(I,1) = R(I,J) * W(J,1) + D(I,1)
DO 130 L= 1,49
LL= L+1
DO 122 I=1, MESH
122 W(I,L+1) = (W(I,L) / D(I,L)) * W(I,1)
RESID(1) = 0.0
RESID (LL) = 0.0
DO 125 J=1, MESH
DIF(J,L) = W(J,L+1) - W(J,L)
125 RESID (LL) = RESID (LL) + DIF(J,L) * DIF(J,L)
RESID (LL) = SQRTF (RESID(LL))
IF (L-2) 127,127,126

C CHECK FOR DIVERGENCE OF APPROXIMATIONS

126 IF (RESID(LL) -RESID(LL-1) ) 127,230,230
127 DO 130 I=1, MESH
DO 130 J=1, MESH
130 D(I,L+1) = R(I,J)*W(J,L+1) + D(I,L+1)
GO TO 131
230 LL=LL-1
131 DO 132 I=1, MESH
132 X(I,N) = W(I,LL)

C OPTIONAL WRITING OF APPROXIMATIONS

IF (SENSE SWITCH 3) 133,140
133 WRITE OUTPUT TAPE 3, 134
134 FORMAT (28H1 SUCCESSIVE APPROXIMATIONS )
DO 135 J=1,25
135 WRITE OUTPUT TAPE 3 , 136, N,J,(W(I,J), I=1,MESH), RESID(J)
136 FORMAT (4HORUN 12, 3H J=12,1P10E10.3/(1PE21.3,1P9E10.3 ))
140 CONTINUE

C GEOMETRY FACTOR FOR 45 DEGREE RUNS

IF (SENSE SWITCH 4) 142,150
142 DO 146 N=1, NRUNS
DO 146 I=1, MESH
146 X(I,N) = X(I,N) * 2.25
150 DO 69 J=1, NRUNS

C COMPUTE SUM OF COUNTS AND AVERAGE ENERGY

SUM (J) = 0.0
ESUM (J) = 0.0
DO 68 L = 1, MESH
ESUM (J) = ESUM (J) + E (L)*X(L,J)
68 SUM (J) = SUM (J) + X (L,J)
69 ESUM (J) = ESUM (J) / SUM (J)

C WRITE SMOOTHED INPUT SPECTRUM AND UNFOLDED SPECTRUM

90 WRITE OUTPUT TAPE 3, 92
DO 91 J =1, NRUNS

```

```

91 WRITE OUTPUT TAPE 3, 93, J, ( B (I,J), I = 1, MESH )
92 FORMAT ( 41 H0 SPECTRA ADJUSTED FOR GAIN AND SMOOTHED )
93 FORMAT ( 11HORUN NUMBER I2,1P10E10.3/(13H 1P10E10.3)
94 FORMAT (26H TOTAL COUNTS F10.1 , 15H AVERAGE ENERGY
X F8.3 )
WRITE OUTPUT TAPE 3, 96
96 FORMAT (25HUNFOLDED GAMMA SPECTRA )
DO 95 J = 1, NRUNS
WRITE OUTPUT TAPE 3, 93, J, ( X (I,J), I=1, MESH )
95 WRITE OUTPUT TAPE 3, 94, SUM (J) , ESUM (J)

```

C MULTIPLY UNFOLDED SPECTRUM BY RESPONSE MATRIX TO CHECK

```

WRITE OUTPUT TAPE 3,320
320 FORMAT (14HOCHECK SPECTRA )
DO 325 N=1, NRUNS
DO 324 I=1, MESH
DO 324 J=1, MESH
324 Y(I,N) = Y(I,N) + R(I,J) *X(J,N)
325 WRITE OUTPUT TAPE 3, 93, N, (Y(I,N), I=1, MESH)

```

C OPTIONAL SMOOTHING AFTER UNFOLDING

```

IF (SENSE SWITCH 2) 240, 97
240 WRITE OUTPUT TAPE 3, 250
250 FORMAT (26H SMOOTHED UNFOLDED SPECTRA )
DO 350 N=1, NRUNS
MINUS = MESH - 1
DO 340 L=2, MINUS
340 Y(L,N) = 0.25*X(L-1,N) + 0.5*X(L,N) + 0.25*X(L+1,N)
Y(MESH,N) = 0.25* X(MINUS,N) + 0.75* X(MESH,N)
Y(1,N) = 0.75*X(1,N) + 0.25* X(2,N)
DO 345 L=1, MESH
345 X(L,N) = Y(L,N)
350 WRITE OUTPUT TAPE 3, 93, N, (X(I,N), I=1, MESH)
97 CONTINUE
END FILE 3
REWIND 3
100 END ( 0,1,0,0,0 )

```

SUBROUTINE GAINAJ (F,H,NBOXES,GAIN, THRES, EMAX)

```

DIMENSION E(50), EA(50), H(50), G(50), F(50)
BOTE = THRES * GAIN
TOPE = EMAX * GAIN
DO 10 N=1, NBOXES
BOXES = NBOXES
P=N
E(N) = (((TOPE-BOTE) /BOXES) * (P-0.5)) + BOTE
G(N) = F(N)/GAIN
10 EA(N)=(((EMAX-THRES)/BOXES) * (P-0.5)) / + THRES
IF ( GAIN - 1.0 ) 60,60,14

```

C GAIN TO BE INCREASED

```

14 H(1) = G(1) - (G(2)-G(1))*(E(1)-EA(1))/(E(2)-E(1))
15 DO 50 N=2, NBOXES
DO 30 L=2, N

```

```

M=N-L+1
IF (EA(N)-E(M)) 30,30,45
30 CONTINUE
45 H(N) = G(M) + (G(M+1)-G(M))*(EA(N)-E(M))/(E(M+1)-E(M))
50 CONTINUE
55 GO TO 90

C GAIN TO BE DECREASED

60 DO 80 N=1,NBOXES
  NLESS = NBOXES - N
  DO 70 L=1,NLESS
    M=N+L
    IF (EA(N) -E(M)) 75,75,70
  70 CONTINUE
  72 H(N) = G(NBOXES) *(G(NBOXES)/G(NBOXES-1))**((EA(N)-E(NBOXES))/
  X (E(NBOXES)-E(NBOXES-1)) )
  GO TO 80
  75 H(N) = G(M) -(G(M)-G(M-1)) * (E(M)-EA(N))/(E(M)-E(M-1))
  80 CONTINUE
  90 RETURN
  95 END (0,1,0,0,1)

```

SUBROUTINE RESPON (MESH, EMAX, THRES,R)

```

DIMENSION R(50,50) , E(50)
FLMESH = MESH

```

C LOCATE ENERGY INTERVALS

```

DO 12 J=1, MESH
  EINDEX = J
  10 E(J) = (( EMAX-THRES ) /FLMESH ) * ( EINDEX- 0.5 ) + THRES
  DO 12 K = 1, MESH
  12 R (J,K ) = 0.0

```

C LOCATE PULSE HEIGHT INTERVALS

```

15 DO 60 J = 1, MESH
  DO 50 I = 1, MESH
  ELEM = 0.0

```

C AVERAGE RESPONSE OVER 10 PULSE HEIGHT INTERVALS

```

DO 25 L = 1,10
  XINDEX = 10* ( I-1 ) + L
  X = (( EMAX-THRES) / (FLMESH*10.0)) * (XINDEX-0.5) + THRES
  ELL = L
  IF (X- 1.25*E(J)) 25,25,55
  25 ELEM = ELEM + CURVE(E(J),X)
  50 R (I,J) = R (I,J) + ELEM /10.0
  55 R (I,J) = R (I,J) + ELEM / ELL
  60 CONTINUE
  DO 70 I=1,MESH
  DO 70 J=1,MESH
  70 R(I,J) = R(I,J) * 100.0/ FLMESH
  RETURN
  END (0,1,0,0,1)

```

FUNCTION CURVE (E,X)

C PHOTO AND ESCAPE PEAKS

PHOT1 = 0.0
PHOT2 = 0.0
PHOT3 = 0.0
C = 0.361
U = 0.0815 * ((E)**0.5)

C CONSTANTS FOR 10 PERCENT RESOLUTION AT 0.66 MEV

IF (E-0.65) 5,7,7
5 HITE1 = 0.00459 * E**(-0.033)
GO TO 8
7 HITE1 = 0.00253 * E**(-1.46)
8 PHOT1 = HITE1 * EXPF(-(X-E)**2.0 / (C*U**2.0))
IF (E-1.75) 11,9,9
9 HITE2 = 1.437*HITE1*LOGF(E/1.75) /2.303
HITE3 = 0.569*HITE1*LOGF(E/1.75) /2.303
PHOT2 = HITE2 * EXPF(-(X-E+0.51)**2.0 / (C*U**2.0))
PHOT3 = HITE3 * EXPF(-(X-E+1.02)**2.0 / (C*U**2.0))
IF (X-0.4) 10,102,102
102 IF (X-0.6) 103,103,10

C ANNIHILATION PEAK

103 ANNHT = 1.2 * (HITE2 + HITE3)
ANNIH = ANNHT * EXPF(-(X-0.51)**2.0 / 0.00122)
GO TO 11
10 ANNIH = 0.0
11 IF (E-1.0) 14,12,12

C COMPTON DISTRIBUTION

12 COMPEJ = E-0.25
13 GO TO 20
14 IF (E-0.5) 17,15,15
15 COMPEJ = 0.9 * E - 0.15
16 GO TO 20
17 COMPEJ = 0.6 * E
20 CONTINUE
COMAR = 0.0077 - 0.001806 / (E+0.235)
COMPHT = COMAR / ((E+COMPEJ) * 10.0)

C SCATTER PEAK

121 IF (X-0.5) 22,21,21
21 SCATR = 0.0
GO TO 24
22 SCATHT = 0.455*COMPHT
SCATPS = 0.145 + 0.0675*E
SCWID = 0.08
SCATR = SCATHT * EXPF (-(X-SCATPS)**2.0 / (C*SCWID**2.0))

C COMPTON DISTRIBUTION WITH ESCAPE PEAKS

```
24 IF (E-1.75) 25,25,30
25 IF (X-COMPEJ) 26,26,27
26 COMPT = COMPHT
   GO TO 50
27 IF (X-E) 28,28,29
28 COMPT = COMPHT * (E-X) / (E-COMPEJ)
   GO TO 50
29 COMPT = 0.0
   GO TO 50
30 IF (X-E+1.22) 31,31,34
31 COMPT = COMPHT
32 GO TO 50
34 IF (X-E+0.87) 35,38,38
35 IF (HITE2 - COMPHT) 31,31,135
135 COMPT = COMPHT + (HITE2-COMPHT)*((X-E+1.22)/0.35)
36 GO TO 50
38 IF (X-E+0.51) 39,42,42
39 COMPT = HITE2
40 GO TO 50
42 IF (X-COMPEJ) 43,45,45
43 COMPT = HITE2 + (0.1*COMPHT) * ((X-E+0.51)/(COMPEJ-E+0.51))
44 GO TO 50
45 IF (X-E) 46,48,48
46 COMPT = (HITE2 + 0.1 * COMPHT) * (E-X) / (E-COMPEJ)
47 GO TO 50
48 COMPT = 0.0
50 CONTINUE
55 CURVE = PHOT1 + PHOT2 + PHOT3 + SCATR + COMPT + ANNIH
   RETURN
   END (0,1,0,0,1)
```

REFERENCES

1. J.F. Mollenauer, Effects of Angular Momentum on Gamma-Ray Production in Compound-Nucleus Reactions (Ph.D. Thesis), Lawrence Radiation Laboratory Report 9724, June 1961.
2. N. Starfelt and H. W. Koch, Phys. Rev. 102, 1598 (1956).
3. J. H. Hubbell and N. E. Scofield, IRE Trans. Nuclear Sci. NS-5, 1957 (1958).
4. N. E. Scofield, A Technique for Unfolding Gamma-Ray Scintillation Spectrometer Pulse-Height Distributions, U.S. Naval Radiological Defense Laboratory Report USNRDL- TR 447, 1960.
5. A. B. Smith, P. R. Fields, and A. M. Friedman, Phys. Rev. 104, 699 (1956).

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