2

GJBX-169 '79

science Applications, INC.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ANALYSIS OF AIRBORNE RADIOMETRIC DATA
VOLUME 4
MAZNAI CODE FOR GAMMA-RAY
SPECTRAL ENHANCEMENT

By
J. H. Reed
D. C. Shreve
S. M. Sperling

January 17, 1979

Science Applications, Inc.
P. O. Box 2351
La Jolla, California 92037

Work performed, in part, under Bendix Field Engineering
Corporation, Grand Junction Operations
Subcontract No. 77-041-L

Prepared for
U.S. Energy Research and Development Administration
Grand Junction, Colorado 81501

MASTER

SCIENCE APPLICATIONS, LA JOLLA, CALIFORNIA
ALBUQUERQUE • ANN ARBOR • ARLINGTON • ATLANTA • BOSTON • CHICAGO • HUNTSVILLE
LOS ANGELES • McLEAN • PALO ALTO • SANTA BARBARA • SUNNYVALE • TUCSON

P.O. Box 2351, 1200 Prospect Street, La Jolla, California 92037

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

"This report was prepared as an account of work sponsored in part by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of the contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus product or process disclosed, or represents that its use would not infringe privately owned rights."

CONTENTS

1.	INTRODUCTION	3
2.	DESCRIPTION OF MAZNAI METHODOLOGY	5
3.	DETECTOR RESPONSE FUNCTION	15
4.	MAZNAI USER'S GUIDE	21
5.	REFERENCES	25
APPENDIX A - MAZNAI - CODE LISTING		A-1
APPENDIX B - REPRINT OF REFERENCE 5		B-1

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

1. INTRODUCTION

In gamma-ray spectrometry measurements, an energy distribution of gamma-rays is viewed by a spectrometer which in turn produces a data set. This data is the result of a complex detection process and generally suffers from loss of resolution due to this detection process and to statistical noise. It is the purpose of the MAZNAI computer program to remove the degrading effects of the detector, to minimize the effects of statistical fluctuations, and to construct an enhanced image spectrum that corresponds as closely as possible to the spectrum of radiation incident on the detector.

The MAZNAI methodology and code has evolved over a period of several years. The mathematical basis is provided by the formulation of an optimization function, W , consisting of the sum of a posteriori and a priori information. For those interested in a detailed description of the formulation of a W -function the Science Application, Inc. (SAI) report to the Defense Nuclear Agency⁽¹⁾ authored by Martin Sperling is recommended. In the present version of MAZNAI, the W -function has been designed for the processing of "peaky" data such as gamma-ray and x-ray spectra that contained discrete lines superimposed on a continuum. The a posteriori portion of W is a function of the instrumental response. Therefore, an accurate response function of the detector must be provided for satisfactory operation. The a priori portion contains all the information known prior to the measurement. For example, peaks tend to be gaussian shaped and the remainder of the spectrum tends to be a smoothly varying continuum.

Section 2 of this report gives a brief description of the MAZNAI methodology, Section 3 discusses detector response functions. Section 4 is the user's guide which describes particular details of the preparation of the data necessary for running the code.

Appendix A contains the code listing. For completeness, the Berger and Seltzer Publication (Ref 5) which is the basis for the adopted detector response function parameterization - is included as Appendix B.

2. DESCRIPTION OF MAZNAI METHODOLOGY

Gamma-ray spectrometers are usually linear in their behavior. They produce expected data sets related to object spectra by an integral equation of the form

$$D_i = N \int K(E_+, E_-) \bar{\phi}(E) dE; \quad (1)$$

where

$$E_+ = \frac{1}{2}(E_i + E)$$

is the average of the incident particle energy, E , and the energy deposited in the spectrometer when an event is detected in its i -th channel, E_i , where

$$E_- = E_i - E$$

is the difference between these two energies; where $K(E_+, E_-)$, the spectrometer response, is the probability of a count being detected in the i -th channel when a quantum of radiation is incident on the spectrometer; and where N is the total number of events detectable over the full range of deposition energies, from zero to infinity. Generally the dependence of K on E_+ is slow, so that over a sufficiently narrow energy interval, K may be approximated as dependent on E_- alone. In this case, the integral relating object and data becomes a convolution integral, the so-called folding integral. The German name for convolution, "faltung," is the origin of the terms "folding" and "unfolding".

The conceptualization of unfolding as a process of deconvolution is in error in two regards: first, as we have already seen, the folding integral has a dependence on E_+ , and is therefore not a convolution in the strictest sense. Second, the

introduction of noise into the sequence of information flow makes the sequence irreversible, destroying perfect symmetry between the spectrometer and the unfolding processor, separating the values of the expected and the observed data and making the image spectrum only an estimate of the object. Consequently, the most accurate inverse of the folding integral does not compute the most accurate unfolded spectrum.

The approach to spectral unfolding in which a function is optimized as the spectral estimate is varied, is based on Bayesian statistics. In brief, the expectation value of the spectrum is given by the integral

$$\phi(E) = \int_{\text{all } \bar{\phi}} \bar{\phi} f(\bar{\phi}|D) d\bar{\phi}, \quad (2)$$

where $f(\bar{\phi}|D)$ is the conditional probability that the spectral vector assumes the value $\bar{\phi}$ when the data vector assumes the observed value D , and where the range of integration is over all physically allowable spectra. This solution is an impractical one, however, because of the high dimensionality of the integral as determined by the number of degrees of freedom of the spectrum. Fortunately, $f(\bar{\phi}|D)$ tends to have a maximum in $\bar{\phi}$ closely localized at the expectation value. Therefore, optimization techniques can be applied to approximating that vector value.

It is difficult to formulate $f(\bar{\phi}|D)$ directly, because doing so requires thinking backward from the observed data to the object spectrum. Thinking forward requires use of the equivalent formulation

$$f(D|\bar{\phi}) f(\bar{\phi})/f(D) = f(\bar{\phi}|D), \quad (3)$$

where $f(D|\bar{\phi})$ is the conditional probability of observing data D when the object spectrum $\bar{\phi}$ is measured, and where $f(\bar{\phi})$ and $f(D)$ are the a priori probability distributions of spectrum and data,

respectively. Since the optimization is one in which the spectrum is varied, the $f(D)$ denominator behaves as an arbitrary constant which can be omitted without affecting the final result.

Another practical matter is that probabilities are awkward to work with, primarily because of their extreme numerical range and consequently sudden gradients. Likelihoods, defined as the logarithms of probabilities, have been useful in this regard, the Bayesian likelihood having the form

$$L(\bar{\phi}|D) = L_{\text{a posteriori}}(D|\bar{\phi}) + L_{\text{a priori}}(\bar{\phi}) . \quad (4)$$

Optimizing the a posteriori term corresponds to what is conventionally known as the maximum likelihood technique, while inclusion of the a priori term generally regularizes the solution in the presence of statistical counting fluctuations and poorly conditioned response matrices. This formulation was applied to nuclear physics many years ago by Fermi, and was described in Jay Orear's Notes on Statistics for Physicists⁽²⁾. Analogous formulations have been suggested by A.N. Tikhonov⁽³⁾ and by D.L. Phillips⁽⁴⁾.

The negative of the likelihood is sometimes referred to as the information, information function, or information functional, and it decomposes into an analogous sum of a posteriori and a priori terms:

$$W(\bar{\phi}|D) = W_{\text{a posteriori}}(D|\bar{\phi}) + W_{\text{a priori}}(\bar{\phi}) . \quad (5)$$

The rationale behind this alternate definition is that likelihood has remained an isolated and ad hoc construct, while the concept of information is interwoven into a rich theory with many related insights and applications. This usage of the term information might be questioned by some purists, who would

insist that information is a statistical concept only, attributable to a communication channel but not to a specific message, and measurable only in terms of entropy. However, as long as there do in fact exist two separate words, "information" and "entropy", and as long as it is understood that entropy is the expectation value of information, which itself is a random variable, the technical vocabulary is enriched and no confusion can arise. Furthermore, this technical usage is in good accord with colloquial practice.

In unfolding NaI data with discrete and continuum spectral components, the problem naturally arises of determining the presence and energy of all resolvable gamma-ray lines. Two methods immediately suggest themselves: (1) perform a peak search on the NaI data using a peak search algorithm, or (2) unfold the data using one of the conventional unfolding algorithms, incorporating the spectrometer energy resolution into the response matrix and stressing the algorithm toward maximum resolution, then apply the peak search algorithm or read the spectral graph manually. These methods have serious limitations. Peak search algorithms are notoriously poor at resolving doublets and triplets aggregated within data by energy spacings small with respect to intrinsic resolution. This problem is aggravated by the presence of Compton edges and above 1 MeV by single and double escape peaks. Unfolding the data before searching removes the competing edges and escape peaks but in practice does little or nothing to improve resolution beyond the limit set by intrinsic detector characteristics. Attempts to exceed this limit generally result in the appearance of paradoxical oscillations, readily mistaken for actual peaks.

These oscillations are a consequence of the contrastingly different frequency contents of signal and noise ("frequency content" referring to the presence in data of wavelike components as revealed by Fourier analysis). Signal bandwidth is limited by spectrometer resolution, narrowing in frequency as

intrinsic resolution broadens in energy. In the vicinity of the limiting bandwidth, the signal power spectrum falls rapidly to small values. Noise represented by statistical counting fluctuations holds its power virtually unchanged to arbitrarily unchanged to arbitrarily high frequencies. Consequently, any attempt to improve the spectral resolution by linear techniques produces a corresponding upward weighting of all high frequency components, with increased dominance of noise over signal. This is a characteristic of linear system, not a fundamental information theoretic limitation. If, for example, all peaks sit on a continuum-free zero baseline, the resolution limit can readily be exceeded by the spectrum that minimizes an information function in the form of Eq. (5), with a positively constrained estimation space. This non-linear technique is effective for super-resolution because paradoxical oscillations about a zero baseline have a much stronger tendency to swing positive and negative than to remain strictly positive, resulting from involvement of lower frequencies in the latter case. Consequently, a weak regularization function, $W_{\text{a priori}}$ is able to suppress oscillations without degrading algorithmic resolution.

In the MAZNAI implementation, a non-zero baseline or continuum is incorporated by treating the spectral estimate in the j -th image energy channel as the superposition of a continuum and a discrete component,

$$Q_j = Q_j^C + Q_j^D \quad (6)$$

The solution is iterative, with a low-pass Legendre filter used to keep high-frequency oscillations from building up in the continuum estimate. Derivation of the $(m+1)$ -th estimate is illustrated in Figure 1. Initialization at a large continuum/discrete ratio, and convergence of the continuum only from the over-estimated side, ensures the continuing presence of a zero-baseline discrete structure.

Figure 1. Simplified MAZNAI Block Diagram.

Examples of MAZNAI spectral enhancement are shown in Fig 2 and 3. The existence of all enhanced lines in Fig. 2 and 3 have been verified by separate Ge(Li) measurements. The example in Fig. 3 is of particular interest since it represents the spectrum from a single isotope ($\text{Ag}^{110\text{m}}$) and it, therefore, provides us the opportunity of evaluating the effectiveness of MAZNAI in estimating gamma-ray intensities. The ratio of the MAZNAI estimated intensity, I_M , to intensity based the known branching ratio, I_B , is indicated in parenthesis above each enhanced peak. In this case, the errors in the I_M 's are all less than or equal to five percent. In general, if the code has converged (smoothing indicator <1) then those peaks with the greatest intensities tend to have accuracies consistent with statistics and resolution capabilities. Peaks with the smallest intensities tend to be systematically underestimated, and peaks below some recognition threshold are absent from the discrete component but may in groups influence the continuum.

Simulation studies have shown MAZNAI capable of resolving doublets, triplets, and quadruplets. The absence of subsidiary oscillations is characteristic of this technique.

Figure 2. Example of MAZNAI Unfolding (Uranium Ore with 3 x 3 inch NaI Detector).

Figure 3. MZNAI Unfolding with Source Spectrum (Sliver-110 with 3 x 3 inch NaI Detector Source from GeLi Data). Values above MAZE-enhanced Peaks are ratios of image to object line intensities with ratio at 1384 keV.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

3. DETECTOR RESPONSE FUNCTION

In the unfolding process, one requires precise knowledge of the response of the detector to monoenergetic gamma-rays with energies ranging from about 100 keV to nearly 3 MeV, namely, the detector response function. The determination and representation of the detector response function is a major prerequisite to the use of MAZNAI on experimental data.

The following description of the mathematical representation of the detector response function is based on the Berger and Seltzer paper (Appendix B.)

The response function $R(E_o, h)$ can be written as the convolution of an energy deposition spectrum $D(E_o, E)$ and a resolution function $G(E, h)$, multiplied by the detection efficiency $\eta(E_o)$:

$$R(E_o, h) = \eta(E_o) \int_0^{E_o} D(E_o, E) G(E, h) dE$$

The various quantities in equation 1 have the following meaning:

- $R(E_o, h)$ is the probability that a gamma ray incident with energy E_o will give rise to a pulse with a height between h and $h + dh$.
- $\eta(E_o)$ is the probability that the incident gamma ray will have at least one interaction in the detector.
- $D(E_o, E)dE$ is the probability that the gamma ray, if it interacts with the detector at all, will deposit an amount of energy between E and $E+dE$.
- $G(E, h)dh$ is the probability that the deposition of energy E will give rise to a pulse with a height between h and $h + dh$.

The assumed normalization of the response function is such that the integral of $R(E_0, h)$ over all h is equal to $n(E_0)$. Berger and Seltzer calculated the energy deposition spectrum $D(E_0, E)$ of a 3" dia by 3" NaI detector using the Monte Carlo based code ETRAN. The authors of this document have used the same code to calculate the energy disposition spectrum of a 5" dia by 6" long NaI detector.

For each sampled Monte Carlo cascade, consisting of the history of the incident gamma-ray and the histories of all secondary photons and charged particles, the energy E deposited in the detector is scored as the difference between the incident gamma-ray energy E_0 and the sum of the energies carried away by escaping electrons, positrons or photons. By sampling large numbers of such cascades (typically 10,000 to 50,000), estimates of the energy deposition spectrum are obtained. This spectrum has the form of a line spectrum plus a continuum $C(E_0, E)$:

$$D(E_0, E) = C(E_0, E) + P_0 \delta(E - E_0) + P_1 \delta(E - E_0 + mc^2) \\ + P_2 \delta(E - E_0 + 2mc^2) + P_3 \delta(E - \bar{E}_f)$$

where δ is the delta function and mc^2 the electron rest energy. P_0 is the probability that the entire gamma-ray energy E_0 is deposited in the detector. P_1 and P_2 are the probabilities that all of the energy is deposited with the exception of the amounts mc^2 or $2mc^2$ carried away by one or two unscattered annihilation quanta. P_3 is the probability that all energy is deposited except that carried away by unscattered K X-rays from iodine (with a weighted average energy $\bar{E}_f = 29$ keV).

The quantity P_0 can also be interpreted as the relative area under the total absorption peak of the response function. Similarly, P_1 and P_2 are the relative areas under the single and double annihilation radiation escape peaks, and P_3 is the relative area under the fluorescence radiation escape peak.

It is advantageous to express the continuous part of the energy deposition spectrum $C(E_0, E)$, in terms of dimensionless functions C_j , ($j = 1, 2, 3, 4$) which depend on dimensionless energy-related variables x , y and z . This representation of the data minimizes the explicit dependence on E_0 , and facilitates interpolation with respect to E_0 and E .

For $E_0 \leq 1.2$ MeV, we set

$$C(E_0, E) = C_1(E_0, x) (1 + mc^2 / 2E_0) / E_0$$

where

$$x = E(1 + mc^2 / 2E_0) / E_0$$

For $E_0 > 1.2$ MeV, we set

$$C(E_0, E) = C_2(E_0, y) / (E_0 - 2mc^2)$$

$$\text{for } 0 \leq E < E_0 - 2mc^2$$

$$C(E_0, E) = C_3(E_0, z) / 2mc^2$$

$$\text{for } E_0 - 2mc^2 \leq E < E_0 - mc^2$$

$$C(E_o, E) = C_4(E_o, z) / 2mc^2$$

$$\text{for } E_o - mc^2 \leq E \leq E_o$$

where

$$y = E / (E_o - 2mc^2)$$

and

$$z = (E - E_o + 2mc^2) / 2mc^2$$

Now, given the P_i 's and the C_j 's, the response of a given detector to any monoenergetic gamma-ray can be estimated by interpolating between the energy deposition spectra and folding the result with the measured detector resolution.

The usual means of representing the detector resolution as a function of energy is:

$$R(\%) = R_o (E_s / E)^n$$

when R_o is the percent resolution $[FWHM(keV) / E_s(keV) \times 100]$ at E_s , the standard energy of Cs^{137} (.6616 MeV). This simple relationship holds well for most NaI(Tl) detectors over the energy range of interest.

The ETRAN energy deposition calculations do not take into account small angle scattering from the detector housing. This phenomenon is found to be significant when comparing calculated detector responses to experimental

detector responses. The calculated values of the P_i 's and C_j 's must be adjusted to account for this effort. Hence, a combination of calculated energy deposition functions and experimental data is necessary to produce accurate detector response functions.

It is essential that accurate detector response function be available if optimum results are to be obtained from the MAZNAI code.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

4. MAZNAI USER'S GUIDE

This section presents the input format of the information necessary for MAZNAI. Appendix A contains a line image listing of a complete input file. The response function input variable names correspond to the tables listed in Ref. 5 which is included as Appendix B.

MAZNAI input items:

Card image 1: (experimental parameters) format (3I5, 4F10.0, 3I5)

NR: number of recorded channels (≤ 260)
NC: number of analyzed channels (≤ 260)
MAXIT: maximum number of iterations
DE: energy/channel (MeV)
EZERO: energy (MeV) of lower boundary of recorded channels
RES: resolution of NaI detector at .661 MeV (%)
TAU: smoothing parameter
IPRNT: print control flat
 = 0: no diagnostic printout
 = 1: diagnostic printout of information including
 the response function and intermediate
 iterations.

Card image 2: (response function parameters) format (7I10)

NELOW: number of energies below 1.2 MeV
NEHI: number of energies above 1.2 MeV
NXDAT: number of data points of continuum below 1.2 MeV
NYDAT: number of data points of continuum above 1.2 MeV
 and below second escape peak

NZDATL: number of data points between the first and second escape peaks

NZDATH: number of data points between the first escape peak and the full energy peak

IEDEP: = 0: energy deposition function input
= 1: scaled energy deposition function input

Card image 3: format (10F8.5)

POL_i, i = 1, NELOW: full energy peak probabilities below 1.2 MeV

Card image 4: format (10F8.5)

POH_i, i = 1, NEHI: full energy peak probabilities above 1.2 MeV

Card image 5: format (10F8.5)

P3_i, i = 1, NELOW: Iodine K x-ray escape probabilities

Card image 6: format (10F8.5)

Pl_i, i = 1, NEHI: first escape peak probabilities

Card image 7: format (10F8.5)

P2_i, i = 1: second escape peak probabilities

Card image 8: format (10F8.5)

EDATL_i, i = 1, NELOW: energies of data below 1.2 MeV

Card image 9: format (10F8.5)

EDATH_i, i = 1, NEHI: energies of data above 1.2 MeV

Card image 10: format (10F8.5)

XR_i, i = 1, NYDAT: energy-related variable $x^{(5)}$

Card image 11: format (10F8.5)

YR_i, i = 1, NYDAT: energy-related variable $y^{(5)}$

Card image 12: format (10F8.5)

ZR_i , $i = 1$, NZDATL + NZDATH: energy-related variable z ⁽⁵⁾

Card image 13: format (10F8.5)

$RPL_{i,j}$, $i = 1$, NELOW; $j = 1$, $2 * NXDAT - 2$: continuum response function corresponding to energies below 2.1 MeV. The number of actual card images read in depends on previously defined parameters.⁽⁵⁾

Card image 14: format (10F8.5)

$RPH_{i,j}$, $i = 1$, NEHI; $j = 1$, $2 * (NYDAT + NZDATL + NZDATH) - 6$: continuum response function corresponding to energies above 1.2 MeV. The number of actual card images, again, depends on previously defined parameters.

Card image 15: format (80A1)

This card contains an 80-character title which will be printed on the output file.

Card image 16: format (10F8.0)

C_i , $i = 1$, NR: experimental data representing the number of counts per channel

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

5. REFERENCES

1. Sperling, S. M., "Spectral Unfolding: Its Mathematical Basis, Implementation and Application with MAZE 2", Final Report, DNA 2990F, October 1972.
2. Orear, J. 1958. Notes on Statistics for Physicists. University of California Radiation Laboratory Report UCRL-8417.
3. Tikhonov, A. N., 1963. "The Solution of Incorrectly Posed Problem and the Method of Regularization.", Doklady Akad, Nauk SSSR. IJI, No. 3: 501-504.
4. Phillips, D. L. 1962. J. Assoc. Comp. Mach. 9: 87.
5. M. J. Berger and S. M. Seltzer, "Response Functions for Sodium Iodide Scintillation Detectors" NI & M 104, pp 317-332, October 1972.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

APPENDIX A

MAZNAI

1. CODE LISTING

The following is a listing of the MAZNAI code. Below is a list of the names of the routines that make up the MAZNAI code in the order of their appearance.

1. Main routine
2. MAZNAI
3. ASET
4. RESOL
5. INTEN
6. VBOUND
7. VLOG
8. VEXP
9. VPICT
10. VPICT1
11. VPICTL
12. INTRP
13. NORM
14. ALFBET
15. PGEN
16. PGENT
17. RUNSUM
18. INTGRL
19. ERROR
20. FIT
21. SLOPE
22. CURVE
23. ENDP
24. XPRINT

Also included is a completed listing of a 160 channel sample problem input sequence.


```

      PROGRAM INPUT
C     PROGRAM INPUT(TAPE8,INPUT,OUTPUT,PUNCH,TAPES=INPUT,TAPE6=OUTPUT,
C     1 TAPE7=PUNCH)
      DIMENSION Q(300,2),SIGMA(300),QD(300),QC(300)
      DIMENSION RPL(15,55),RPH(13,60)
      DIMENSION POL(20),POH(20),P1(20),P2(20),P3(20)
      DIMENSION ERR(300)
      COMMON/      /ALFA(300,30),BETA(300,30),H1(300,30),H2(300,30)
      1 ,SAB(300),SBQ(300)
      COMMON/DATA/DE,EZERDP,ERM,RES,NC,NR,IPRNT,IPUN,NRUNS
      1,APARM,BPARM,CPARM
      COMMON/XYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
      COMMON/NS/NELOW,NEHI,NXDAT,NYDAT,NZDATH,NZDATH
      COMMON/JUNK/J1(300),J2(300),JA
      COMMON /LRG/ A(10000)
      ERM=0.511
      READ(5,1001) NR,NC,MAXIT,DE,EZERO,RES,TAU,IPRNT,IPUN,NRUNS
1001  FORMAT(3I5,4F10.5,3I5)
      EZERP=EZERO-(.5*FLOAT(NC-NR))*DE
      WRITE(6,1002) NR,NC,EZERO,DE,RES,MAXIT,TAU,IPRNT
1002  FORMAT(1H1,8X,3HNR=,I4,7X,3HNC=,I4,5X,6HEZERO=,F9.5,7X,3HDE=,
      1F9.5,7X,4HRES=,F6.2,1H(,5X,6HMAXIT=,I4,7X,4HTAU=,F9.5,5X,
      26HIPRNT=,I2)
      CALL RESOL(SIGMA)
      CALL ASET(SIGMA)
      READ(5,5001) NELOW,NEHI,NXDAT,NYDAT,NZDATH,NZDATH,IEDEP
5001  FORMAT(7I10)
      READ(5,5000)(POL(I),I=1,NELOW)
      READ(5,5000)(POH(I),I=1,NEHI)
      READ(5,5000)(P3(I),I=1,NELOW)
      READ(5,5000)(P1(I),I=1,NEHI)
      READ(5,5000)(P2(I),I=1,NEHI)
      READ(5,5000)(EDATL(I),I=1,NELOW)
      READ(5,5000)(EDATH(I),I=1,NEHI)
5000  FORMAT(10F8.5)
      READ(5,5000)(XR(I),I=1,NXDAT)
      READ(5,5000)(YR(I),I=1,NYDAT)
      NZ=NZDATH+NZDATH
      READ(5,5000)(ZR(I),I=1,NZ)
      NHI=2*(NYDAT+NZDATH+NZDATH)-6
      NX=2*NXDAT-2
      DO 10 I=1,NX
      10 READ(5,5000)(RPL(J,I),J=1,NELOW)
      DO 11 I=1,NHI
      11 READ(5,5000)(RPH(J,I),J=1,NEHI)
1004  FORMAT(10F8.5)
1006  FORMAT(5X,8HRPL(J,I),3X,10F8.5)
1007  FORMAT(5X,8HRPH(J,I),3X,10F8.5)
      CALL INTEN(POL,POH,P1,P2,P3)
      IF(IEDEP.EQ.1) GO TO 150
C     IEDEP=1 IMPLIES ENERGY DEPOSITION READ
C     IDEP=0 IMPLIES CS ACCORDING TO BURGER AND SELTZER
      DO 110 J=1,NELOW
      E=EDATL(J)
      CE=(1.+ERM/(2.*E))/E
      DO 100 I=1,NX
      RPL(J,I)=RPL(J,I)*CE
100  CONTINUE
110  CONTINUE
      NY=2*NYDAT-2

```

```

DO 140 J=1,NHI
E=EDATH(J)
CY=1./(E-2.*ERM)
DO 120 I=1,NY
RPH(J,I)=RPH(J,I)*CY
120 CONTINUE
NZ1=NY+1
DO 130 I=NZ1,NHI
RPH(J,I)=.5*RPH(J,I)/ERM
130 CONTINUE
140 CONTINUE
150 CONTINUE
CALL INTRP(RPL,RPH)
CALL ALFBET
DO 7631 I=1,14
JJ=10*I
DO 7384 K=1,NC
QD(K)=0.
QC(K)=0.
7384 CONTINUE
QD(JJ)=1.
CALL PGEN(QC,QD)
CALL XPRINT(NR,QC,SHRESFN )
7631 CONTINUE
CALL MAZNAI(Q,TAU,MAXIT)
DO 5 I=1,NC
QD(I)=Q(I,2)
QC(I)=Q(I,1)-Q(I,2)+1.
5 CONTINUE
IF(IPUN.EQ.1) WRITE(7,201) (QD(I),I=1,NC)
IF(IPUN.EQ.1) WRITE(7,201) (QC(I),I=1,NC)
201 FORMAT(8E10.4)
CALL VPICTL(QD,NC,SH DISC,SHRETE )
CALL VPICTL(QC,NC,SHCONTI,SHNUUM )
CALL ERROR(Q(1,1),QD,QC,SIGMA,ERR)
CALL XPRINT(NC,ERR,SHERR )
STOP
END
SUBROUTINE MAZNAI(Q,TAU,MAX)

```

C MAZE3 IS A HIGH-RESOLUTION REFOCUSING CODE FOR SPECTRAL DATA REDUC
C ITS PRINCIPLE OF OPERATION IS THAT OF MINIMIZING AN INFORMATION FU
C CONSISTING OF THE SUM OF A DATA-INFORMATION PART, A CONTINUUM-INFU
C PART, AND A DISCRETE-INFORMATION PART, BY MOVING THE SPECTRAL ESTI
C ACCORDING TO FIRST AND SECOND DERIVATIVES OF THE INFORMATION PARTS
C THE CALLING PROGRAM MUST DIMENSION (C, A, AND Q) ACCORDING TO THE
C DIMENSIONS OF THE PROBLEM AND THE PARAMETER DEFINITIONS.
C C IS THE COUNT VECTOR. 'A' CONSISTS OF ALL RESPONSE MATRIX ELEMEN
C GREATER THAN 1.E-6, STORED IN THE SEQUENCE ROW1,ROW2,ROW3,..... U
C COMPLETION OF EXECUTION, Q IS THE SUPER-RESOLVED SPECTRUM, STORED
C THE FIRST NC ELEMENTS REPRESENT THE CONTINUUM PLUS DISCRETE SPECTR
C AND THE SECOND NC ELEMENTS REPRESENT THE DISCRETE SPECTRUM. THE
C CONTINUUM SPECTRUM MAY BE OBTAINED BY SUBTRACTING Q(J,2) FROM Q(J,
C FOR J=1,NC. TAU IS THE SMOOTHING PARAMETER, NOMINALLY = 1, INCREA
C MORE REGULARIZATION, DECREASE FOR LESS.

```

DIMENSION EPEAK(100),ENLOW(100),PKH(100),ENHI(100),ICHPK(100)
DIMENSION Q(300,2),DWDQ(300,4),DEL(300,8),DELSUM(300,4),

```

```

1 EFF(300),P(300),QT(300),C(900),TITL(80)
COMMON/DATA/DE,EZEROP,ERM,RES,NC,NR,IPRNT,IPUN,NRUNS
COMMON/JUNK/J1(300),J2(300),JA
COMMON /LRG/ A(10000)
EQUIVALENCE(DE(1,5),DELSUM(1,1))
DOT=1.
ITCHK=1
5000 CONTINUE
READ(5,2002) TITL
2002 FORMAT(80A1)
WRITE(6,2002) TITL
READ(5,2001) (C(I),I=1,NR)
2001 FORMAT(10F8.0)
DOT=1.
NC1=NC-1
NC2=NC-2
NMAX=2+NC**2/JA
BETA=0.
DO 1 J=1,NC
1 EFF(J)=0.
CSUM=0.
K=0
DO 2 I=1,NR
IF(C(I).LE.0.) C(I)=C(I)+.1
CSUM=CSUM+C(I)
QT(I)=1.
2 CONTINUE
CALL PGENT(QT,EFF)
DO 201 J=1,NC
IF(EFF(J).LE.0.) EFF(J)=1.E-5
201 CONTINUE
IF(IPRNT.EQ.1) CALL XPRINT(NC,EFF,5H EFF )
EPASS=0.
DO 3 J=1,NC
3 EPASS=EPASS+EFF(J)
Q(1,2)=SQRT(CSUM/EPASS)
Q(1,1)=CSUM/EPASS-Q(1,2)
C DELSUM(1,3)=Q(1,1)
C DELSUM(1,4)=Q(1,2)
DELSUM(1,3)=ALOG(Q(1,1))
DELSUM(1,4)=ALOG(Q(1,2))
DO 4 J=1,NC
DELSUM(J,1)=0.
DELSUM(J,2)=0.
DELSUM(J,3)=DELSUM(1,3)
DELSUM(J,4)=DELSUM(1,4)
Q(J,1)=Q(1,1)
4 Q(J,2)=Q(1,2)
9000 FORMAT(1H1)
WRITE(6,9000)
DO 5 M=1,MAX
IF(IPRNT.EQ.1) WRITE(6,1002)M
1002 FORMAT(8H **** M=,I3)
L=0
SOLD=SDATA
103 SDATA=0.
L=L+1
K=0
DO 11 J=1,NC
11 QT(J)=Q(J,1)+Q(J,2)

```

```

CALL PGEN(P,QT)
DO 10 I=1,NR
SDATA=SDATA-C(I)*ALOG(P(I)/C(I))+P(I)-C(I)
10 CONTINUE
IF(M.EQ.1) GO TO 106
IF(SDATA.LT.SOLD.OR.L.EQ.2) GO TO 105
C GO TO 105
DOT=DOT*DOT1
DOT1=0.
DO 104 J=1,NC
Q(J,2)=Q(J,2)*EXP(-DELSUM(J,2))
DELSUM(J,2)=0.
104 DOT1=DOT1+EFF(J)*Q(J,2)
DOT1=(CSUM-DOT1)/DOT
IF(DOT1.LE.0.) DOT1=1.
DO 114 J=1,NC
114 Q(J,1)=DOT1*Q(J,1)
GO TO 103
DO 107 J=1,NC
107 DELSUM(J,2)=DEL(J,3)+DELSUM(J,2)
C 107 DELSUM(J,2)=Q(J,2)
KOLD=(M-1)/20
KIN=M/20
IF(KIN.EQ.KOLD) GO TO 725
CALL XPRINT(NC,QT,5HSPECT)
IF(IPUN.EQ.1) WRITE(7,301)(P(I),I=1,NR)
IF(IPUN.EQ.1) WRITE(7,301)(QT(J),J=1,NC)
IF(IPUN.EQ.1) WRITE(7,301)(Q(J,2),J=1,NC)
CCCCC ANALYZE Q(J,I)
KK=0
SUMQ=0.
DO 720 J=2,NC1
IF(Q(J,2).LT.1.) GO TO 720
IF(Q(J-1,2).LT.1.) GO TO 710
IF(Q(J+1,2).LT.1.) GO TO 705
IF(Q(J,2).LE.Q(J-1,2).AND.Q(J,2).LE.Q(J+1,2)) GO TO 702
IF(KK.EQ.0) KK=1
SUMQ=SUMQ+Q(J,2)
IF(Q(J,2).GE.Q(J-1,2).AND.Q(J,2).GE.Q(J+1,2)) GO TO 701
GO TO 720
C701 FIND CENTER OF PEAK
701 AL=ALOG(Q(J-1,2)/Q(J,2))
AL=AL/ALOG(Q(J,2)/Q(J+1,2))
X1=J-1
X2=J
X3=J+1
X0=AL*(X3*X3-X2*X2)+X1*X1-X2*X2
X0=X0/(2.*(AL-1.))
EPEAK(KK)=(X0+.5)*DE+EZEROP
ICHPK(KK)=J
GO TO 720
710 KK=KK+1
ENLOW(KK)=J*DE+EZEROP
SUMQ=SUMQ+Q(J,2)
IF(Q(J+1,2).GE.1.) GO TO 720
ENHI(KK)=(J+1.)*DE+EZEROP
PKH(KK)=SUMQ
SUMQ=0.
EPEAK(KK)=(J+.5)*DE+EZEROP
GO TO 720

```

```

702 PKH(KK)=SUMQ+Q(J,2)/2.
    SUMQ=Q(J,2)/2.
    ENHI(KK)=(J+.5)*DE+EZEROP
    KK=KK+1
    ENLOW(KK)=ENHI(KK-1)
    GO TO 720
705 PKH(KK)=SUMQ+Q(J,2)
    ENHI(KK)=(J+1.)*DE+EZEROP
    SUMQ=0.
720 CONTINUE
    WRITE(6,731)M
731 FORMAT(24H ANALYSIS OF PEAKS AFTER ,I4,12H ITERATIONS /
1 1H ,37HELOW EHI EPEAK COUNTS )
C DO 730 LK=1,KK
    LK=1
    WRITE(6,740)ENLOW(LK),ENHI(LK),EPEAK(LK),PKH(LK)
740 FORMAT(1H ,3F10.3,F10.2)
725 CONTINUE
106 DO 6 J=1,NC
C DELSUM(J,3)=Q(J,1)
C DFLSUM(J,4)=Q(J,2)
    DELSUM(J,3)=DELSUM(J,3)+DELSUM(J,1)
    DELSUM(J,4)=DELSUM(J,4)+DELSUM(J,2)
    DWDQ(J,1)=DELSUM(J,3)
    DWDQ(J,3)=DELSUM(J,4)
6 CONTINUE
    DO 7 K=2,4,2
C IF(K.EQ.2) BETA=0.
    IF(K.EQ.2) BETA=2.
    IF(K.EQ.4) BETA=0.
    GAMMA=.5*BETA**2
    L=K-1
    DWDQ(1,K)=2.*(DWDQ(1,L)-DWDQ(2,L))-(DWDQ(2,L)-DWDQ(3,L))
    DWDQ(2,K)=-3.*(DWDQ(1,L)-DWDQ(2,L))+3.*(DWDQ(2,L)-DWDQ(3,L))
    *- (DWDQ(3,L)-DWDQ(4,L))
    DO 8 J=3,NC2
8 DWDQ(J,K)=(DWDQ(J-2,L)-DWDQ(J-1,L))-3.*(DWDQ(J-1,L)-DWDQ(J,L))
    *+3.*(DWDQ(J,L)-DWDQ(J+1,L))-(DWDQ(J+1,L)-DWDQ(J+2,L))
    DWDQ(NC1,K)=(DWDQ(NC1-2,L)-DWDQ(NC2,L))-3.*(DWDQ(NC2,L)
    *-DWDQ(NC1,L))+3.*(DWDQ(NC1,L)-DWDQ(NC,L))
    DWDQ(NC,K)=(DWDQ(NC2,L)-DWDQ(NC1,L))-2.*(DWDQ(NC1,L)-DWDQ(NC,L))
    DWDQ(1,K)=GAMMA*DWDQ(1,K)+BETA*(DWDQ(1,L)-DWDQ(2,L))
    DO 108 J=2,NC1
    R=-(DWDQ(J-1,L)-DWDQ(J,L))+(DWDQ(J,L)-DWDQ(J+1,L))
108 DWDQ(J,K)=GAMMA*DWDQ(J,K)+BETA*R
7 DWDQ(NC,K)=GAMMA*DWDQ(NC,K)-BETA*(DWDQ(NC1,L)-DWDQ(NC,L))
    DO 9 J=1,NC
    DEL(J,2)=-DWDQ(J,2)-DWDQ(J,1)
9 DEL(J,4)=-DWDQ(J,4)-DWDQ(J,3)
    DOT=0.
    DOT1=0.
    DO 109 J=1,NC
    DOT=DOT+DEL(J,2)**2
109 DOT1=DOT1+DEL(J,4)**2
    DOT=SQRT(DOT)
    IF(DOT1.LE.0.) DOT1=1.
    DOT1=TAU/SQRT(DOT1)
9002 FORMAT(3X,15H AFTER STEP M =,I4,20H, DATA INFORMATION =,G10.3,19H
    * COS(DATA,DISCR) =,E10.3,8H GRAD =,E10.3,16H COS(NEW,OLD) =,F10.
    *3)

```

```

      K=M-1
      WRITE(6,9002) K,SDATA,R34,R3,R36
      SI=2.*SDATA/FLOAT(NR)
      IF(SI.LT.1.0) GO TO 40
      IF(M.EQ.MAX) GO TO 5
      DO 12 J=1,NC
12    DWDQ(J,3)=0.
      K=0
      DO 13 I=1,NR
13    QT(I)=(C(I)-P(I))/P(I)
      CALL PGENT(QT,DWDQ(1,3))
      R=0.
      R34=0.
      R3=0.
      R36=0.
      R6=0.
      DO 14 J=1,NC
        DWDQ(J,1)=DWDQ(J,3)
        DEL(J,1)=DWDQ(J,1)/EFF(J)
        DEL(J,3)=DWDQ(J,3)/EFF(J)
        DEL(J,4)=DOT1*DEL(J,4)
        R=R+DEL(J,3)**2
        R34=R34+DEL(J,3)*DEL(J,4)
        R6=R6+DEL(J,6)**2
        DEL(J,3)=DEL(J,3)+DEL(J,4)
        R3=R3+DEL(J,3)**2
        R36=R36+DEL(J,3)*DEL(J,6)
14    CONTINUE
      R=SQRT(R)
      DOT=R/DOT
      DO 19 J=1,NC
        DEL(J,2)=DOT*DEL(J,2)
19    DEL(J,1)=DEL(J,1)+DEL(J,2)
      R6=SQRT(R6)
      R3=SQRT(R3)
      R34=R34/(R*TAU)
      R3R6=R3*R6
      IF(R3R6.LE.0.) R3R6=1.
      R36=R36/R3R6
9003  FORMAT(/3X,50HLEGENDE EXPANSION CANNOT BE EXECUTED BECAUSE NMAX
      * 13H EXCEEDS NC/2)
      IF(2*NMAX.LE.NC) GO TO 120
      WRITE(6,9003)
      RETURN
120  R=20./NMAX**2
      DO 119 N=1,NMAX
        AN=N-1
        DWDQ(N,2)=0.
        DWDQ(NC+1-N,2)=2.*(AN+.5)*.7** (AN*AN*R)/FLOAT(NC1)
        IF(AN.LE.0.) AN=1.0
119  DWDQ(NC+1-N,4)=(AN-1.)/AN
        DOT=2./FLOAT(NC1)
        DOT1=1.+DOT
        DO 15 K=1,2
          DO 15 J=1,NC
            IF(K.EQ.1) GO TO 121
            DEL(J,1)=0.
121  X=DOT*FLOAT(J)-DOT1
          DO 15 N=1,NMAX
            L=NC+1-N

```

```

      IF(N.GT.2) GO TO 116
      IF(N.EQ.2) GO TO 115
      PN=1.
      GO TO 16
115  PN=X
      GO TO 16
116  R=X*PN1
      PN=DWDQ(L,4)*(R-PN2)+R
16   PN2=PN1
      PN1=PN
      GO TO (117,118),K
117  R=DWDQ(L,2)*PN
      DWDQ(N,2)=DWDQ(N,2)+R*DEL(J,1)
      GO TO 15
118  DEL(J,1)=DEL(J,1)+DWDQ(N,2)*PN
15  CONTINUE
      R=R36*R36
      DO 34 J=1,NC
      DELSUM(J,1)=DEL(J,1)
      DELSUM(J,2)=DELSUM(J,2)+R
34  CONTINUE
      DOT=0.0
      DOT1=0.0
      DO 35 J=1,NC
      Q(J,1)=Q(J,1)*EXP(DELSUM(J,1))
      Q(J,2)=Q(J,2)*EXP(DEL(J,3)+DELSUM(J,2))
      DOT=DOT+EFF(J)*Q(J,1)
      DOT1=DOT1+EFF(J)*Q(J,2)
35  CONTINUE
      IF(DOT.LE.0.) DOT=1.0
      DOT1=(CSUM-DOT1)/DOT
      IF(DOT1.LE.0.) DOT1=1.
      DO 135 J=1,NC
135  Q(J,1)=DOT1*Q(J,1)
5   CONTINUE
9001 FORMAT(/4X,21HSMOOTHING INDICATOR =,G10.3,23H, SMOOTHING PARAMETER
      * =,G10.3)
40  WRITE(6,9001) SI,TAU
      IF(IPUN.EQ.1) WRITE(7,301) (P(I),I=1,NR)
      CALL VPICTL(P,NR,SHREFOL,SHD SPC )
      DO 36 I=1,NR
36  P(I)=SQRT(C(I))-SQRT(P(I))
      CALL VPICTL(C,NR,SH DA,SHTA )
      WRITE(6,9004)
      WRITE(6,9005) CSUM
9004 FORMAT (1H0)
9005 FORMAT (7X,38HTHE SUM OF THE INPUT DATA IS EQUAL TO ,G10.3)
      CALL VPICTL(P,NR,SHDEVIA,SHATIONS )
      QSUM=0.
      DO 37 J=1,NC
      Q(J,1)=Q(J,1)+Q(J,2)
      Q(J,2)=Q(J,2)+1.
      IF (J.GT.(NC-6)) GO TO 37
      IF (J.GT.6) QSUM=QSUM+Q(J,1)
37  CONTINUE
      CALL VPICTL(Q,NC,SH SPEC,SHTRUM )
      WRITE(6,9006) QSUM
      IF(IPUN.EQ.1) WRITE(7,301) (C(I),I=1,NR)
      IF(IPUN.EQ.1) WRITE(7,301) (P(I),I=1,NR)
C   IF(IPUN.EQ.1) WRITE(7,301) (Q(I),I=1,NC)

```

```

301 FORMAT(8E10,4)
9006 FORMAT(/5X,40HNO. OF COUNTS IN CHANNELS 7 THRU (NC-6)=,G10.3)
      ITCHCK=ITCHCK+1
      IF(ITCHCK,LE,NRUNS) GO TO 5000
      RETURN
      END
      SUBROUTINE ASET(SIGMA)
      DIMENSION SIGMA(1)
      COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
      COMMON/JUNK/J1(300),J2(300),JJ
      COMMON /LRG/ A(10000)
      GAUSS(SIG,S,T)=(EXP(-.5*((T-S)/SIG)**2))/(2.5066283*SIG)
      ZERO=.5*(NC-NR)
      JMIN=1
      JJ=0
      DO 2 I=1,NR
      SUM=0.
      T=I
      J1(I)=JMIN
      DO 3 J=JMIN,NC
      S=J-ZERO
      IF((T-S)/SIGMA(J),LT,10.) GO TO 50
      G=0.
      GO TO 51
50 G=GAUSS(SIGMA(J),S,T)
51 CONTINUE
      IF(S.LE.T.AND,G.LT,1.E-6) GO TO 4
      IF(S.GT.T.AND,G.LT,1.E-6) GO TO 5
      JJ=JJ+1
      A(JJ)=G
      SUM=SUM+G
      GO TO 3
4 J1(I)=J1(I)+1
3 J2(I)=J
5 CONTINUE
      MIN=JJ-J2(I)+J1(I)
      DO 100 KK=MIN,JJ
100 A(KK)=A(KK)/SUM
      2 JMIN=J1(I)
      WRITE(6,9002)JJ
9002 FORMAT(5X,33HTHE RESPONSE FUNCTION,A,REQUIRES ,15,18H STORAGE LOCA
      *TIONS)
      RETURN
      END
      SUBROUTINE RESOL(SIGMA)
      DIMENSION SIGMA(1)
      COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
      ERESOL=.66164
      RESPR=.3416
      DO 1 J=1,NC
      XJ=J
      E=DE*(XJ-.5)+EZEROP
      IF(E.LT.,1) E=.1
      IF(E.LE,0.46) GO TO 10
      RES=8.279
      RESPR=0.367
      GO TO 11
10 RES=8.479
      RESPR=.299
11 CONTINUE

```



```

R=RES*(ERESOL/E)**RESPR
N=R*E*.01
SIGMA(J)=.42466091*W/DE
1 CONTINUE
RETURN
END
SUBROUTINE INTEN(POL,POH,P1,P2,P3)
COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
DIMENSION E(300),POL(20),POH(20),P1(20),P2(20),P3(20)
DIMENSION XX(300),DD(300),SL(300)
COMMON/XYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
COMMON/NS/NELOW,NEHI,NXDAT,NYDAT,NZDATL,NZDATH
COMMON/PEAK/PK(300,5)
EN(T)=(T-.5)*DE+EZEROP
ECOM(E)=(2.*E*E)/(ERM+2.*E)
K=0
DO 10 J=1,NC
E(J)=0.
DO 10 I=1,5
10 PK(J,I)=0.
DO 50 J=1,NC
XJ=J
E(J)=EN(XJ)
IF(E(J).GT.1.2) GO TO 60
K=K+1
50 CONTINUE
60 N=K
IF(N.EQ.0) GO TO 70
M=NELOW+4
IF(IPRNT.EQ.1) CALL XPRINT(NELOW,EDATL,SHEDATL )
IF(IPRNT.EQ.1) CALL XPRINT(NELOW,POL,SHPOL )
IF(IPRNT.EQ.1) CALL XPRINT(NELOW,P3,SHP3 )
IF(IPRNT.EQ.1) CALL XPRINT(NEHI,EDATH,SHEDATH )
IF(IPRNT.EQ.1) CALL XPRINT(NEHI,POH,SHPHI )
IF(IPRNT.EQ.1) CALL XPRINT(NEHI,P1,SHP1 )
IF(IPRNT.EQ.1) CALL XPRINT(NEHI,P2,SHP2 )
CALL FIT(NELOW,M,EDATL,POL,N,E,PK(1,1),XX,DD,SL)
IF(IPRNT.EQ.1) CALL XPRINT(N,PK(1,1),SHPOL )
CALL FIT(NELOW,M,EDATL,P3,N,E,PK(1,4),XX,DD,SL)
IF(IPRNT.EQ.1) CALL XPRINT(N,PK(1,4),SHP3 )
DO 65 I=1,N
IF((PK(I,1)+PK(I,4)).GE.1.) PK(I,4)=1.-PK(I,1)
65 CONTINUE
IF(K.EQ.NC) GO TO 85
70 KK=0
K=K+1
DO 80 J=K,NC
XJ=J
E(J)=EN(XJ)
KK=KK+1
IF(E(J).GT.EDATH(NEHI)) GO TO 100
80 CONTINUE
M=NEHI+4
CALL FIT(NEHI,M,EDATH,POH,KK,E(K),PK(K,1),XX,DD,SL)
IF(IPRNT.EQ.1) CALL XPRINT(KK,PK(K,1),SHPOL )
CALL FIT(NEHI,M,EDATH,P1,KK,E(K),PK(K,2),XX,DD,SL)
IF(IPRNT.EQ.1) CALL XPRINT(KK,PK(K,2),SHP1 )
CALL FIT(NEHI,M,EDATH,P2,KK,E(K),PK(K,3),XX,DD,SL)
IF(IPRNT.EQ.1) CALL XPRINT(KK,PK(K,3),SHP2 )
85 DO 90 J=1,NC

```

```

        PK(J,5)=1.-PK(J,1)-PK(J,2)-PK(J,3)-PK(J,4)
        IF(PK(J,5).LT.0. ) GO TO 200
90      CONTINUE
        IF(IPRNT.EQ.1) CALL XPRINT(NC,PK(1,5),SHCONTN )
        RETURN
100     CONTINUE
        WRITE(6,6001)
6001    FORMAT(1H ,25HENERGY EXCEEDS MAX ENERGY )
        STOP
200     WRITE(6,6000)
6000    FORMAT(1H ,15HPEAKS GT 1 )
        STOP
        END
        SUBROUTINE VBOUND(V,N,V1,V2)
C-----
C          V1=MINIMUM(V)
C          V2=MAXIMUM(V)
C-----
        DIMENSION V(N)
        V1=V(1)
        V2=V(1)
        DO 1 I=1,N
        V1=AMIN1(V1,V(I))
1       V2=AMAX1(V2,V(I))
        RETURN
        END
        SUBROUTINE VLOG(V,W,N)
C-----
C          UPON RETURN W CONTAINS LOG(V).
C-----
        DIMENSION V(N),W(N)
        DO 1 I=1,N
        IF(V(I).LT.1.E-30) GO TO 2
        W(I)=ALOG(V(I))
        GO TO 1
2       W(I)=ALOG(1.E-30)
1       CONTINUE
        RETURN
        END
        SUBROUTINE VEXP(V,W,N)
C-----
C          UPON RETURN W CONTAINS EXP(V)
C-----
        DIMENSION V(N),W(N)
        DO 1 I=1,N
1       W(I)=EXP(V(I))
        RETURN
        END
        SUBROUTINE VPIC(V,N,WORD1,WORD2)
C-----
C          V IS PLOTTED ON THE LINE PRINTER AND DUMPED.
C          WORD1 AND WORD2 FORM A 10-LETTER LABEL.
C          THE FORM IS 'C1C2C3C4C5'.
C-----
        DIMENSION V(N)
9000    FORMAT(1X,8HMINIMUM=,G10.3,94X,8HMAXIMUM=,G10.3)
9001    FORMAT(1X,11HVECTOR DUMP,I4,10G11.4)
9002    FORMAT(/)
9003    FORMAT(1H1////)
9004    FORMAT(1H1)

```

```

CALL VBOUND(V,N,V1,V2)
WRITE(6,9004)
CALL VPICT1(V,V1,V2,N,WORD1,WORD2)
WRITE(6,9000) V1,V2
LAST=MOD(N+14,66)
LEFT=66-LAST
LEFT1=LEFT
IF(LEFT.GT.61) LEFT1=61
NEED=(N/10)+1
IF(NEED.GT.LEFT1) GO TO 2
NSKIP=LEFT-LEFT1
IF(NSKIP.EQ.0) GO TO 5
DO 1 I=1,NSKIP
1 WRITE(6,9002)
5 CONTINUE
GO TO 3
2 WRITE(6,9003)
3 CONTINUE
WRITE(6,9002)
WRITE(6,9002)
DO 4 I1=1,N,10
I2=I1+9
IF(I2.GT.N) I2=N
WRITE(6,9001) I1,(V(I),I=I1,I2)
4 CONTINUE
RETURN
END
SUBROUTINE VPICT1(V,A1,A2,N,WORD1,WORD2)
DIMENSION V(N)
DIMENSION VLINE(130)
9000 FORMAT(1H1,130A1)
9001 FORMAT(1X,130(1HX))
9002 FORMAT(1X,130A1)
9003 FORMAT(1X,30(1HX),2A5,88(1HX))
DATA BLANK,TRI,QUAD,PLUS,AMINUS,ZERO/1H,1H>,1HX,1H+,1H-,1HO/
DY=(A2-A1)/125.
IF (DY.LE.1.E-6) DY=1.E-6
DY2=DY/2.
YMIN=A1-DY2
YMAX=A2+DY2
JZERO=(-YMIN/DY)+3.
DO 1 J=1,130
IF(J.LT.JZERO) VLINE(J)=AMINUS
IF(J.EQ.JZERO) VLINE(J)=ZERO
IF(J.GT.JZERO) VLINE(J)=PLUS
1 CONTINUE
WRITE(6,9002) VLINE
WRITE(6,9001)
WRITE(6,9001)
DO 10 I=1,N
YJ=V(I)-YMIN
JY=(YJ/DY)+3.
DO 2 J=1,2
2 VLINE(J)=QUAD
DO 3 J=3,128
IF(J.LT.JY) VLINE(J)=TRI
IF(J.GE.JY) VLINE(J)=BLANK
3 CONTINUE
DO 4 J=129,130
4 VLINE(J)=QUAD

```

```

WRITE(6,9002) VLINE
10 CONTINUE
WRITE(6,9001)
WRITE(6,9003) WORD1,WORD2
DO 11 J=1,130
IF(J.LT.JZERO) VLINE(J)=AMINUS
IF(J.EQ.JZERO) VLINE(J)=ZERO
IF(J.GT.JZERO) VLINE(J)=PLUS
11 CONTINUE
WRITE(6,9002) VLINE
RETURN
END
SUBROUTINE VPICTL(V,N,WORD1,WORD2)

```

```

C-----
C      V IS PLOTTED ON THE LINE PRINTER AND DUMPED.
C      WORD1 AND WORD2 FORM A 12-LETTER LABEL.
C      THE FORM IS 'C1C2C3C4C5C6'.
C-----

```

```

      DIMENSION V(N)
9000 FORMAT(1X,8HMINIMUM=,G10.3,69X,8HSEMI-LOG,17X,8HMAXIMUM=,G10.3)
9001 FORMAT(1X,11HVECTOR DUMP,I4,10G11.4)
9002 FORMAT(/)
9003 FORMAT(1H1////)
9004 FORMAT(1H1)
      CALL VLOG(V,V,N)
      CALL VBOUND(V,N,V1,V2)
      WRITE(6,9004)
      V1=0.
      DO 10 I=1,10
      XJ=10.**I
      XJ=ALOG(10.*XJ)
      IF(V2.LT.XJ) GO TO 12
10 CONTINUE
12 V2=XJ
      CALL VPICT1(V,V1,V2,N,WORD1,WORD2)
      V1=EXP(V1)
      V2=EXP(V2)
      WRITE(6,9000) V1,V2
      CALL VEXP(V,V,N)
      LAST=MOD(N+14,66)
      LEFT=66-LAST
      LEFT1=LEFT
      IF(LEFT.GT.61) LEFT1=61
      NEED=(N/10)+1
      IF(NEED.GT.LEFT1) GO TO 2
      NSKIP=LEFT-LEFT1
      IF(NSKIP.EQ.0) GO TO 5
      DO 1 I=1,NSKIP
1 WRITE(6,9002)
5 CONTINUE
      GO TO 3
2 WRITE(6,9003)
3 CONTINUE
      WRITE(6,9002)
      WRITE(6,9002)
      DO 4 I1=1,N,10
      I2=I1+9
      IF(I2.GT.N) I2=N
      WRITE(6,9001) I1,(V(I),I=I1,I2)
4 CONTINUE

```

```

RETURN
END
SUBROUTINE INTRP(RPL,RPH)
DIMENSION RPL(15,55),RPH(13,60)
COMMON/ /ALFA(300,30),BETA(300,30),H1(300,30),H2(300,30)
1 ,SAQ(300),SBQ(300)
COMMON/DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
COMMON/XYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
COMMON/NS/NELOW,NEHI,NXDAT,NYDAT,NZDATH,NZDATH
ENG(T)=(T-.5)*DE+EZEROP
EDIV=ENG(FLOAT(INT((1.2-EZEROP)/DE)+1))+DE*.5
DO 1 J=1,NC
XJ=J
E=ENG(XJ)
IF(E.GT.EDATH(NEHI)) GO TO 26
IF(E.GT.EDIV) GO TO 2
DO 5 JD=1,NELOW
JP=JD-1
IF(E.GT.EDATL(JD)) GO TO 5
IF(JD.EQ.1) GO TO 4
X=(E-EDATL(JP))/(EDATL(JD)-EDATL(JP))
GO TO 6
4 X=E/EDATL(1)
GO TO 6
5 CONTINUE
6 CONTINUE
K=JD
IF(K.EQ.1) GO TO 10
MM=NXDAT-1
DO 13 I=1,MM
M=2*I
ALFA(J,I)=X*(RPL(K,M-1)-RPL(K-1,M-1))+RPL(K-1,M-1)
BETA(J,I)=X*(RPL(K,M)-RPL(K-1,M))+RPL(K-1,M)
13 CONTINUE
GO TO 1
10 MM=NXDAT-1
DO 11 I=1,MM
M=I*2
ALFA(J,I)=X*RPL(K,M-1)
BETA(J,I)=X*RPL(K,M)
11 CONTINUE
GO TO 1
2 DO 15 JD=1,NEHI
JP=JD-1
IF(E.GT.EDATH(JD)) GO TO 15
X=(E-EDATH(JP))/(EDATH(JD)-EDATH(JP))
GO TO 20
15 CONTINUE
20 K=JD
MM=NYDAT+NZDATH+NZDATH-3
DO 25 I=1,MM
M=2*I
ALFA(J,I)=X*(RPH(K,M-1)-RPH(K-1,M-1))+RPH(K-1,M-1)
BETA(J,I)=X*(RPH(K,M)-RPH(K-1,M))+RPH(K-1,M)
25 CONTINUE
1 CONTINUE
CALL NORM
RETURN
26 WRITE(6,1001)
1001 FORMAT(1H1,2X,28HEMAX GREATER THAN MAX ENERGY )

```

```

STOP
END
SUBROUTINE NORM
COMMON/ /ALFA(300,30),BETA(300,30),H1(300,30),H2(300,30)
1 ,SAQ(300),SBQ(300)
COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
COMMON/EXYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
COMMON/NS/NELOW,NEHI,NXDAT,NYDAT,NZDATL,NZDATH
COMMON/PEAK/PK(300,5)
ENG(T)=(T-.5)*DE+EZEROP
ECOM(E)=(2.*E*E)/(ERM+2.*E)
EDIV=ENG(FLOAT(INT((1.2-EZEROP)/DE)+1))+DE*.5
DO 1 J=1,NC
ER2=2.*ERM
XJ=J
E=ENG(XJ)
IF(E.GT.EDIV) GO TO 4
EC=ECOM(E)
MM=NXDAT-1
DO 50 I=1,MM
II=I+1
H1(J,I)=XR(I)*EC
H2(J,I)=XR(II)*EC
50 CONTINUE
ARA=0.0
DO 2I=1,MM
ARA=ARA+0.5*(ALFA(J,I)+BETA(J,I))*(H2(J,I)-H1(J,I))/DE
2 DO 3 I=1,MM
ALFA(J,I)=ALFA(J,I)*PK(J,5)/ARA
3 BETA(J,I)=BETA(J,I)*PK(J,5)/ARA
GO TO 1
4 CONTINUE
ES=E-1.022
EF=E-.511
MY=NYDAT-1
DO 10 I=1,MY
II=I+1
H1(J,I)=YR(I)*ES
H2(J,I)=YR(II)*ES
10 CONTINUE
MZS=MY+1
MZSTOP=MY+NZDATL-1
II=0
DO 11 I=MZS,MZSTOP
II=II+1
I2=II+1
H1(J,I)=E-(1.-ZR(II))*ER2
H2(J,I)=E-(1.-ZR(I2))*ER2
11 CONTINUE
II=II+1
MZS=MZSTOP+1
MZSTOP=MZS+NZDATH-2
DO 12 I=MZS,MZSTOP
II=II+1
I2=II+1
H1(J,I)=E-(1.-ZR(II))*ER2
H2(J,I)=E-(1.-ZR(I2))*ER2
12 CONTINUE
ARA=0.0
N=NYDAT+NZDATL+NZDATH-3

```

```

DO 5 I=1,N
ARA=ARA+0.5*(ALFA(J,I)+BETA(J,I))*(H2(J,I)-H1(J,I))/DE
5 CONTINUE
DO 6 I=1,N
ALFA(J,I)=ALFA(J,I)*PK(J,5)/ARA
6 BETA(J,I)=BETA(J,I)*PK(J,5)/ARA
1 CONTINUE
RETURN
END
SUBROUTINE ALFBET
COMMON/ /ALFA(300,30),BETA(300,30),H1(300,30),H2(300,30)
1 ,SAQ(300),SBQ(300)
COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
COMMON/XYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
COMMON/NS/NELDW,NEHI,NXDAT,NYDAT,NZDATL,NZDATH
ENG(T)=(T-.5)*DE+EZEROP
EDIV=ENG(FLOAT(INT((1.2-EZEROP)/DE)+1))+DE*.5
DO 1 J=1,RC
XJ=J
E=ENG(XJ)
IF(E.GT.EDIV) GO TO 2
NLOW=NXDAT-1
DO 3 I=1,NLOW
H1(J,I)=(H1(J,I)-EZEROP)/DE
H2(J,I)=(H2(J,I)-EZEROP)/DE
V1=ALFA(J,I)
V2=BETA(J,I)
BETA(J,I)=(V2-V1)/(H2(J,I)-H1(J,I))
ALFA(J,I)=0.5*(V1+V2)-0.5*BETA(J,I)*(H1(J,I)+H2(J,I))
3 CONTINUE
GO TO 1
2 CONTINUE
NHI=NYDAT+NZDATL+NZDATH-3
DO 4 I=1,NHI
H2(J,I)=(H2(J,I)-EZEROP)/DE
H1(J,I)=(H1(J,I)-EZEROP)/DE
V1=ALFA(J,I)
V2=BETA(J,I)
BETA(J,I)=(V2-V1)/(H2(J,I)-H1(J,I))
ALFA(J,I)=0.5*(V1+V2)-0.5*BETA(J,I)*(H1(J,I)+H2(J,I))
4 CONTINUE
1 CONTINUE
RETURN
END
SUBROUTINE PGEN(P,Q)
DIMENSION Q(300),P(300),R(300)
COMMON/ /ALFA(300,30),BETA(300,30),H1(300,30),H2(300,30)
1 ,SAQ(300),SBQ(300)
COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
COMMON/XYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
COMMON/NS/NELDW,NEHI,NXDAT,NYDAT,NZDATL,NZDATH
COMMON/PEAK/PK(300,5)
COMMON/JUNK/J1(300),J2(300),JA
COMMON /LRG/ A(10000)
ENG(T)=(T-.5)*DE+EZEROP
E12(HH,6)=(HH+SQRT(HH*HH+1.022*HH*G))/(2.*G)
ECUM(E)=(2.*E*E)/(ERM+2.*E)
XNC=NC+.5
EDIV=ENG(FLOAT(INT((1.2-EZEROP)/DE)+1))+DE*.5
EMAX=ENG(XNC)

```

```

DO 3 J=1,NC
R(J)=0.
3 P(J)=0.
IF(EZEROP,GE,EDIV) GO TO 100
NLOW=NXDAT-1
DO 40 I=1,NLOW
CALL RUNSUM(SAQ,ALFA(1,I),0,NC)
CALL RUNSUM(SBQ,BETA(1,I),0,NC)
DO 1 J=1,NC
XJ=J
E=ENG(XJ)
II=I+1
IF(XR(I).LE.0.) XR(I)=0.0001
E8=XR(II)
EA=XR(I)
E1=E12(E,E8)
E2=E12(E,EA)
IF(E1.GT.EDIV) GO TO 2
E1=(E1-EZEROP)/DE
IF (E1.GT.XNC) GO TO 2
IF(E2.GT.EDIV) E2=EDIV
E2=(E2-EZEROP)/DE
IF(E2.GT.XNC) E2=XNC
IF(E1.LT.1.) GO TO 1
IF(E2.LT.1.) GO TO 1
CALL INTGRL(SNTGRL,SAQ,ALFA(1,I),0,E2,NC)
S1=SNTGRL
CALL INTGRL(SNTGRL,SAQ,ALFA(1,I),0,E1,NC)
S2=SNTGRL
CALL INTGRL(SNTGRL,SBQ,BETA(1,I),0,E2,NC)
S3=SNTGRL
CALL INTGRL(SNTGRL,SBQ,BETA(1,I),0,E1,NC)
S4=SNTGRL
R(J)=R(J)+S1-S2+(XJ-.5)*(S3-S4)
1 CONTINUE
2 CONTINUE
40 CONTINUE
100 CONTINUE
NHI=NYDAT+NZDATL+NZDATH-3
DO 200 I=1,NHI
CALL RUNSUM(SAQ,ALFA(1,I),0,NC)
CALL RUNSUM(SBQ,BETA(1,I),0,NC)
DO 10 J=1,NC
K=I-NYDAT+1
IF(I.GE.(NYDAT+NZDATL-1)) K=K+1
KK=K+1
XJ=J
E=ENG(XJ)
IF(I.GT.NYDAT-1) GO TO 55
II=I+1
IF(YK(I).LE.0.) YR(I)=.001
E2=E/YR(I)+1.022
E1=E/YR(II)+1.022
GO TO 60
55 CONTINUE
E1=E+(1.-ZR(KK))*1.022
E2=E+(1.-ZR(K))*1.022
60 CONTINUE
IF(E1.GT.EMAX) GO TO 20
IF(E2.GT.EMAX) E2=EMAX

```



```

IF(E2,LE,EDIV) GO TO 10
IF(E1,LE,EDIV) E1=EDIV
E1=(E1-EZEROP)/DE
E2=(E2-EZEROP)/DE
IF(E1,LT,1.) GO TO 10
IF(E2,LT,1.) GO TO 10
CALL INTGRL(SNTGRL,SAQ,ALFA(1,I),Q,E2,NC)
S1=SNTGRL
CALL INTGRL(SNTGRL,SAQ,ALFA(1,I),Q,E1,NC)
S2=SNTGRL
CALL INTGRL(SNTGRL,SBQ,BETA(1,I),Q,E2,NC)
S3=SNTGRL
CALL INTGRL(SNTGRL,SBQ,BETA(1,I),Q,E1,NC)
S4=SNTGRL
R(J)=R(J)+S1-S2+(XJ-.5)*(S3-S4)
10 CONTINUE
20 CONTINUE
200 CONTINUE
DO 30 J=1,NC
IF(Q(J),LT,1.E-10) GO TO 30
T=J
E=ENG(T)
R(J)=R(J)+PK(J,1)*Q(J)
DO 31 K=2,4
EN=E-ERM*FLOAT(K-1)
IF(K,EQ,2) EN=E-(.488-.0045*(E-1.022))
IF(K,EQ,4) EN=E-.029
RJ=(EN-EZEROP)/DE+.5
JJ=INT(RJ)
IF(JJ,LE,0) GO TO 31
IF(JJ,GE,NC) GO TO 31
W2=RJ-FLOAT(JJ)
R(JJ)=R(JJ)+(1.-W2)*PK(J,K)*Q(J)
R(JJ+1)=R(JJ+1)+W2*PK(J,K)*Q(J)
31 CONTINUE
30 CONTINUE
K=0
DO 50 I=1,NR
JMIN=J1(I)
JMAX=J2(I)
DO 51 J=JMIN,JMAX
K=K+1
51 P(I)=P(I)+A(K)*R(J)
50 CONTINUE
RETURN
END
SUBROUTINE PGENT(P,Q)
DIMENSION Q(300),P(300),R(300)
COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
COMMON/PEAK/PK(300,5)
COMMON/EXYZ/EDATL(15),EDATH(13),XR(30),YR(30),ZR(30)
COMMON/JUNK/J1(300),J2(300),JA
COMMON /LRG/ A(10000)
COMMON/NS/NELDH,NEHI,MXDAT,NYDAT,MZDATL,MZDATH
COMMON/ /ALFA(300,30),BETA(300,30),H1(300,30),H2(300,30)
1 ,SAQ(300),SBQ(300)
ENG(T)=(T-.5)*DE+EZEROP
H12(E,G)=(2.*G+E*E)/(.511+2.*E)
XNC=NC+.5
EDIV=ENG(FLOAT(INT((1.2-EZEROP)/DE)+1))+DE*.5

```

```

      EMAX=ENG(XNC)
      DEL=1./DE
      DO 5 J=1,NC
      R(J)=0.0
      H1(J,1)=1.0
      XJ=J
      H2(J,1)=XJ-.5
5      Q(J)=0.0
      K=0
      DO 50 I=1,NR
      JMIN=J1(I)
      JMAX=J2(I)
      DO 52 J=JMIN,JMAX
      K=K+1
52      R(J)=R(J)+P(I)*A(K)
50      CONTINUE
      CALL RUNSUM(SAQ,H1(1,1),R,NC)
      CALL RUNSUM(SBQ,H2(1,1),R,NC)
      IF(EZEROP.GT.1.2) GO TO 100
      N=NXDAT-1
      DO 40 I=1,N
      DO 1 J=1,NC
      XJ=J
      E=ENG(XJ)
      IF(E.GT.EDIV) GO TO 2
      II=I+1
      EB=XR(II)
      E2=H12(E,EB)
      E2=(E2-EZEROP)/DE
      IF(E2.LT.0.) GO TO 1
      EA=XR(I)
      E1=H12(E,EA)
      E1=(E1-EZEROP)/DE
      IF(E1.LT.0.) E1=0.
      IF(E2.GT.NC) E2=XNC
      IF(E1.GT.NC) GO TO 1
      CALL INTGRL(SNTGRL,SAQ,H1(1,1),R,E2,NC)
      S1=SNTGRL
      CALL INTGRL(SNTGRL,SAQ,H1(1,1),R,E1,NC)
      S2=SNTGRL
      CALL INTGRL(SNTGRL,SBQ,H2(1,1),R,E2,NC)
      S3=SNTGRL
      CALL INTGRL(SNTGRL,SBQ,H2(1,1),R,E1,NC)
      S4=SNTGRL
      Q(J)=Q(J)+ALFA(J,I)*(S1-S2)+BETA(J,I)*(S3-S4)
1      CONTINUE
2      CONTINUE
40      CONTINUE
100     CONTINUE
      NH=NYDAT+NZDATL+NZDATH-3
      DO 200 I=1,NH
      K=I-NYDAT+1
      IF(I.GE.(NYDAT+NZDATL-1)) K=K+1
      KR=K+1
      DO 10 J=1,NC
      XJ=J
      II=I+1
      E=ENG(XJ)
      IF(E.LE.EDIV) GO TO 10
      E6=E-1.022

```

```

      IF (I.GT.(NYDAT-1)) GO TO 250
      E1=YR(I)*ES
      E2=YR(II)*ES
      GO TO 18
250  CONTINUE
      E1=E-2.*ERM*(1.-ZR(K))
      E2=E-2.*ERM*(1.-ZR(KK))
18   CONTINUE
      E1=(E1-EZEROP)/DE
      E2=(E2-EZEROP)/DE
      IF (E2.LT.0.) GO TO 10
      IF (E1.LT.0.) E1=0.
      IF (E2.GT.NC) E2=XNC
      IF (E1.GT.NC) GO TO 10
      CALL INTGRL(SNTGRL,SAQ,H1(1,1),R,E2,NC)
      S1=SNTGRL
      CALL INTGRL(SNTGRL,SAQ,H1(1,1),R,E1,NC)
      S2=SNTGRL
      CALL INTGRL(SNTGRL,SBQ,H2(1,1),R,E2,NC)
      S3=SNTGRL
      CALL INTGRL(SNTGRL,SBQ,H2(1,1),R,E1,NC)
      S4=SNTGRL
      Q(J)=Q(J)+ALFA(J,I)*(S1-S2)+BETA(J,I)*(S3-S4)
10   CONTINUE
20   CONTINUE
200  CONTINUE
      DO 30 J=1,NC
      T=J
      E1=ENG(T)
      Q(J)=Q(J)+PK(J,1)*R(J)
      EN=E1+.029
      RJ=(EN-EZEROP)*DEL+.5
      JJ=INT(RJ)
      IF (JJ.LE.0) GO TO 25
      IF (JJ.GT.(NC-1)) GO TO 25
      W2=RJ-FLOAT(JJ)
      Q(JJ)=Q(JJ)+(1.-W2)*PK(JJ,4)*R(J)
      JJ1=JJ+1
      Q(JJ1)=Q(JJ1)+W2*PK(JJ1,4)*R(J)
25   CONTINUE
      IF (E1.LE..178) GO TO 30
      EN=E1+1.022
      RJ=(EN-EZEROP)*DEL+.5
      JJ=INT(RJ)
      IF (JJ.LE.0) GO TO 31
      IF (JJ.GT.(NC-1)) GO TO 31
      W2=RJ-FLOAT(JJ)
      Q(JJ)=Q(JJ)+(1.-W2)*PK(JJ,3)*R(J)
      JJ1=JJ+1
      Q(JJ1)=Q(JJ1)+W2*PK(JJ1,3)*R(J)
31   IF (E1.LE..689) GO TO 30
      EN=E1+(.488-.0045*(E1-1.022))
      RJ=(EN-EZEROP)*DEL+.5
      JJ=INT(RJ)
      IF (JJ.LE.0) GO TO 30
      IF (JJ.GT.(NC-1)) GO TO 30
      W2=RJ-FLOAT(JJ)
      Q(JJ)=Q(JJ)+(1.-W2)*PK(JJ,2)*R(J)
      JJ1=JJ+1
      Q(JJ1)=Q(JJ1)+W2*PK(JJ1,2)*R(J)

```

```

30  CONTINUE
    RETURN
    END
    SUBROUTINE RUNSUM(SUM,X,Y,N)
    DIMENSION SUM(N),X(N),Y(N)
    SUM(1)=X(1)*Y(1)
    DO 1 I=2,N
    SUM(I)=SUM(I-1)+X(I)*Y(I)
1   CONTINUE
    RETURN
    END
    SUBROUTINE INTGRL(SNTGRL,SUM,X,Y,BOUND,N)
    DIMENSION X(N),Y(N),SUM(N)
    IBOUND=BOUND
    SNTGRL=SUM(IBOUND)+(BOUND-IBOUND)*X(IBOUND+1)*Y(IBOUND+1)
    RETURN
    END
    SUBROUTINE ERROR(QMIN,QD,QC,SIG,ERR)
    DIMENSION QMIN(1,1),SIG(1),ERR(1),AP(300),P(300),Q(300)
    DIMENSION QD(1),QC(1)
    COMMON /DATA/ DE,EZEROP,ERM,RES,NC,NR,IPRNT
    CALL PGEN(P,QMIN)
    DO 10 K=1,NC
    SIG(K)=3.
10  ERR(K)=0.
    DO 100 K=1,NC
    DO 50 J=1,NC
    Q(J)=0.
    X=(FLOAT(J-K))**2/(2.*SIG(K)**2)
    Y=(FLOAT(J-K))**2/(FLOAT(NR)**2/2.)
    IF(X.GT.10.) GO TO 40
    Q(J)=QD(K)*EXP(-X)
40  IF(Y.GT.10.) GO TO 50
    Q(J)=Q(J)+QC(K)*EXP(-Y)
50  CONTINUE
    CALL PGEN(AP,Q)
    SUM=0.
    APM=0.
    DO 55 I=1,NR
55  APM=AMAX1(AP(I),APM)
    N=0
    DO 60 I=1,NR
    IF(AP(I).GT.APM*1.E-5) N=N+1
    SUM=SUM+AP(I)*AP(I)/P(I)
60  CONTINUE
    XN=N
    IF (SUM.LE.0.) GO TO 100
    ERR(K)=QMIN(K,1)*SQRT(SQRT(XN)/SUM)
100 CONTINUE
    RETURN
    END
    SUBROUTINE FIT(N,M,X,D,NFIT,XFIT,FITT,XX,DD,SL)
    DIMENSIONX(1),D(1),XX(1),DD(1),XFIT(1),FITT(1,1),SL(1)
C-----
C    N=NUMBER OF DATA POINTS
C    M=N+4
C    D=DATA AT VALUES OF X
C    NFIT=NUMBER OF FIT DATA POINTS
C    FIT INTERPOLATED DATA
C-----

```

```

      DD 10 I=1,N
      II=I+2
      XX(II)=X(I)
      DD(II)=D(I)
C 10 CONTINUE
      ESTIMATE 2 ADDITIONAL POINTS AT EACH END
      IF(IPRNT.EQ.1) CALL XPRINT(N,X,SHX= )
      IF(IPRNT.EQ.1) CALL XPRINT(N,D,SHD= )
      N2=N-2
      IF(IPRNT.EQ.1) CALL XPRINT(NFIT,XFIT,SHXFIT= )
      NI=N-1
      NP1=N+3
      NP2=N+4
      CALL ENDP(X(3),X(2),X(1),D(3),D(2),D(1),XX(2),XX(1),DD(2),DD(1))
      CALL ENDP(X(N2),X(N1),X(N),D(N2),D(N1),D(N),XX(NP1),XX(NP2),
1 DD(NP1),DD(NP2))
      IF(IPRNT.EQ.1) WRITE(6,6000) DD(1),DD(2),DD(NP1),DD(NP2)
6000 FORMAT(1H,4F10.5)
C CALCULATE SLOPES AT ALL DATA POINTS
      DD 20 I=1,N
      I1=I+1
      I2=I+2
      I3=I+3
      I4=I+4
      I5=I+5
      CALL SLOPE(XX(I),DD(I),XX(I1),DD(I1),XX(I2),DD(I2),XX(I3),DD(I3),
1 ,XX(I4),DD(I4),SL(I2))
20 CONTINUE
C ESTIMATE POINTS AT XFIT
      IF(IPRNT.EQ.1) CALL XPRINT(N,SL,SHSLOPE )
      DD 40 K=1,NFIT
      DD 30 I=1,M
      IF(XFIT(K).GT.XX(I)) GO TO 30
      J=I-1
      CALL CURVE(XX(J),DD(J),SL(J),XX(I),DD(I),SL(I),XFIT(K),FITT(K,1))
      GO TO 40
30 CONTINUE
40 CONTINUE
      IF(IPRNT.EQ.1) CALL XPRINT(NFIT,FITT,SHFITT )
      RETURN
      END
C SUBROUTINE SLOPE(X1,Y1,X2,Y2,X3,Y3,X4,Y4,X5,Y5,T3)
      ESTIMATE SLOPE AT POINT 3
      XM4=(Y5-Y4)/(X5-X4)
      XM3=(Y4-Y3)/(X4-X3)
      XM2=(Y3-Y2)/(X3-X2)
      XM1=(Y2-Y1)/(X2-X1)
      IF(XM1.EQ.XM2.AND.XM3.EQ.XM2) GO TO 10
      A=ABS(XM4-XM3)
      B=ABS(XM2-XM1)
      T3=(A*XM2+B*XM3)/(A+B)
      RETURN
10 T3=(XM2+XM3)/2.
      RETURN
      END
C SUBROUTINE CURVE(X1,Y1,T1,X2,Y2,T2,XP,YP)
C CALCULATES YP GIVEN ADJECENT DATA POINTS AND SLOPES
C
      Y=Y2-Y1

```

```

X=X2-X1
R=Y/X
P2=(3.*R-2.*T1-T2)/X
P3=(T1+T2-2.*R)/(X*X)
DX=XP-X1
YP=Y1+T1*DX+P2*DX*DX+P3*DX*DX*DX
RETURN
END
SUBROUTINE ENDP(X1,X2,X3,Y1,Y2,Y3,X4,X5,Y4,Y5)

```

C
C
C

ESTIMATE TWO ADDITIONAL POINTS AT THE END OF THE DATA

```

X4=X3-X1+X2
X5=2.*X3-X1
Y4=(X4-X3)*(2.*(Y3-Y2)/(X3-X2)-(Y2-Y1)/(X2-X1))+Y3
Y5=(X5-X4)*(2.*(Y4-Y3)/(X4-X3)-(Y3-Y2)/(X3-X2))+Y4
RETURN
END
SUBROUTINE XPRINT(N,V,WORD)
DIMENSION V(N)
1001 FORMAT(///5X,11HLISTING OF ,A5)
1002 FORMAT(2X,8HLOCATION,I4,10G11.4)
WRITE(6,1001) WORD
DO 1 I1=1,N,10
I2=I1+9
IF(I2.GT.N) I2=N
WRITE(6,1002) I1,(V(I),I=I1,I2)
1 CONTINUE
RETURN
END

```

160	160	200	.01	.1	8.	.05	1	1	
	14	7	21	6	6	8	1		
.884	.828	.786	.740	.668	.650	.615	.586	.560	.504
.464	.444	.402	.369						
.369	.330	.300	.263	.224	.184	.175			
.01000	.00650	.00400	.00350	.00300	.00280	.00230	.00220	.00205	.00160
.00140	.00130	.00120	.00120						
.00033	.00161	.00388	.0111	.0271	.0450	.0501			
.0001	.00030	.00070	.0026	.0079	.0170	.0250			
.155	.213	.279	.335	.393	.411	.478	.513	.555	.662
.764	.835	.930	1.114						
1.114	1.290	1.461	1.780	2.160	2.750	3.103			
.000	.100	.200	.300	.400	.500	.600	.700	.800	.900
.950	.975	1.0	1.05	1.1	1.2	1.3	1.4	1.5	1.7
2.3									
0.0	.20	.40	.60	.80	1.0				
.000	.100	.200	.300	.400	.500	.500	.600	.700	.750
.800	.850	.90	1.0						
.199	.264	.327	.228	.350	.298	.271	.248	.224	.176
.148	.133	.112	.096	.	.	.	.	.	.
.212	.264	.327	.235	.360	.327	.279	.248	.234	.179
.151	.135	.115	.096	.	.	.	.	.	.
.212	.264	.327	.235	.360	.327	.279	.248	.234	.179
.151	.135	.115	.096	.	.	.	.	.	.
.220	.271	.327	.239	.335	.347	.279	.248	.224	.186
.148	.135	.120	.098	.	.	.	.	.	.
.220	.271	.327	.239	.335	.347	.279	.248	.224	.186
.148	.135	.120	.098	.	.	.	.	.	.
.220	.274	.327	.224	.336	.355	.279	.251	.227	.191
.155	.139	.127	.098	.	.	.	.	.	.
.220	.274	.327	.224	.336	.355	.279	.251	.227	.191
.155	.139	.127	.098	.	.	.	.	.	.
.216	.279	.327	.199	.321	.348	.275	.251	.235	.194
.161	.149	.129	.099	.	.	.	.	.	.
.216	.279	.327	.199	.321	.348	.275	.251	.235	.194
.161	.149	.129	.099	.	.	.	.	.	.
.212	.280	.333	.181	.311	.334	.279	.254	.239	.199
.167	.148	.129	.102	.	.	.	.	.	.
.212	.280	.333	.181	.311	.334	.279	.254	.239	.199
.167	.148	.129	.102	.	.	.	.	.	.
.205	.295	.339	.172	.306	.313	.279	.257	.241	.199
.165	.148	.127	.104	.	.	.	.	.	.
.205	.295	.339	.172	.306	.313	.279	.257	.241	.199
.165	.148	.127	.104	.	.	.	.	.	.
.221	.451	.374	.185	.311	.305	.283	.255	.243	.193
.165	.153	.137	.108	.	.	.	.	.	.
.221	.451	.374	.185	.311	.305	.283	.255	.243	.193
.165	.153	.137	.108	.	.	.	.	.	.
.267	.576	.473	.270	.345	.313	.268	.248	.231	.193
.169	.158	.141	.119	.	.	.	.	.	.
.267	.576	.473	.270	.345	.313	.268	.248	.231	.193
.169	.158	.141	.119	.	.	.	.	.	.
.414	.625	.654	.280	.410	.341	.324	.299	.253	.222
.192	.173	.152	.136	.	.	.	.	.	.
.414	.625	.654	.280	.410	.341	.324	.299	.253	.222
.192	.173	.152	.136	.	.	.	.	.	.
.414	.607	.549	.243	.321	.341	.291	.265	.242	.209
.192	.196	.155	.147	.	.	.	.	.	.

.414	.607	.549	.243	.321	.341	.291	.265	.242	.209
.192	.196	.155	.147	.	.	.	.	.	.
.432	.549	.490	.224	.271	.270	.252	.237	.213	.176
.153	.151	.129	.125	.	.	.	.	.	.
.432	.549	.490	.224	.271	.270	.252	.237	.213	.176
.153	.151	.129	.125	.	.	.	.	.	.
.337	.412	.315	.203	.165	.185	.165	.193	.147	.117
.117	.089	.084	.061	.16	.	.	.	.	.
.337	.412	.315	.203	.165	.185	.165	.193	.147	.117
.117	.089	.084	.061	.16	.	.	.	.	.
.294	.361	.233	.104	.117	.128	.107	.070	.058	.052
.037	.035	.025	.027	.	.	.	.	.	.
.294	.361	.233	.104	.117	.128	.107	.070	.058	.052
.037	.035	.025	.027	.	.	.	.	.	.
.104	.362	.223	.072	.107	.107	.071	.068	.055	.040
.031	.032	.025	.024	.	.	.	.	.	.
.104	.362	.223	.072	.107	.107	.071	.068	.055	.040
.031	.032	.025	.024	.	.	.	.	.	.
.104	.394	.274	.052	.122	.099	.074	.062	.055	.042
.037	.030	.031	.007	.	.	.	.	.	.
.104	.394	.274	.052	.122	.099	.074	.062	.055	.042
.037	.030	.031	.007	.	.	.	.	.	.
.225	.363	.286	.031	.117	.114	.090	.085	.073	.039
.021	.000	.000	.000	.	.	.	.	.	.
.225	.363	.286	.031	.117	.114	.090	.085	.073	.039
.021	.000	.000	.000	.117	.11	.	.	.	.
.243	.362	.286	.043	.175	.149	.079	.067	.034	.065
.	.	.	.	.	.	.	.	.	.
.243	.362	.286	.043	.175	.149	.079	.067	.034	.065
.	.	.	.	.	.	.	.	.	.
.276	.508	.334	.031	.136	.044	.000	.000	.000	.000
.	.	.	.	.	.	.	.	.	.
.276	.508	.334	.031	.136	.044	.000	.000	.000	.000
.	.	.	.	.	.	.	.	.	.
.423	.659	.339	.028	.000	.000	.000	.000	.000	.000
.	.	.	.	.	.	.	.	.	.
.423	.659	.339	.028	.000	.000	.000	.000	.000	.000
.	.	.	.	.	.	.	.	.	.
.691	.656	.233	.000	.000	.000	.000	.000	.000	.000
.	.	.	.	.	.	.	.	.	.
.10200	.08880	.07340	.05590	.04660	.02780	.02520	.	.	.
.09930	.08780	.07340	.05590	.04460	.03000	.02540	.	.	.
.09930	.08780	.07340	.05590	.04460	.03000	.02540	.	.	.
.09780	.08580	.07340	.05590	.04340	.03220	.02550	.00000	.00000	.00000
.09780	.08580	.07340	.05590	.04340	.03220	.02550	.00000	.00000	.00000
.09630	.08480	.07340	.05590	.04340	.03440	.02580	.00000	.00000	.00000
.09630	.08480	.07340	.05590	.04340	.03440	.02580	.00000	.00000	.00000
.09630	.08480	.07340	.05590	.04660	.03660	.02640	.00000	.00000	.00000
.09630	.08480	.07340	.05590	.04660	.03660	.02640	.00000	.00000	.00000
.09630	.08430	.07340	.05590	.04860	.03900	.03400	.00000	.00000	.00000
.09630	.08430	.07340	.05700	.05270	.04800	.04780	.00000	.00000	.00000
.09630	.08070	.07180	.05700	.05310	.04800	.05100	.00000	.00000	.00000
.09630	.08070	.07180	.05700	.05310	.04800	.05100	.00000	.00000	.00000
.09780	.08070	.07180	.05920	.05470	.04800	.05250	.00000	.00000	.00000
.09780	.08070	.07180	.05920	.05470	.04800	.05250	.00000	.00000	.00000
.10100	.08070	.07180	.06130	.05630	.05120	.05150	.00000	.00000	.00000
.10100	.08070	.07180	.06130	.05630	.05120	.05150	.00000	.00000	.00000
.10200	.08480	.07500	.06450	.05880	.05120	.05100	.00000	.00000	.00000

.10200	.08480	.07500	.06450	.05880	.05120	.05100	.00000	.00000	.00000
.10500	.09290	.08300	.07140	.06490	.05150	.05050	.00000	.00000	.00000
.10500	.09290	.08460	.07960	.06690	.06390	.06350	.00000	.00000	.00000
.11700	.10400	.09100	.08610	.06900	.06870	.07090	.00000	.00000	.00000
.11700	.10400	.09100	.08610	.06900	.06870	.07090	.00000	.00000	.00000
.12800	.11800	.11000	.09250	.09320	.09100	.07090	.00000	.00000	.00000
.12800	.11800	.11000	.09250	.09320	.09100	.07090	.00000	.00000	.00000
.15800	.12600	.11200	.09470	.06320	.06350	.06350	.00000	.00000	.00000
.15800	.12600	.11200	.09470	.06320	.06350	.06350	.00000	.00000	.00000
.07220	.06860	.04310	.05270	.03200	.03200	.02840	.00000	.00000	.00000
.07220	.06860	.04310	.05270	.03200	.03200	.02840	.00000	.00000	.00000
.02210	.01210	.02000	.02370	.01200	.01200	.02120	.00000	.00000	.00000
.02210	.01210	.02000	.02370	.01200	.01200	.02120	.00000	.00000	.00000
.02410	.02320	.02000	.01290	.00608	.00959	.00709	.00000	.00000	.00000
.02410	.02320	.02000	.01290	.00608	.00959	.00709	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
TITLE									
10170.	10170.	10610.	10680.	10810.	10790.	11200.	11770.	12710.	12740.
12560.	12220.	11830.	11690.	11540.	11570.	11290.	11330.	11230.	11240.
10960.	11100.	10820.	10810.	11040.	11000.	11270.	11230.	11220.	11290.
11600.	12060.	12860.	13300.	13740.	13180.	11770.	10500.	9212.	8675.
8209.	7679.	7390.	7323.	7131.	7091.	7076.	7166.	7773.	9049.
12030.	17430.	25660.	35120.	43620.	46930.	44430.	37710.	29110.	22040.
17110.	13830.	12390.	11690.	11390.	11310.	10160.	8566.	7366.	6464.
6116.	6527.	8177.	10670.	14290.	17760.	20410.	21600.	21160.	19090.
16850.	14680.	12450.	9973.	7980.	5950.	4332.	3146.	2401.	1937.
1735.	1500.	1540.	1484.	1489.	1512.	1441.	1530.	1501.	1470.
1499.	1397.	1303.	1273.	1273.	1209.	1066.	968.	971.	891.
856.	817.	793.	772.	777.	794.	886.	988.	1268.	1683.
2049.	2583.	3092.	3497.	3633.	3554.	3284.	3052.	2652.	2319.
2092.	2046.	2153.	2118.	2210.	2251.	2193.	2074.	1869.	1519.
1329.	1111.	890.	769.	654.	523.	489.	375.	307.	233.
200.	151.	116.	100.	80.	58.	54.	62.	62.	48.

APPENDIX B

REFERENCE 5

REPRINTED WITH THE PERMISSION
OF NORTH-HOLLAND PUBLISHING CO.

(Berger and Seltzer, NI&M 104, 317-332 (1972))

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

RESPONSE FUNCTIONS FOR SODIUM IODIDE SCINTILLATION DETECTORS*

M. J. BERGER and S. M. SELTZER

National Bureau of Standards, Washington, D.C. 20234, U.S.A.

Received 19 April 1972

The response of sodium iodide detectors to gamma rays has been calculated by a method that takes into account the multiple scattering and escape from the detector of the incident gamma rays as well as of the secondary charged particles and bremsstrahlung. The method is applicable to gamma rays with arbitrarily high energies, and its accuracy has been verified by comparisons with experimental response functions at energies up to 20 MeV. A systematic tabulation has been made of the response functions for 3" x 3" detectors irradiated with broad parallel beams of gamma rays, at energies between 100 keV and 20 MeV. These results are given in a parametrized form

which makes it easy to interpolate with respect to incident gamma-ray energy. A few response functions have also been calculated for detectors irradiated with 50 MeV gamma rays. Exploratory calculations have shown that 3" x 3" detectors are "omnidirectional" in the sense that the shape of the response function depends very little on the direction of the incident gamma-ray beam. Therefore, the tabulated data for broad parallel beams incident perpendicularly can, in good approximation, also be applied to other source geometries, e.g. the case of a detector exposed to an isotropic gamma-ray flux.

1. Introduction

Increasingly complex and sophisticated methods are being used for the conversion of observed NaI pulse-height distributions into true gamma-ray spectra. These methods require accurate and detailed information about the detector response function which describes the stochastic relation between the pulse-heights and the energies of the incident gamma rays. The calculations reported here were undertaken in order to provide a reliable standard set of response functions as input for a conversion system developed by Trombka¹⁻³) and his associates at Goddard Space Flight Center (NASA).

A large amount of experimental and calculated response function data has accumulated over the years. [For a good review, and references to the literature, see, e.g., Neiler and Bell⁴), and Van Lieshout et al.⁵].] The new contributions from our work are the following:

- The loss of energy from the NaI detector due to the escape of secondary charged particles and bremsstrahlung is treated by a more detailed and realistic transport calculation than in previous work. This allows accurate determination of the response function for arbitrarily high energies of the incident gamma rays.
- The validity of the calculations has been checked by numerous comparisons with experimental data, both old and recent, at energies up to 20 MeV.
- A systematic tabulation has been made of the response functions for detectors with a commonly

used size (3" x 3") exposed to broad parallel beams of gamma rays. These results are given at 21 energies between 100 keV and 20 MeV, in a form which permits easy interpolation to any energy.

- The dependence of the response function on the direction of the incident gamma-rays has been investigated.

2. Components of the response function

The response function $R(E_0, h)$ can be written as the convolution of an energy deposition spectrum $D(E_0, E)$ and a resolution function $G(E, h)$, multiplied by the detection efficiency $\eta(E_0)$:

$$R(E_0, h) = \eta(E_0) \int_0^{E_0} D(E_0, E) G(E, h) dE. \quad (1)$$

The various quantities in eq. (1) have the following meaning:

$R(E_0, h)dh$ is the probability that a gamma ray incident with energy E_0 will give rise to a pulse with a height between h and $h + dh$.

$\eta(E_0)$ is the probability that the incident gamma ray will have at least one interaction in the detector.

$D(E_0, E)dE$ is the probability that the gamma ray, if it interacts with the detector at all, will deposit an amount of energy between E and $E + dE$.

$G(E, h)dh$ is the probability that the deposition of energy E will give rise to a pulse with a height between h and $h + dh$.

The assumed normalization of the response function is such that the integral of $R(E_0, h)$ over all h is equal to

* This work was carried out with the joint support of NASA and the Office of Naval Research.

$\eta(E_0)$. The evaluation of the detection efficiency is a geometrical problem which has been solved analytically for various cases of interest⁶⁻⁸). The efficiency values from our Monte Carlo calculation were used primarily to check the correctness of our sampling procedures.

3. Calculation of the energy deposition spectrum

The calculation of $D(E_0, E)$ is a multiple scattering problem involving photons, electrons and positrons. The multiple Compton scattering of photons and their eventual escape from, or absorption in, the detector were simulated by random sampling, in direct analogy to the physical processes⁹). This was done for the incident gamma-rays as well as for all secondary photons (bremsstrahlung, annihilation quanta, fluorescence radiation), using cross sections for Compton scattering, photoelectric absorption and pair production taken from a compilation by Hubbell¹⁰). The multiple scattering of the electrons and positrons set in motion in gamma-ray interactions (photoelectrons, Compton electrons, electron-positron pairs) was treated by a Monte Carlo model in which, instead of sampling all successive interactions, the combined effect of many successive scattering was taken into account with the use of analytical multiple-scattering theory¹¹). Each electron track to be simulated was divided into many short segments; the multiple-scattering angular deflection in each segment was sampled from the Goudsmit-Saunderson¹²) distribution, and the energy loss from the Landau¹³) distribution. In each path segment the electron was given a chance to set in motion secondary (knock-on) electrons in inelastic collisions [according to the Møller¹⁴) cross section], to produce characteristic X-rays via K-shell ionization [according to the Kolbenstvedt¹⁵) cross section], and to emit bremsstrahlung [according to a combination of Born-approximation cross sections with semi-empirical corrections described elsewhere¹⁶)]. Positrons were treated as if they were electrons, except that the emission of annihilation quanta (from positrons at rest) was allowed to occur.

Monte Carlo histories were terminated when the electron or photon escaped from the detector or when its energy dropped to a value below 10 keV. Electron histories were also terminated when the energy of the electron fell to a value smaller than 4% of the incident gamma-ray energy, provided this took place deep enough in the detector so that the residual electron range was smaller than the distance to the nearest detector boundary*. All energy remaining upon termination of a Monte Carlo history was considered to have been deposited in the detector. Because of the

10 keV cut-off, only fluorescence radiation from the K-shell of iodine had to be included.

For each sampled Monte Carlo cascade, consisting of the history of the incident gamma ray and the histories of all secondary photons and charged particles, the energy E deposited in the detector was scored as the difference between the incident gamma-ray energy E_0 and the sum of the energies carried away by escaping electrons, positrons or photons. By sampling large numbers of such cascades (typically 10000 to 50000), estimates of the energy deposition spectrum were obtained. This spectrum has the form of a line spectrum plus a continuum $C(E_0, E)$:

$$D(E_0, E) = C(E_0, E) + P_0\delta(E - E_0) + P_1\delta(E - E_0 + mc^2) + P_2\delta(E - E_0 + 2mc^2) + P_3\delta(E - \bar{E}_f), \quad (2)$$

where δ is the delta function and mc^2 the electron rest energy. P_0 is the probability that the entire gamma-ray energy E_0 is deposited in the detector. P_1 and P_2 are the probabilities that all of the energy is deposited with the exception of the amounts mc^2 or $2mc^2$ carried away by one or two unscattered annihilation quanta. P_3 is the probability that all energy is deposited except that carried away by unscattered K X-rays from iodine (with a weighted average energy $\bar{E}_f = 29$ keV)[†]. The quantity P_0 can also be interpreted as the relative area under the *total absorption peak* of the response function. Similarly, P_1 and P_2 are the relative areas under the *single* and *double annihilation radiation escape peaks*, and P_3 is the relative area under the *fluorescence radiation escape peak*.

The computation of gamma-ray Monte Carlo histories was relatively fast. Neglecting secondary electrons, only ≈ 0.5 min of time on an IBM 360/91 computer was needed to trace the histories of 10000 gamma rays incident on a 3" $\times$ 3" detector. The cost of tracing electron Monte Carlo histories was much higher. For example, with the inclusion of all charged-particle and bremsstrahlung secondaries, the time required to follow the cascades generated by 10000 gamma rays incident on a 3" $\times$ 3" detector was ≈ 5 min for an

* This cut-off procedure greatly speeded up the calculation, but resulted in a slight underestimate of the bremsstrahlung emitted by low-energy electrons. From the examination of tabulated bremsstrahlung efficiency values (ref. 17) and from trial calculations with different cut-off procedures, we reached the conclusion that the effect of the adopted cut-off procedure on the calculated energy deposition spectra was negligible.

† Actually the computer program gives information about individual escape peaks associated with the escape of $K_{\alpha 1}$, $K_{\alpha 2}$, $K_{\beta 1}$ and $K_{\beta 2}$ quanta whose energies are 28.612, 28.317, 32.295 and 33.047 keV, and whose relative intensities are 0.542, 0.279, 0.148 and 0.031, respectively.

TABLE I
Values of the exponent n in eq. (4) for the detector resolution, derived from various sets of experimental data.

Author	Energy	n
Trombka ^a	0.279 MeV to 2.76 MeV	0.32
Trombka ^b	0.032 MeV to 2.76 MeV	0.34
Ferguson et al. ^c	0.030 MeV to 1.332 MeV	0.34
Steyn ^d	0.073 MeV to 2.754 MeV	0.375
McGowan ^e	0.081 MeV to 1.850 MeV	0.33

^a Priv. comm; analysis of expt. data obtained at Goddard SFC.

^b Priv. comm; analysis of expt. data of Heath (ref. 19).

^c Priv. comm; analysis of data obtained at Howard University.

^d Ref. 18.

^e Our least-squares analysis of McGowan's data from Oak Ridge National Laboratory as reported by Kelley et al. ⁽²⁰⁾.

incident gamma-ray energy of 2 MeV, ≈ 12 min at 20 MeV and ≈ 24 min at 50 MeV.

4. Determination of the resolution function

It is well known that the resolution function $G(E, h)$ can be closely approximated by a Gaussian whose mean value $\bar{h}$ is proportional* to E and whose standard deviation $\sigma(E)$ must be obtained from experimental data. The resolution of the detector is defined to be the ratio

$$r(E) = 100 W(E)/E \text{ (percent)}, \quad (3)$$

where $W = 2\sigma\sqrt{2 \log 2}$ is the full width at half maximum of the Gaussian. The energy dependence of the detector resolution can be expressed by a power law,

$$r(E) = r(E')(E'/E)^n, \quad (4)$$

where E' is a reference energy which – in agreement with common usage – we take to be the energy of ^{137}Cs gamma rays (0.661 MeV). As discussed later in section 8, the magnitude of $r(0.661)$ typically ranges from 7% to 12%.

On the basis of simple statistical arguments it has often been assumed that the power n in eq. (4) has the value $\frac{1}{2}$. However, a better fit to the experimental data can be obtained with $n \approx \frac{1}{3}$, as pointed out by Trombka and Adler⁽³⁾ and Steyn⁽¹⁸⁾. Table I summarizes various analyses of experimental data, by Trombka (using his own data as well as those of Heath⁽¹⁹⁾), by Ferguson (priv. comm.), by Steyn⁽¹⁸⁾ and by Kelley et al.⁽²⁰⁾. These analyses have led us to adopt in our work the value $n = 0.34$.

* The proportionality applies provided that a possible non-linearity of channel number versus energy has been removed by an appropriate correction [see, e.g. Heath⁽¹⁹⁾].

5. Some comparisons at low energies

Even though this paper is focussed mainly on the response function at high energies, it is well to begin by making a few comparisons at low energies where charged-particle motion and escape are unimportant.

Various authors have calculated, at energies from 10 to 100 keV, the ratio of the fluorescence escape peak to the total absorption peak, P_3/P_0 . At 100 keV, for the case of perpendicular incidence on a large detector, an approximate analytical calculation by Axel⁽²¹⁾ gave the value 0.04, a similar calculation by Fioratti and Piermattei⁽²²⁾ the value 0.0365, a Monte Carlo calculation by Israel et al.⁽²³⁾ the value 0.042, and the present work the value 0.040. These results are on the whole consistent with each other, and have been shown by Fioratti and Piermattei to be in approximate agreement with the experimental data. Heath⁽¹⁹⁾ obtained the experimental value 0.056 for a 3" $\times$ 3" detector.

We now turn to the comparison of calculated and experimental values of the total absorption peak, P_0 , at an energy of 0.661 MeV. Table 2 contains comparisons, for the case of a narrow pencil beam, between results of our program [using cross sections from Hubbell⁽¹⁰⁾ and from an earlier tabulation by Grodstein⁽²⁴⁾], previous calculated values of Berger and Doggett⁽²⁵⁾ and Miller and Snow⁽²⁶⁾, and experimental values of Jarczyk et al.⁽²⁷⁾, Schmidt⁽²⁸⁾ and Foote and Koch⁽²⁹⁾. In table 3, comparisons are made, for the case of a broad parallel beam, between our results, the calculations of Miller and Snow⁽²⁶⁾ and Giannini et al.⁽³⁰⁾, and experimental values of Jarczyk et al.⁽²⁷⁾. The following conclusions can be drawn from these comparisons:

- The agreement between the various calculations is, by and large, satisfactory.

TABLE 2
Comparison of calculated and experimental values of the total absorption peak, P_0 , for detectors irradiated with a narrow pencil beam of 0.661-MeV gamma rays.

Detector size	Calculated				Experimental		
	This work ^a	This work ^b	Berger and Doggett ⁽²⁵⁾	Miller and Snow ⁽²⁶⁾	Jarczyk et al. ⁽²⁷⁾	Schmidt ⁽²⁸⁾	Footc and Koch ⁽²⁹⁾
1" × 1"	0.384	0.367	0.377				
2" × 2"	0.574	0.559			0.51		
3" × 3"	0.703	0.689			0.65		
4" × 4"	0.790	0.779					
5" × 4"	0.818	0.808	0.821	0.819	0.74	0.71	0.8

^a Using gamma-ray cross sections from Hubbell⁽¹⁰⁾. ^b Using gamma-ray cross sections from Grodstein⁽²¹⁾.

TABLE 3
Comparison of calculated and experimental values of the total absorption peak, P_0 , for detectors irradiated with a broad parallel beam of 0.661-MeV gamma rays.

Detector size	Calculated			Experimental
	This work	Miller and Snow ⁽²⁶⁾	Giannini et al. ⁽³⁰⁾	Jarczyk et al. ⁽²⁷⁾
2" × 2"	0.478	0.470	0.461	0.40
3" × 3"	0.569			0.50
4" × 4"	0.664	0.652		
5" × 4"	0.698			0.58

b. In the cases examined, the change in the value of P_0 resulting from the use of different cross sections ranges from 1.2% for large detectors to 4.5% for small detectors*.

c. The experimental values of P_0 tend to be significantly lower than the calculated values, by as much as 10–20%.

These discrepancies are most probably due to the fact that the calculations were done for an idealized bare detector and failed to take into account the scattering (and backscattering) of radiation into the detector from surrounding material. Some Monte Carlo calculations have already been made by Nardi⁽³¹⁾ and Steyn et al.⁽³²⁾ that include the effects of gamma-ray scattering in the cladding material around the NaI crystals and in the photomultiplier tube. Nardi has also demonstrated that there are additional perturbations of the response function which must be due to scattered gamma-rays from other pieces of equipment, walls, etc. Still to be done are high-energy response function

calculations which include the effects of the scattering (and backscattering) of secondary electrons in surrounding materials.

6. Effect of charged-particle and bremsstrahlung escape on the response function

In order to explore the effect of the escape of electrons, positrons and bremsstrahlung, we have carried out response-function calculations not only with the complete Monte Carlo model but also with a simplified model in which these effects were omitted. A typical comparison of the results obtained with the two models is given in fig. 1, for the case of a narrow pencil beam of 10.83 MeV electrons incident on a 3" × 3" detector. Use of the simplified model results in a considerable overestimate of the total absorption peak and the first and second annihilation radiation escape peaks, and a corresponding underestimate of the low-pulse-height tail of the response function. Fig. 2 compares the peak parameters P_0 , P_1 , P_2 and P_3 obtained with the two Monte Carlo models for gamma-rays with energies between 100 keV and 20 MeV incident on a 3" × 3" detector. The differences begin to be noticeable at 3 MeV where they amount to $\approx 10\%$,

* The differences, although small, are statistically significant. They are based on samples of 10000 histories, calculated twice with different cross sections, but using the same sequence of random numbers.

Fig. 1. Effect on the response function of the escape of bremsstrahlung and charged particles from the detector. Dashed curve was calculated with omission of these effects.

Fig. 2. Total absorption peak (P_0), single and double annihilation radiation escape peaks (P_1 and P_2) and iodine K-shell fluorescence escape peak (P_3). Dashed curves are calculated disregarding the escape of bremsstrahlung and secondary charged particles.

and then rapidly increase at higher energies. The correct values of P_1 and P_2 reach a peak at 5 MeV and rapidly decrease at higher energies, whereas the results from the simplified model continue to rise. The effects of charged-particle and bremsstrahlung escape are clearly important enough to justify the computational effort that goes into the calculation of electron transport.

7. Comparisons with previous high-energy calculations

Various approximations have been used in the past to calculate charged-particle and bremsstrahlung escape from sodium iodide detectors. Zerby and Moran³³) evaluated the spectrum of the bremsstrahlung emitted by an electron in the course of being slowed down to rest in an unbounded sodium iodide medium. They used the continuous-slowing-down approximation and assumed the radiative energy loss to be small compared to the collision energy loss. The Zerby-Moran spectrum was used in response-function calculations by Zerby and Moran³⁴), Miller and Snow²⁶), and Weitkamp³⁵).

Fig. 3. Experimental response function of Koch and Wyckoff (points), and corresponding Monte Carlo result (curve), for a beam of 15 MeV electrons incident on a $5'' \times 5''$ detector. The experimental beam spread was approximated in the calculation by assuming a uniform beam with a 2 cm diameter. Assumed resolution $r(0.661) = 12\%$.

Zerby and Moran neglected electron motion altogether. Miller and Snow assumed the electrons to travel in a straight line, through a distance equal to the electron range. Giannini et al.³⁰⁾ made two improvements: they used a more accurate bremsstrahlung spectrum, derived without the assumption that the radiative loss is relatively small; they improved the treatment of electron transport through use of a Monte Carlo model introduced by Wilson³⁶⁾ which assumes initial straight-line travel followed by terminal diffusion.

In the present calculation the electron paths were divided into many segments whose length was chosen so that the average energy decrease per segment was 5%. The energy loss sampled for each segment took into account energy-loss straggling. The change of electron energy and direction was traced from segment to segment. This provided the basis for an accurate estimate of electron escape from the detector, and for the accurate evaluation of the angular and energy distribution of the bremsstrahlung emitted in the detector.

The validity of the method used for the calculation

of electron and bremsstrahlung transport has been confirmed in various ways. Good agreement has been obtained in comparisons with the following experimental results: (a) the response of silicon detectors to electrons with energies up to 1 MeV³⁷⁾; (b) the backscattering of 1 MeV electrons from a large NaI detector, as measured by Titus³⁸⁾; (c) the emission of bremsstrahlung from a thick tungsten target as measured by O'Dell et al.^{16,39)}; (d) the response of a $5'' \times 5''$ NaI detector to 15 MeV electrons as measured by Koch and Wyckoff⁴⁰⁾, this comparison is shown in fig. 3.

Figs. 4a and b compare energy deposition spectra obtained by Miller and Snow²⁶⁾ at 8 MeV, and by Giannini et al.³⁰⁾ at 12 MeV, with our results. The low-energy part of our spectrum is considerably higher than that of Miller and Snow, and somewhat higher than that of Giannini. Comparisons of the total absorption peaks and first and second annihilation escape peaks are given in table 4. The Miller-Snow values for P_0 , P_1 and P_2 exceed ours by 38%, 37% and 81%, respectively. The Giannini values for P_0 and P_1 are about the same as ours, but their P_2 -value is 52% higher.

The Miller-Snow and Giannini results are based on Monte Carlo samples of 10000 gamma-rays with at least one interaction in the detector, and ours on a sample of 10000 incident gamma rays. The differences between the results from the different calculations are

several times larger than the statistical uncertainties, and are presumably due to the differences in the Monte Carlo models. The trend of the discrepancies is not unexpected. Inasmuch as the energy deposition spectra under discussion pertain to a broad parallel beam

Fig. 4. Energy deposition spectra from different calculations. Arrows indicate positions of the total absorption peak and of the single and double annihilation radiation escape peaks. Areas under these peaks are given in table 4. a) Comparison with Monte Carlo calculation of Miller and Snow⁽²⁶⁾. b) Comparison with Monte Carlo calculation of Giannini et al.⁽³⁰⁾.

TABLE 4
Comparison of various calculated results for the total absorption peak (P_0) and the single and double annihilation radiation escape peaks (P_1 and P_2). The data apply to broad parallel beams.

		P_0	P_1	P_2
Source energy 8 MeV 4" x 4" detector	Miller and Snow	0.192	(0.194)	(0.0491)
	This work	0.139	0.142	0.0270
Source energy 12 MeV 3" x 3" detector	Giannini et al.	0.0425	(0.0755)	(0.0402)
	This work	0.0414	0.0753	0.0276

Entries in parentheses were obtained by subtracting the continuum contribution from the tabulated $D(E_0, E)$ -histogram.

TABLE 5
Detector resolution $r(0.661)$, as defined by eq. (4), for various source-detector combinations for which experimental and calculated response functions are compared in figs. 5-7

Figure	Experimenter	$r(0.661)$ (percent)	Method of determination
5a,b	Heath ¹⁹⁾	8.3	Measured at 0.661 MeV
5c	Lazar ¹¹⁾	8.5	Measured at 0.479 MeV
6a	Metzger (priv. comm.)	7.3	Measured at 0.661 MeV
6b	Trombka et al. ¹²⁾	7.4	Measured at 0.661 MeV
6c	Jarczyk et al. ²⁷⁾	7.7	Through comparison of expt. and calc. response functions in fig. 6c
7	Kockum and Starfelt ⁴³⁾	11.5	Measured at 1.28 MeV

incident perpendicularly, the secondary electrons and bremsstrahlung would penetrate straight into the detector if it were not for multiple scattering. When the assumption of straight-line motion is replaced by a more realistic transport treatment, the chance of energy escape through the lateral surface of the detector is enhanced, and the absorption and escape peaks are lowered.

8. Comparisons with high-energy experiments

At energies above 3 MeV the experimental determination of NaI detector response functions becomes increasingly difficult because monoenergetic sources are lacking and background problems are usually severe. High-quality experimental data have been obtained in a limited number of cases; however, interpolation in these data with respect to incident gamma-ray energy is hardly feasible. It appears to be most advantageous to use the available experimental data to check the validity of calculational methods, and then to rely on systematic computations for the production of extensive response function libraries.

At high energies it is hard to determine the values of P_0 , P_1 and P_2 by measuring the areas under the peaks of the experimental response functions, because the

width of the Gaussian resolution function is not small compared to the separation of the peak energies. Comparisons with calculated results are therefore best made for the response function itself in the peak region.

Fig. 5. Response functions for detectors irradiated with gamma rays from point-isotropic sources. Points are experimental and curves are calculated. a) Comparison with an experimental response function obtained by Heath¹⁹⁾ with a radioactive ^{24}Na source at a distance of 10 cm from the detector. b) Comparison with an experimental response function obtained by Heath¹⁹⁾ with a radioactive ^{35}S source at a distance of 10 cm from the detector. c) Comparison with an experimental response function obtained by Lazar with a ^{210}Bi source at a distance of 9.3 cm from the detector. Dashed curve represents experimental data in region of very high background.

The values of the experimental detector resolution $r(0.661)$ used in the comparisons are listed in table 5. The calculated response functions are normalized to one incident gamma-ray photon, so that the area under each curve is equal to the detection efficiency. The experimental data are usually presented as relative number of counts versus channel number. We have renormalized them so as to obtain the best agreement with the calculated response function in the pulse-height region including the total absorption and first and second escape peaks.

Fig. 6. Response functions for detectors irradiated by broad parallel beams. Points are experimental and curves are calculated. a) Comparison with an experimental response function obtained by Metzger (private communication) with a ^{241}Am ^{14}C (α, γ) source. b) Comparison with an experimental response function obtained by Trombka with gamma rays from radiative capture of thermal neutrons in Ni. The calculation takes into account the following five most prominent lines of the gamma-ray spectrum: 8.999, 8.533, 7.819, 7.536 and 6.837 MeV, for which the numbers of photons/100 neutrons are, respectively: 41.65, 18.74, 9.04, 4.93, 11.91.

Fig. 7. Response functions for detectors irradiated by narrow beams. a) Comparison with an experimental response function (dashed curve) obtained by Jarzyck et al.²⁷⁾ with a $^{14}\text{N}(n, \gamma)$ source. b) Comparison with an experimental response function (points) obtained by Kockum and Starfelt¹³⁾ with a $^3\text{H}(p, \gamma)$ source.

Figs. 5a, b and c show comparisons with experimental results of Heath¹⁹⁾ and Lazar⁴¹⁾ for point-isotropic gamma-ray sources located on the detector axis. Figs. 6a and b show comparisons with results of Metzger (private communication) and Trombka et al.⁴²⁾ obtained with broad parallel beams.

Figs. 7a and b show comparisons with results obtained by Jarzcyk et al.²⁷⁾ and by Kockum and Starfelt⁴²⁾ with narrow beams. The various experiments cover incident gamma-ray energies between 3 MeV and 20 MeV.

The trends indicated by the various comparisons are rather similar. There is good agreement between calculated and experimental results in the upper third of the pulse-height distribution, a region which includes the total absorption peak and the first and second annihilation radiation escape peaks. At pulse heights below this region the experimental response functions typically exhibit a rise, often rather steep, to values that greatly exceed the theoretical values*. Kockum and Starfelt explained this rise in their data as due to background from neutron and gamma-ray contamination. Similarly, Jarzcyk et al. reported their response functions only in the region of large pulse heights, because of the strong background at lower pulse heights.

- * By contrast, there is good agreement between experiment and calculation for the electron response function measured by Koch and Wyckoff at 15 MeV, as shown in fig. 3. In this case, with an electron beam as radiation source, the background problem was minimal.

In the absence of techniques for eliminating such background it will remain necessary to rely on calculations for the lower two-thirds of the pulse-height distribution.

9. Response functions at 50 MeV

Response functions for incident gamma-ray energies above 20 MeV are of potential interest for a number of applications. It has been shown by Hofstadter and coworkers^{44,45)} that very large NaI crystals can be successfully used as total absorption spectrometers for electrons and photons in the energy range of 0.1 to 15 GeV. At more moderate energies, monoenergetic gamma-ray beams with energies of 30 to 40 MeV are coming into use⁴⁶⁾, in experimental arrangements that utilize the annihilation of positrons in flight. In gamma-ray astronomy the occurrence of gamma-ray fluxes with energies up to 50 MeV or higher has been reported⁴⁸⁻⁵⁰⁾. We have made a few exploratory calculations of response functions at 50 MeV, for detector sizes that appear to be readily available commercially. The results are shown in fig. 8.

10. Response function tabulations

The most commonly used NaI detector for single-crystal gamma-ray spectroscopy is the 3" x 3" detector. We now present data from which one can easily construct the response function for such a detector, for incident gamma-ray energies between 100 keV and 20 MeV. The results are for a broad parallel beam

Fig. 8. Calculated response functions for detectors irradiated with broad parallel beams of 50 MeV gamma rays. Assumed detector resolution is $r(0.661) = 7.5\%$.

TABLE 6
Calculated values of the total absorption peak, P_0 , single and double annihilation radiation escape peaks, P_1 and P_2 , and the iodine K-shell fluorescence radiation escape peak, P_3 . Results pertain to broad parallel beams incident perpendicularly on the endface of a $3'' \times 3''$ detector.

E_0 (MeV)	P_0	P_3	E_0 (MeV)	P_0	P_1	P_2
0.1	0.958	0.0382	1.2	0.425	0.00005	0.00007
0.15	0.963	0.0169	1.5	0.370	0.0056	0.0025
0.2	0.946	0.0101	2.0	0.304	0.0234	0.0099
0.3	0.875	0.0055	3.0	0.225	0.0643	0.0257
0.4	0.779	0.0038	4.0	0.178	0.0979	0.0366
0.5	0.697	0.0029	5.0	0.143	0.114	0.0425
0.6	0.627	0.0024	6.0	0.117	0.119	0.0446
0.8	0.534	0.0019	8.0	0.0793	0.112	0.0419
1.0	0.471	0.0016	10.0	0.0567	0.0951	0.0327
1.2	0.425	0.0014	12.0	0.0425	0.0720	0.0248
			15.0	0.0259	0.0444	0.0161
			20.0	0.0092	0.0198	0.0074

incident on the flat endface of a cylindrical detector. As will be discussed in section 11, $3'' \times 3''$ detectors are sufficiently symmetric so that the response function (divided by the detection efficiency), $R(E_0, h)/\eta(E_0)$, is rather independent of the directional distribution of the incident gamma-ray beam. The tabulated results can therefore be applied, at least approximately, to various other beam geometries of interest, for example the case of an isotropic gamma-ray flux that may be of interest in gamma-ray astronomy.

Monte Carlo calculations of the energy deposition spectrum $D(E_0, E)$ have been carried out for 20 values of E_0 between 100 keV and 20 MeV, in each case with a sample of 50000 incident gamma rays. The resulting values of the peak parameters P_0 , P_1 and P_2 (and the values of P_3 at energies up to 1.2 MeV) are given in table 6. The standard deviation of P_1 is

$$[P_1(1 - P_1)/50000]^{1/2}.$$

We have found it advantageous to express the continuous part of the energy deposition spectrum, $C(E_0, E)$, in terms of dimensionless functions C_j , ($j=1,2,3,4$) which depend on dimensionless energy-related variables x , y and z . The representation of the data has been arranged so as to minimize the explicit dependence on E_0 , and to facilitate interpolation with respect to E_0 and E .

For $E_0 \leq 1.2$ MeV, we set

$$C(E_0, E) = C_1(E_0, x)(1 + mc^2/2E_0)/E_0, \quad (5)$$

where

$$x = E(1 + mc^2/2E_0)/E_0. \quad (6)$$

For $E_0 > 1.2$ MeV, we set

$$C(E_0, E) = C_2(E_0, y)/(E_0 - 2mc^2), \quad (7a)$$

$$\text{for } 0 \leq E < E_0 - 2mc^2,$$

$$C(E_0, E) = C_3(E_0, z)/2mc^2, \quad (7b)$$

$$\text{for } E_0 - 2mc^2 \leq E < E_0 - mc^2,$$

$$C(E_0, E) = C_4(E_0, z)/2mc^2, \quad (7c)$$

$$\text{for } E_0 - mc^2 \leq E \leq E_0,$$

where

$$y = E/(E_0 - 2mc^2) \quad (8)$$

and

$$z = (E - E_0 + 2mc^2)/2mc^2. \quad (9)$$

The functions C_j are given in table 7. By comparing the results of different Monte Carlo runs, and by examining the dispersion of the data prior to smoothing, we arrived at the estimate that the statistical error (relative standard deviation) of most of the $C(E_0, E)$ -values is approximately 5, 8, 11 and 13% for $E_0 = 1.6, 12$ and 20 MeV, respectively. The estimated statistical accuracy of the response functions obtained with the use of the data in tables 6 and 7 is 3% or better in the peak region, and 5–15% in the continuum region.

We have developed a spline interpolation program, utilizing an algorithm given by Ahlberg et al.⁵¹, in order to construct the response function from the tabulated data. The program performs a simple interpolation with respect to E_0 in table 6, and a double interpolation, with respect to E_0 and x , y or z , on the data in table 7. Finally, the program convolutes the energy deposition spectrum with a Gaussian resolution function according to eq. (1). A family of response functions generated in this manner for $E_0 = 2, 3, 4, \dots, 20$ MeV is shown in fig. 9.

TABLE 7
Calculated values of the continuous part of the energy deposition spectrum, for broad parallel beams incident perpendicularly on the endface of a $3'' \times 3''$ detector.

E_0 (MeV)	0.10	0.15	0.20	0.30	0.40	0.50	0.60	0.80	1.00	1.20
x	$C_1(E_0, x)$									
0.00	0.00000	0.00000	0.00062	0.0403	0.128	0.200	0.255	0.323	0.359	0.373
0.05	0.00045	0.00615	0.0202	0.0835	0.176	0.252	0.304	0.359	0.390	0.411
0.10	0.00090	0.00870	0.0259	0.0940	0.191	0.270	0.320	0.372	0.401	0.421
0.20	0.00181	0.0105	0.0314	0.112	0.206	0.281	0.336	0.390	0.414	0.429
0.30	0.00142	0.00960	0.0310	0.114	0.213	0.291	0.348	0.410	0.435	0.446
0.40	0.00057	0.00790	0.0272	0.108	0.209	0.294	0.358	0.418	0.451	0.467
0.50	0.00069	0.00735	0.0260	0.0970	0.200	0.290	0.355	0.427	0.470	0.495
0.60	0.00220	0.00855	0.0226	0.0880	0.190	0.279	0.352	0.442	0.497	0.530
0.70	0.00975	0.0193	0.0350	0.0940	0.183	0.269	0.347	0.459	0.530	0.583
0.80	0.0168	0.0380	0.0502	0.120	0.201	0.280	0.357	0.496	0.597	0.677
0.90	0.0238	0.0505	0.0855	0.166	0.254	0.345	0.433	0.591	0.720	0.820
0.95	0.0280	0.0635	0.105	0.193	0.294	0.391	0.485	0.653	0.795	0.917
0.975	0.0310	0.0707	0.113	0.207	0.308	0.408	0.507	0.680	0.835	0.970
1.00	0.0115	0.0165	0.0230	0.0440	0.0880	0.177	0.266	0.435	0.523	0.597
1.10	0.00051	0.00183	0.00412	0.0118	0.0228	0.0299	0.0330	0.0303	0.0237	0.0164
1.20	0.00003	0.00075	0.00188	0.00315	0.00338	0.00288	0.00151	0.00001	0.00000	0.00000

E_0 (MeV)	1.2	1.5	2.0	3.0	4.0	5.0	6.0	8.0	10.0	12.0	15.0	20.0
y	$C_2(E_0, y)$											
0.00	0.0672	0.155	0.238	0.276	0.269	0.246	0.229	0.200	0.178	0.155	0.132	0.118
0.05	0.0715	0.163	0.240	0.276	0.271	0.247	0.231	0.213	0.204	0.199	0.194	0.197
0.10	0.0728	0.166	0.241	0.277	0.272	0.248	0.233	0.222	0.220	0.226	0.238	0.260
0.20	0.0735	0.167	0.242	0.278	0.275	0.252	0.243	0.243	0.251	0.265	0.297	0.326
0.30	0.0740	0.168	0.243	0.279	0.282	0.265	0.260	0.267	0.283	0.303	0.334	0.390
0.40	0.0744	0.169	0.245	0.289	0.300	0.290	0.286	0.300	0.323	0.351	0.400	0.490
0.50	0.0752	0.170	0.247	0.298	0.319	0.319	0.322	0.350	0.387	0.430	0.497	0.625
0.60	0.0757	0.171	0.257	0.317	0.348	0.364	0.377	0.416	0.473	0.535	0.634	0.810
0.70	0.0760	0.172	0.268	0.340	0.385	0.422	0.455	0.515	0.597	0.697	0.843	1.09
0.80	0.0767	0.173	0.279	0.378	0.431	0.492	0.556	0.692	0.830	0.975	1.18	1.51
0.90	0.0774	0.174	0.297	0.419	0.527	0.657	0.795	1.16	1.35	1.59	1.90	2.15
0.95	0.0777	0.175	0.303	0.438	0.590	0.780	1.00	1.47	1.94	2.29	2.57	2.54
0.975	0.0779	0.175	0.307	0.452	0.605	0.790	1.02	1.54	2.11	2.60	2.90	2.68
1.00	0.0780	0.175	0.309	0.466	0.614	0.785	1.00	1.47	1.94	2.18	2.19	1.90

E_0 (MeV)	1.2	1.5	2.0	3.0	4.0	5.0	6.0	8.0	10.0	12.0	15.0	20.0
z	$C_3(E_0, z)$											
0.00	0.450	0.373	0.347	0.350	0.388	0.430	0.451	0.439	0.402	0.351	0.261	0.128
0.10	0.460	0.399	0.363	0.370	0.396	0.430	0.451	0.439	0.391	0.339	0.253	0.138
0.20	0.478	0.424	0.388	0.381	0.397	0.412	0.427	0.417	0.374	0.325	0.247	0.124
0.30	0.501	0.464	0.423	0.388	0.376	0.375	0.376	0.356	0.309	0.260	0.189	0.0899
0.35	0.519	0.485	0.437	0.380	0.344	0.319	0.298	0.262	0.222	0.180	0.128	0.0690
0.40	0.542	0.502	0.455	0.378	0.320	0.276	0.241	0.192	0.157	0.127	0.0910	0.0496
0.45	0.574	0.521	0.461	0.370	0.305	0.259	0.223	0.171	0.134	0.107	0.0756	0.0406
0.50	0.603	0.542	0.467	0.368	0.304	0.258	0.222	0.168	0.129	0.0986	0.0675	0.0371

E_0 (MeV)	1.2	1.5	2.0	3.0	4.0	5.0	6.0	8.0	10.0	12.0	15.0	20.0
z	$C_4(E_0, z)$											
0.50	0.608	0.588	0.549	0.491	0.450	0.421	0.398	0.363	0.300	0.269	0.134	0.0715
0.60	0.700	0.662	0.611	0.536	0.478	0.432	0.393	0.332	0.268	0.204	0.129	0.0634
0.70	0.853	0.797	0.726	0.613	0.535	0.460	0.396	0.294	0.222	0.167	0.108	0.0521
0.75	0.976	0.904	0.751	0.562	0.450	0.374	0.318	0.239	0.187	0.147	0.0971	0.0414
0.80	0.434	0.385	0.327	0.259	0.217	0.187	0.164	0.129	0.103	0.0818	0.0514	0.0204
0.85	0.0996	0.0945	0.0876	0.0775	0.0695	0.0631	0.0575	0.0483	0.0383	0.0285	0.0169	0.0052
0.90	0.0100	0.0132	0.0153	0.0161	0.0152	0.0137	0.0122	0.0092	0.0068	0.0048	0.0025	0.0007
1.00	0.0001	0.0003	0.0005	0.0007	0.0007	0.0006	0.0005	0.0003	0.0002	0.0001	0.0001	0.0000

Fig. 9. Set of response functions constructed with use of the data given in tables 6 and 7. Assumed resolution $r(0.661) = 7.5\%$. Curves are normalized so that the area under each is equal to $45\eta(E_0)$. Results pertain to the case of a broad parallel beam incident on the flat endface of a $3'' \times 3''$ detector.

11. Other irradiation geometries

The irradiation geometry can be characterized in terms of the differential flux of gamma rays at the detector site, i.e. the number $n(\theta, \varphi)$ of gamma rays per unit solid angle that cross a unit area of surface perpendicular to the propagation vector $u = (\sin\theta \cos\varphi, \sin\theta \sin\varphi, \cos\theta)$. The angles θ and φ are spherical coordinates in a system whose polar axis coincides with the symmetry axis of the cylindrical detector.

One case of interest is the oblique broad parallel beam, characterized by a differential flux distribution

$$n(\theta, \varphi) = n_0 \delta(\cos\theta - \cos\theta_0) \delta(\varphi - \varphi_0), \quad (10)$$

where n_0 is a normalization constant and δ the delta function. The number of gamma rays entering the detector through one of the flat endfaces is $n_0 \pi R^2 \cos\theta_0$, that entering through the other endface is zero, and the number entering through the lateral surface is $n_0 2RL \sin\theta_0$, where R and L are the radius and length of the detector.

If the differential flux is isotropic, i.e. with a distribution

$$n(\theta, \varphi) = n_0/4\pi, \quad (11)$$

one finds, after integrating over all directions of incidence, that the number of gamma rays entering through each flat endface is $n_0 \pi R^2/4$, and the number entering through the lateral surface is $n_0 \pi RL/2$. Of course one might want to adjust these numbers in order to take into account that one flat endface is usually shielded, at least partially, by the photomultiplier tube, and that the lateral surface may be surrounded by other materials such as anti-coincidence shields.

Another case, which arose in the analysis by Trombka of lunar data from the Apollo 15 mission, is that of a detector with its flat endface pointing toward the surface of the moon. There is a thin layer of radioactive material on the lunar surface due to cosmic-ray bombardment. It is a good approximation to assume that the gamma ray flux from the lunar surface is isotropic over one hemisphere ($0 \leq \cos\theta \leq 1$). In this case, which we shall denote as that of a 2π -isotropic flux, the number of gamma rays entering through one of the endfaces is $n_0 \pi R^2/4$, that entering through the other endface is zero, and that entering through the lateral surface is $n_0 \pi RL/4$.

Taking into account the spherical shape of the lunar

TABLE 8

Detection efficiency $\eta(E_0)$ and peak parameters P_0 , P_1 and P_2 of the energy deposition spectrum, for broad parallel beams incident at an angle θ_0 with respect to the detector axis, and for the case of a 2π -isotropic flux. Numbers in parentheses indicate the estimated statistical uncertainty in the last significant figures.

E_0 (MeV)	θ_0	η	P_0	P_1	P_2
0.661	0°	0.877	0.597 (4)		
	60°	0.652	0.578 (7)		
	90°	0.781	0.592 (9)		
	2 π -iso.	0.681	0.569 (6)		
6.13	0°	0.622	0.114 (2)	0.119 (2)	0.0447 (12)
	60°	0.423	0.103 (3)	0.114 (3)	0.0482 (24)
	90°	0.522	0.105 (5)	0.115 (5)	0.0490 (31)
	2 π -iso.	0.447	0.106 (3)	0.115 (4)	0.0458 (23)
12.0	0°	0.656	0.0425 (11)	0.0720 (15)	0.0248 (9)
	2 π -iso.	0.476	0.0375 (20)	0.0642 (26)	0.0261 (17)

surface one can show that gamma rays arriving at the detector site must have obliquity cosines greater than $\cos\theta_{\min} = [1 - R_M^2/(R_M + H)^2]^{1/2}$, where R_M ($=1738$ km) is the radius of the moon and H is the height of the detector above the lunar surface. A typical height in the Apollo 15 experiment was $H=111$ km, corresponding to $\cos\theta_{\min}=0.341$. We note that for $H=0$ one has the limiting case of a 2π -isotropic flux as defined above, and for $H \rightarrow \infty$ the limiting case of a broad parallel beam incident perpendicularly. As discussed below, the shapes of the response functions in the two limiting cases are quite close to each other, so that one can dispense with Monte Carlo calculations for intermediate values of H .

We have explored the influence of the irradiation geometry on the response of $3'' \times 3''$ detectors at three energies (0.661, 6.13 and 12 MeV). Results of these calculations are given in table 8 for the following circumstances: broad parallel beams incident at angles of 0°, 60° or 90°, and the case of a 2π -isotropic flux as defined above. It can be seen that the peak parameters P_0 , P_1 and P_2 of the energy deposition spectrum are nearly independent of the beam geometry. The small observed differences are either within, or not far outside, the limits of the statistical error. When complete response functions are plotted one finds that their shape (but not their normalization) is almost the same in all the cases studied. The normalization factor, i.e. the detection efficiency $\eta(E_0)$, depends more strongly on the irradiation geometry, and can be determined rather simply, without recourse to elaborate Monte Carlo calculations. For convenience we give in table 9 a set of efficiency values for $3'' \times 3''$ detectors exposed to a

TABLE 9

Detection efficiency $\eta(E_0)$ for a $3'' \times 3''$ detector irradiated by a broad parallel beam incident perpendicularly on the endface ($\theta_0 = 0^\circ$), and for the case of a 2π -isotropic flux.

E_0 (MeV)	$\theta_0 = 0^\circ$	2 π -iso.
0.1	1.000	0.988
0.15	1.000	0.964
0.2	1.000	0.930
0.3	0.988	0.851
0.4	0.956	0.785
0.5	0.924	0.737
0.6	0.894	0.700
0.8	0.843	0.645
1.0	0.802	0.605
1.2	0.768	0.573
1.5	0.728	0.537
2.0	0.684	0.499
3.0	0.641	0.463
4.0	0.624	0.449
5.0	0.620	0.446
6.0	0.621	0.447
8.0	0.629	0.454
10.0	0.643	0.464
12.0	0.656	0.476
15.0	0.675	0.491
20.0	0.702	0.514

2π -isotropic flux [obtained with a computer program of Trombka¹⁾] and compare them with corresponding values for a broad parallel beam incident perpendicularly.

We would like to thank Dr. Trombka for encouragement, support and much helpful advice. We are also indebted to Drs. Ferguson and Metzger for putting unpublished data at our disposal, and to Mr. M. J. Silverstein for computational assistance.

References

- 1) J. I. Trombka and R. L. Schmadebeck, Nucl. Instr. and Meth. **62** (1968) 253.
- 2) J. I. Trombka and R. L. Schmadebeck, National Aeronautics and Space Adm. Report NASA SP-3044 (1968).
- 3) I. Adler and J. I. Trombka, *Geochemical exploration of the moon and planets* (Springer, Berlin, 1970).
- 4) J. H. Neiler and P. R. Bell, *Alpha-, beta- and gamma-ray spectroscopy*, vol. 1 (ed. K. Siegbahn; North-Holland Publ. Co., Amsterdam, 1968) p. 245.
- 5) R. van Lieshout, A. H. Wapstra, R. A. Ricci and R. K. Giergis, *Alpha-, beta- and gamma-ray spectroscopy*, vol. 1 (ed. K. Siegbahn; North-Holland Publ. Co., Amsterdam, 1968) p. 501.

- ⁶⁾ A. Schaarschmidt and H. J. Keller, Nucl. Instr. and Meth. **72** (1968) 82.
- ⁷⁾ I. Petr, A. Adams and J. B. Birks, Nucl. Instr. and Meth. **95** (1971) 253.
- ⁸⁾ J. I. Trombka, to be published in Nucl. Instr. and Meth.
- ⁹⁾ U. Fano, L. V. Spencer and M. J. Berger, *Handbuch der Physik*, vol. 38/2 (Springer, Berlin, 1959) p. 660.
- ¹⁰⁾ J. H. Hubbell, Nat. Bur. Std. Publ. NSRDS-NBS 29 (1969).
- ¹¹⁾ M. J. Berger, *Methods in computational physics*, vol. 1 (Academic Press, New York, 1963) p. 135.
- ¹²⁾ S. Goudsmit and J. L. Saunderson, Phys. Rev. **57** (1940) 24.
- ¹³⁾ L. Landau, J. Phys. USSR **8** (1944) 201.
- ¹⁴⁾ C. Møller, Ann. Physik **14** (1932) 568.
- ¹⁵⁾ H. Kolbenstvedt, J. Appl. Phys. **38** (1967) 4785.
- ¹⁶⁾ M. J. Berger and S. M. Seltzer, Phys. Rev. C **2** (1970) 621.
- ¹⁷⁾ M. J. Berger and S. M. Seltzer, National Aeronautics and Space Adm. Report NASA SP-3012 (1954).
- ¹⁸⁾ J. J. Steyn, M. A. Sc. Thesis (University of Toronto, 1951).
- ¹⁹⁾ R. L. Heath, U.S. AEC Publ. IDO-16889-1 & 2 (1964).
- ²⁰⁾ G. G. Kelley, P. R. Bell, R. C. Davis and N. H. Lazar, IRE Trans. Nucl. Sci. NS-3 (1956) 57.
- ²¹⁾ P. Axel, Brookhaven Nat. Lab. Publ. BNL 271 (1953).
- ²²⁾ M. P. Fioratti and S. R. Piermattei, Nucl. Instr. and Meth. **96** (1971) 605.
- ²³⁾ H. I. Israel, D. W. Lier and E. Storm, Nucl. Instr. and Meth. **91** (1971) 141.
- ²⁴⁾ G. W. Grodstein, Nat. Bur. Std. Circ. no. 583 (1957).
- ²⁵⁾ M. J. Berger and J. Doggett, Nat. Bur. Std. J. Res. **56** (1956) 355; Rev. Sci. Instr. **27** (1956) 269.
- ²⁶⁾ W. F. Miller and W. J. Snow, Rev. Sci. Instr. **31** (1960) 39; Argonne Nat. Lab. Report ANL-6318 (1961).
- ²⁷⁾ L. Jarczyk, H. Knoepfel, J. Lang, R. Müller and W. Wölfl, Nucl. Instr. and Meth. **17** (1962) 310.
- ²⁸⁾ C. T. Schmidt, IRE Trans. Nucl. Sci. NS-7 (1960) 25.
- ²⁹⁾ R. S. Foote and H. W. Koch, Rev. Sci. Instr. **25** (1954) 746.
- ³⁰⁾ M. Giannini, P. R. Oliva and M. C. Ramorino, Nucl. Instr. and Meth. **81** (1970) 104; Comitato Nazionale Energia Nucleare (Rome) Report RT/FI (69) 38 (1969); Comitato Nazionale Energia Nucleare (Rome) Report RT/FI (69) 15 (1969).
- ³¹⁾ E. Nardi, Nucl. Instr. and Meth. **83** (1970) 331.
- ³²⁾ J. J. Steyn, R. Huang and D. W. Harris, Trans. Am. Nucl. Soc. **14** (1971) 125.
- ³³⁾ C. D. Zerby and H. S. Moran, Oak Ridge Nat. Lab. Report ORNL 2454 (1958).
- ³⁴⁾ C. D. Zerby and H. S. Moran, Nucl. Instr. and Meth. **14** (1962) 115; Oak Ridge Nat. Lab. Report ORNL-3169 (1961).
- ³⁵⁾ C. Weitkamp, Nucl. Instr. and Meth. **23** (1963) 10.
- ³⁶⁾ R. R. Wilson, Phys. Rev. **79** (1950) 204; **84** (1951) 100.
- ³⁷⁾ M. J. Berger, S. M. Seltzer, S. E. Chappell, J. C. Humphreys and J. W. Motz, Nucl. Instr. and Meth. **69** (1969) 181.
- ³⁸⁾ F. Titus, Nucl. Instr. and Meth. **89** (1970) 93.
- ³⁹⁾ A. A. O'Dell, Jr., C. W. Sandifer, R. B. Knowlen and W. D. George, Nucl. Instr. and Meth. **61** (1958) 340.
- ⁴⁰⁾ H. W. Koch and J. M. Wyckoff, Nat. Bur. Std. J. Res. **56** (1956) 319.
- ⁴¹⁾ N. H. Lazar, IRE Trans. Nucl. Sci. NS-5 (1958) 138.
- ⁴²⁾ J. I. Trombka, E. Eller, G. A. Oswald, M. J. Berger and S. M. Seltzer, USAEC Report CONF-710402, vol. 3 (1971).
- ⁴³⁾ J. Kockum and N. Starfelt, Nucl. Instr. and Meth. **4** (1959) 171.
- ⁴⁴⁾ R. Hofstadter, E. B. Hughes, W. L. Lakin and I. Sick, Nature **221** (1969) 228.
- ⁴⁵⁾ E. B. Hughes, R. L. Ford, R. Hofstadter, L. H. O'Neill and J. N. Otis, IEEE Trans. Nucl. Sci. NS-17 (1970) 14.
- ⁴⁶⁾ R. A. Alvarez, B. L. Berman, R. R. Lasher, T. W. Phillips and S. C. Fultz, Phys. Rev. C **4** (1971) 1673.
- ⁴⁷⁾ H. Beil, R. Bergère and A. Veyssière, Nucl. Instr. and Meth. **67** (1969) 293.
- ⁴⁸⁾ G. W. Clark, G. P. Garmire and W. L. Kraushaar, Astrophys. J. Letters **153** (1968) L203.
- ⁴⁹⁾ D. A. Kniffen and C. E. Fichtel, Astrophys. J. Letters **161** (1970) L157.
- ⁵⁰⁾ F. W. Stecker, J. I. Vette and J. I. Trombka, Nature (Phys. Sci.) **231** (1971) 122.
- ⁵¹⁾ J. H. Ahlberg, E. N. Nilson and J. L. Walsh, *The theory of splines and their applications* (Academic Press, New York, 1967).