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GAUSS V
A COMPUTER PROGRAM FOR THE ANALYSIS
OF GAMMA-RAY SPECTRA FROM
Ge (Li) SPECTROMETERS

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ABSTRACT

A description is presented of the computer program GAUSS V which has been written to carry out the analysis of gamma-ray spectra from Ge(Li) spectrometers. This program includes routines to carry out a nonlinear least-squares fit of a Gaussian function to a peak and to compute gamma-ray intensities and energies. In the latter calculation, a correction for the nonlinearity of the system is included. The peaks in the spectrum to be analyzed can be identified either manually by the user or automatically by a peak location routine. Complete descriptions of the experimental and input options are given as well as the card formats.

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I. INTRODUCTION

For the last several years, lithium-drifted germanium detectors have been used for the measurement of gamma-ray spectra. As illustrated in Figure 1, these spectra consist of a series of narrow (typically less than 2 keV wide for gamma-ray energies below 1 MeV) peaks on a continuous background. These spectra are represented by a set of equally spaced data points obtained from a multichannel analog-to-digital converter (ADC). The GAUSS V computer program has been written to carry out the analysis of such gamma-ray spectra by fitting a Gaussian function to the data points in each peak. The Gaussian peak position can then be used to determine the gamma-ray energy, and the area can be used to obtain the gamma-ray intensity. These two computations require a knowledge of the nonlinearities of the spectrometer and of the detector efficiency.

This report constitutes a complete manual for the use of GAUSS V including a description of the mathematical methods used and of the various

Fig. 1. Typical gamma-ray spectrum from a Ge(Li) spectrometer for energy calibration obtained for sources of ^{139}Ce , $^{95\text{m}}\text{Tc}$, ^{192}Ir , ^{113}Sn , ^{137}Cs , ^{94}Nb , ^{95}Zr , ^{95}Nb , and ^{46}Sc . The energies of the gamma rays are given in keV.

input control functions. The mathematical procedures are summarized in Section II and the input variables are discussed in Section III. Examples of the commonly used input forms and samples of the output are given in Section IV. In Section V, some techniques for the measurement of intensities and precise gamma-ray energies are discussed. The appendices provide details on the computer programs involved in handling library tapes for spectral data and linearity and efficiency tables.

The first version of this program, GAUSS I, was used in the analysis of the photopeaks of gamma-ray spectra from NaI(Tl) detectors^[1,2] and has been described in detail.^[3] Another version,^[4] GAUSS III, was used successfully in the determination of precise gamma-ray energies from spectra from Ge(Li) spectrometers.^[5] GAUSS V has also been used for precise gamma-ray energy measurements.^[6] Since the features of this program that are of interest for NaI(Tl) spectrometers and non-Gaussian peaks are the same as those discussed in References 1,3, this report will be concerned exclusively with those feature of GAUSS V that are related to the analysis of gamma-ray spectra from Ge(Li) spectrometers.

GAUSS V is written in FORTRAN IV and is compiled on an IBM 360/75 computer. The program is dimensioned to fit up to five Gaussians in one set of data points, and to handle up to 300 peaks including up to 50 calibration lines per spectrum. For large problems (eg, more than 10 spectra each with more than 50 peaks), the program can locate, analyze and determine the energies and intensities of four to five peaks per second. To facilitate the handling of different kinds of problems, there are four different input forms which require different amounts of input information. For a typical spectrum with 100 peaks, this input can be as small as four cards, in which case the program locates the peaks and determines the parameters needed for each fit. For the same problem, the user can specify this information, which requires about 200 input cards. This program and its automatic peak location routine have been used to analyze over 2000 spectra, generally with 20 to 300 peaks.

II. MATHEMATICAL METHODS

The basic purpose of GAUSS V is to analyze a set of data points that make up a peak resulting from the interaction of a gamma-ray with a Ge(Li) detector. In the program, the peak is represented by a Gaussian function and the underlying spectral background by a linear function. The basic mathematical operation is the nonlinear least-squares fit by which the parameters of the Gaussian (ie, the height Y , width W , and position X) are determined. In addition to this fitting process, there are routines which carry out other operations. One is a peak location routine which identifies the peaks in a spectrum and for each peak (1) makes an initial estimate of the values of the Gaussian parameters, (2) determines the underlying spectral background, and (3) selects the range of data points to be used in the fit. If these operations are not done with this automatic routine, they must be done manually (ie, the user supplies the information as part of the program input). After all of the peak fits have been carried out the program computes the gamma-ray energies and intensities.

For reference in this discussion as well as the following sections, the sequence of the various computations is illustrated in the operational flow chart in Figure 2.

Before discussing the details of these mathematical operations, it may be instructive to describe one possible mode of use of the program. Let us assume that a complex spectrum (eg, over 200 peaks including several multiplets) is to be analyzed to obtain good intensities for all of the observed peaks. If the energies of several of the peaks are known, these can be used for the energy calibration. In the initial analysis the automatic peak location routine is used to determine the energies and intensities of most of the peaks. In these peak fits, the Gaussian parameters Y , W , and X are all allowed to vary. Typically three problems will occur in such an analysis. First, there will be wide variations in the computed peak widths. Next, some of the multiplets will be analyzed only as singlets. Third, due to the presence of neighboring peaks and Compton edges, some of the backgrounds may be incorrect. Two steps are generally necessary to solve all of these problems. First, the analysis of the weak peaks and the multiplets is improved by fixing the widths of these Gaussians at values determined from the strong, single peaks in the spectrum. Second, the changes in the backgrounds and the fits to the multiplets

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Fig. 2. Operational flowchart for GAUSS V.

require that the user supply the input parameters for these peaks manually. The second analysis carried out in this manner generally provides satisfactory answers for all of the peaks, although at times further modifications may be necessary.

The mathematical operations in GAUSS V are described in the following sections in the order of their use (ie, peak location, peak fits, and energy calculations). In this chapter no indication is given concerning the options available. These are discussed in the next two chapters.

1. PEAK LOCATION AND INITIAL PARAMETER ESTIMATES

1.1 Peak Location Method

For spectra from Ge(Li) detectors, the best gamma-ray energies and intensities are often obtained by manual (ie, visual) selection of the parameters for the peak fit. However, since these spectra often contain ≈ 100 peaks, manual selection of the peaks is not practical when large numbers of spectra are analyzed. Therefore, GAUSS V provides for automatic location of the peaks as well as manual identification.

Several methods of automatically locating peaks have been described in the literature.^[7] The method used here^[8] involves the computation of the correlation function of blocks of the experimental spectrum with a Gaussian function. The width of this Gaussian is chosen to approximate the width of the experimental peaks. After subtraction of a "background", the positive points in the correlation function represent possible peaks.

The general equation for this correlation process are given in Reference 8. Specifically, for the k^{th} point in the spectrum, the value C_k of the correlation function is computed over a range M of data points from channel $k - M/2$ to channel $k + M/2$. For this point, the "background" A_k is taken to be the average of the spectral counts y_i ; that is,

$$A_k = \frac{1}{M+1} \sum_{i=k-M/2}^{k+M/2} y_i \quad (1a)$$

The correlation function is then

$$C_k = \sum_{i=k-M/2}^{k+M/2} (y_i - A_k - \sqrt{A_k}) e^{-\left(\frac{x_i - x_k}{b}\right)^2} \quad (1b)$$

where b is the standard deviation associated with the search Gaussian and $WW = 2\sqrt{\ln 2} b$ is the associated full-width-at-half-maximum (FWHM). In

Fig. 3a. Corresponding portions of a gamma-ray spectrum and the associated correlation function from the peak location routine. These show the results for peaks of different widths and peak-to-background ratios and for a doublet.

Fig. 3b. Same as Figure 3a.

these equations the search window width M and the search Gaussian width WW are determined from an estimate (supplied in the input) of the widths $W(x)$ of the experimental peaks. Portions of several correlation functions are shown in Figure 3 along with the corresponding portions of the original spectra. These spectra illustrate the results for peaks of various widths, of various peak-to-background ratios, and for a doublet. Each group of consecutive positive points in the correlation function is considered to be a peak.

One criterion for judging the quality of a peak location method is its ability to find small peaks, while not identifying as peaks too many random fluctuations in the data.

For the routine used here, the sensitivity depends on the values of M (search

window width) and WW (search Gaussian width). These values are given by

$$WW = W(x) \cdot FF4 \quad (2a)$$

and

$$M = W(x) \cdot FF5 \cdot 2 \quad (2b)$$

so the sensitivity can be varied by changing $FF4$ and $FF5$. (In many cases the computer program notation is used for variables so that the relationship with the input options will be clear.) As examples of this dependence, Column 3 of Table 1 gives the number of peaks found for a particular spectrum for various values of $FF4$ and $FF5$. It is clear that the number of peaks identified by this routine increases as $FF4$ decreases, and as $FF5$ increases. A careful visual study of this spectrum indicates the presence of about 80 peaks. Therefore, with the values $FF4 = FF5 = 1.0$, all of the peaks obtained are all real, but some weak peaks are missed. When wishing to identify all of the peaks, we have used $FF4 = 0.7$ and $FF5 = 1.5$. This

TABLE 1

Number of peaks found by peak search routine and number for which Gaussian fit converged for various values of the search parameters FF4 and FF5. These results include those peaks for which there is only one positive point in the correlation function.

<u>FF4</u>	<u>FF5</u>	<u>Number of Peaks</u>		<u>Survival Fraction</u>
		<u>from Search</u>	<u>out of Peak Fit</u>	
0.5	1.0	273	151	0.55
0.7	0.7	82	68	0.83
	1.0	122	89	0.73
	1.5	141	100	0.71
1.0	1.0	63	59	0.94
	1.5	79	72	0.91
	2.0	94	82	0.87
1.5	1.0	50	48	0.96
	2.0	63	62	0.98
2.0	2.0	--	51	--
	3.0	--	59	--

is illustrated in Figure 3b where the doublet structure is identified only for these parameter values. In this case, in Table 1 about 40% of the peaks found are spurious. (Many of the control variables, such as FF4 and FF5, have values stored in GAUSS. These values can be changed when desired by entering the new value as input. The stored values for FF4 and FF5 are 1.0.)

There is a third input variable that can be used to control the sensitivity of the search routine. In "normal" operation, the program requires that at least two consecutive points in the correlation function be positive before these points indicate a peak. The sensitivity for small peaks can be increased by also accepting a "peak" when only one positive point occurs in the correlation function. (The results in Table 1 were obtained for an analysis including the "one-point" peaks.)

Independent of these three sensitivity control variables, the peak fitting routine itself provides some control on the number of peaks for which energies and intensities are obtained. The peak fitting routine described in Section 2.1 does not force the iteration process by which the

Gaussian parameters are determined to converge. In certain cases where the "peak" found by the search routine is, in fact, not a peak, the iteration process diverges and no solution is obtained. Although in some respects this divergence may be considered undesirable, it does provide a way of discarding some of the spurious peaks indicated by the search routine. For the example in Table 1, the number of peaks for which the peak fitting routine converged is given in Column 4, and the fraction that converged is listed in Column 5. These data show that as the number of peaks identified in the search increases, the fraction rejected by the Gaussian fitting routine increases much more rapidly. As a result, there is some waste of computer time when one wishes to be sure of obtaining all of the peaks.

1.2 Peak Fit Parameters

After the approximate locations have been found for the peaks in a spectrum, the next operation is to set up the parameters that are needed for the Gaussian peak fits. These parameters include (1) the range of data points to be used in the fit, (2) the spectral background under the peak, and (3) the initial values of the Gaussian parameters (ie, height Y , width W , and position X). All of these parameters are illustrated in Figure 4. The description of the methods used in the automatic location

Fig. 4. Illustration of the parameters of a Gaussian function and the other parameters involved in a peak analysis.

routine to determine these parameters is followed by those for the manual identification of the peaks.

The initial estimate of the center of the Gaussian X is taken to be the centroid of those data points for which the correlated function has consecutive positive values. The initial estimate of the peak width W is taken from a linear function $W(x)$ supplied by the user. The estimate of the height of the peak Y is taken from the count in the channel nearest to X after subtraction of the spectral background.

The spectral background is represented by a line of zero slope. The magnitude of this background is taken to be the minimum value of the average count in three consecutive channels between X and $X + FF3 \cdot W(x)$. The stored value of $FF3$ is 5.0. If the general slope of the spectrum is negative, the procedure of going out $5 \cdot W(x)$ from the peak center will usually provide a background which is low. This problem can be overcome by the use of a smaller value (eg, 1.5) of $FF3$. The advantage of the larger value is that it allows one to go past a nearby peak to obtain the background value.

The method of selecting the range of data to be used in the peak fit is based on extensive experience in making this choice manually (ie, visually). In any case of conflict (proven or postulated) between obtaining the best possible energies and the best possible intensities, it has been our desire to use a channel selection method that provides the most accurate energy measurements. The method that has been empirically evolved is to use those data points above $Y/2$ on the low-energy side of the peak, and to include one or two channels of a lower count on the high-energy side of the peak (see Figure 4). In the program the first, FC , and the last, LC , channels in the fitting region are given by

$$FC = X - W(x) \cdot FF1 \quad (3a)$$

$$LC = X + 0.5 \cdot W(x) + 1.5 \quad (3b)$$

where the stored value of $FF1 = 0.5$ and FC and LC are truncated to integers. The program then checks the relative height of the points at FC and LC . If the later is higher (ie, $y_{LC} > y_{FC}$) then, LC is increased by one channel (ie, $LC = LC + 1$). To assure that for very narrow peaks there are sufficient points on the low-energy side of a peak, the program also computes

$$FC' = X - FF2. \quad (3c)$$

The stored value of FF2 is 1.5. The program then uses the smaller of FC and FC' as the first channel in the fitting range.

In certain circumstances the peak location routine will identify both members of a doublet. In those cases where two peaks are found with their centers separated by less than $2 \cdot W(x)$ the two peaks are analyzed as singlets as discussed above and also as a doublet. The parameters for the doublet fit are the same as those for the two singlet fits, except the background is taken from the second peak, FC is from the first peak, and LC from the second.

If the peak location routine is not used in an analysis, the initial Gaussian fit parameters must be provided by the user. In the "short" input form, the user must specify the fitting limits FC and LC for each peak to be analyzed as well as the value of the background (and the slope if it is nonzero). In this case the program determines Y as the maximum difference between the experimental count and the background for those data points from FC to LC. The estimate of X is equal to the channel number where this maximum occurs. And the estimate of W again comes from the input function $W(x)$. This input form is especially useful for those cases in which the background or channel range selected by the search routine is not satisfactory.

For the "medium" input form the user must also supply the value of X. This form is used regularly for barely resolved multiplets that are not identified as such by the peak location routine.

2. ANALYSIS OF PEAKS

2.1 Nonlinear Least-Squares Fitting

A least-squares fit is used to determine the values of the variable parameters p_j that minimize the sum of the squares of the deviations of a set of experimental data points y_i from the estimates $\bar{y}_i(p_j)$ for any functional form; that is,

$$R^2 = \sum_{i=1}^n w_i [y_i - \bar{y}_i(p_j)]^2 \quad (4)$$

is minimized, where the w_i are the weights associated with the y_i . The summation is over the n points chosen to be used in the fit.

In the case of the Gaussian function, which is of interest here, $\bar{y}$ is a nonlinear function of the parameters p_j . Thus, in this case, it is necessary to linearize $\bar{y}$ by expanding it in a Taylor series and truncating the series after the first derivatives. Given initial estimates p_j^0 of the parameters, if $p_j = p_j^0 + \delta p_j$, then

$$\bar{y}_i(p_j) \approx \bar{y}_i(p_j^0) + \sum_j \left(\frac{d\bar{y}}{dp_j} \right)_0 \delta p_j \quad (5)$$

For this truncated series, the conditions for R^2 to be a minimum, as a function of the δp_j , are that the set of equations

$$\frac{dR^2}{d(\delta p_j)} = 0 \quad (6)$$

all hold simultaneously. The solution of this set of linear equations gives the values δp_j . Since the higher order derivatives have been neglected in Equation (5), this process does not yield the true minimum of Equation (4). Therefore, Equations (5) and (6) are evaluated and solved again with the p_j^0 replaced by $(p_j^0 + \delta p_j)$. This process is continued until all the δp_j approach zero (ie, are less than some predetermined convergence criteria).

For a complete and rigorous discussion of this method, the reader is referred to Moore and Zeigler^[9] and the references therein.

In GAUSS V, this procedure is used to fit the peaks in a gamma-ray spectrum from a Ge(Li) detector. Here the data points from channel FC to LC are fitted with the function

$$\bar{y}_i = \bar{z}_i + \sum_{j=1}^J \bar{y}_{ij} \quad (7a)$$

Here the spectral background $\bar{z}_i$ is represented by the linear function

$$\bar{z}_i = A + B(x_i - FC) \quad (7b)$$

and the j^{th} component is represented by the Gaussian

$$\bar{y}_{ij} = Y_j e^{-\left(\frac{x_i - X_j}{W_j / 2\sqrt{\ln 2}}\right)^2} \quad (7c)$$

The parameters to be determined in a fit are Y_j , X_j and W_j (see Figure 4). The parameters A and B of the background can also be determined if desired. As many as five Gaussian components can be fitted to one set of data points. (Since the data points are equally spaced, x_i is defined so that it can have only integer values.)

For a fit of a single Gaussian to a set of points, with the background parameters fixed, Equation (6) reduces to a system of 3 simultaneous linear equations in 3 unknowns. The solution of such a set of equations can be indicated conveniently by writing the equations in matrix notation. If M is a symmetric matrix and $\vec{\Delta p}$ and $\vec{V}$ are column vectors, Equation (6) can be written

$$M \cdot \vec{\Delta p} = \vec{V} \quad (8)$$

where for a single Gaussian with parameters Y, W, and X (see Equation (7c))

$$\vec{\Delta p} = (\delta p_1, \delta p_2, \delta p_3) = (\delta Y, \delta X, \delta W) \quad (9a)$$

$$\vec{V} = \left(\sum_i w(y-\bar{y}) \frac{d\bar{y}}{dY}, \sum_i w(y-\bar{y}) \frac{d\bar{y}}{dX}, \sum_i w(y-\bar{y}) \frac{d\bar{y}}{dW} \right) \quad (9b)$$

$$M_{jk} = \sum_i w \frac{d\bar{y}}{dp_j} \frac{d\bar{y}}{dp_k} \quad (9c)$$

(In Equations (9b) and (9c) the index i has been suppressed on w_i , y_i , and $\bar{y}_i$ for simplicity. The generalization of Equation (9) to include more variable parameters is straight forward.)

The solution of Equation (8) is then

$$\Delta p = (M)^{-1} \cdot V \quad (10)$$

As noted above these equations are solved successively with updated estimates of p_j^0 until the parameters converge; that is, $\delta p_j \rightarrow 0$. The parameter values then represent the best Gaussian fit and the matrix M^{-1} contains information about the errors in the parameters.

The convergence criteria stored in the program are such that the iteration process will stop when for each value of j

$$\delta Y_j < 1 \text{ count,}$$

$$\delta X_j < 0.001 \text{ channels, and}$$

$$\delta W_j < 0.001 \text{ channels.}$$

Even if these criteria are not met, the process stops after 10 iterations. (These four values can be modified by placing the new values in the input.) At all points in the iteration process, each parameter is constrained between two limits such that $p_j^l \leq p_j \leq p_j^u$. The values of p^l and p^u in the program are

$$Y^l = 1, \quad Y^u = 10^9$$

$$W^l = 0.1, \quad W^u = 10^2$$

$$X^l = 1, \quad X^u = 10^4.$$

Very rarely, it may be necessary to modify these values in order to obtain a satisfactory analysis of a particular peak. (See Reference 3 for a discussion of the methods used to limit the parameters.)

2.2 Quality of Peak Fits and Errors in the Parameters

The quality of the Gaussian fit to the experimental data defining each peak can be evaluated quantitatively by means of the quantity

$\epsilon^2 = R^2_{\min} / (n-m)$; where $R^2_{\min}$ is the final and smallest value of R^2 from Equation (4), n is the number of points in the fit, and m is the number of variable parameters p_j . It can be shown by statistical arguments [9] that if (a) $\bar{y}(p_j)$ is a linear function of the p_j , (b) the experimental points are actually represented by a function of the form $\bar{y}(p_j)$, and (c) $w_i^{-1/2}$ is a good estimate of the standard deviation of y_i , the values of $R^2_{\min}$ for a large number of identical measurements will have a chi-squared distribution with $(n-m)$ degrees of freedom. Under these assumptions, ϵ^2 will then have a value of about 1.0.

In the case of the analysis of gamma-ray spectra from Ge(Li) spectrometers, there are several reasons for the $R^2_{\min}$ values to deviate from a chi-squared distribution. First, the $\bar{y}(p_j)$ is not a linear function of the parameters. Second, it is common to estimate the error in the count y_i by $\sqrt{y_i}$. However, for very small counts this is not a good estimate due to the statistical variations, and for very large counts it is not a good estimate because of contributions from systematic errors (eg, variations in channel widths in the ADC). Therefore, conditions (a) and (c) above are not met. But most important, the experimental peak shapes are not exactly Gaussian in shape so condition (b) is violated. This deviation from a Gaussian generally consists of two parts: first, "tailing" occurs in the detector and increases the values of y_i on the low-energy side of the peak; and second, a step-like increase in the "background" occurs as one goes from the high-energy to the low-energy side of the peak. Since with a good Ge(Li) detector these deviations from the Gaussian shape will only be detectable (ie, be greater than the statistical fluctuations in the points) for strong peaks, the value of ϵ^2 is expected to increase as the intensity of the peak increases. Another contribution to ϵ^2 occurs if the background line is fixed (which is usually done). Any error in the background will cause an increase in ϵ^2 over its ideal value.

From statistical arguments it can be shown [9] that the estimated variance (ie, the square of the standard deviation σ_j) in the final value of the parameter p_j is given by

$$\text{var } p_j = \sigma_j^2 = \epsilon^2 \cdot (M^{-1})_{jj} \quad (11a)$$

where $(M^{-1})_{jj}$ is the diagonal element of the inverse matrix in

Equation (10). (If $\epsilon^2 < 1.0$ the program uses $\sigma_j^2 = (M^{-1})_{jj}$ instead of the smaller value.) When functions of the Gaussian parameters (such as the peak area) are calculated, the covariance terms must be taken into account. These terms are given by

$$\text{covar } (p_j, p_k) = \epsilon^2 \cdot (M^{-1})_{jk} . \quad (11b)$$

2.3 Modifications of Basic Fitting Method

Any of the parameters that are involved in the Gaussian fitting function or in the background line can be held fixed at their initial values. (This is usually done for the background.) This process is often used for the peak widths in the fitting of weak peaks and for the components of a multiplet.

The program also has available a method of requiring in the fitting process that the value of W be equal to $W(X)$ for the current value of X . (That is, as X changes in the iteration process, the value of W is re-computed.) Since Ge(Li) peaks are very narrow and the initial position estimates are quite accurate, this option has no advantage over fixing the widths at the initial value. Therefore, this option is not used. (See Reference 3 for a description of the methods used to carry out these options.)

3. GAMMA-RAY ENERGIES AND INTENSITIES

Generally the experimenter is interested in the energies and intensities of the gamma-rays which are observed as peaks in a spectrum. In addition to the peak parameters determined from the Gaussian peak fits, these two quantities each involve an auxiliary function that is associated with a particular detector or spectrometer system. For the calculation of intensities, an auxiliary function is necessary to describe the efficiency of the detector as a function of the gamma-ray energy. For the computation of gamma-ray energies it is necessary to describe the correction for the deviation of the spectrometer from a linear relation between the gamma-ray energy and the channel number x . This correction is given as a function of x . In Section 3.1, a description of the method used to store and evaluate these two auxiliary functions is given. In the

succeeding sections, the methods of computing the gamma-ray energies and intensities are described.

3.1 Linearity and Efficiency Tables

The nonlinearity correction and the detector efficiency are represented by functions given in tabular form. Many such tables are available and the user instructs the computer to choose the two tables that are appropriate for the spectrometer system used. The program used to store the tables on either magnetic tape or disc is described in Appendix A.

Each table is composed of one or more sections with the functional values within any one section given for equal increments of the independent variable (ie, E or x). Closely spaced points are used where the function is varying rapidly. Thus, one has the simplicity of interpolation from a table with equally spaced points without requiring an excessive amount of space for the tables.

Interpolation of a value from a table is done in the following manner. Suppose there are NS sections in an efficiency table. For section K, there are NTB(K) points starting at energy E(K) with an energy increment DE(K) between the points. E(NS+1) is the last energy at which an efficiency can be computed. An efficiency can be computed for any energy between E(1) + DE(1) and E(NS+1). For all energies outside of this range, the gamma-ray intensity is set to 0.0. For any other gamma-ray energy EG, the program determines which section of the table is to be used; that is, the Kth section is used if

$$[E(K) + DE(K)] \leq EG < [E(K+1) + DE(K+1)] \quad (12)$$

Within this section, the method of interpolation of the efficiency for the energy EG is by fitting the nearest three table values with a quadratic function and evaluating the quadratic. The first of the three nearest points is given by the index

$$NT = \sum_{J=1}^{K-1} NTB(J) + NTT$$

where

$$NTT = \frac{EG - E(K)}{DE(K)} + 0.5 .$$

Then the efficiency EF is given by

$$EF = A + B \cdot Z + C \cdot Z^2$$

where

$$Z = \frac{EG - E(K)}{DE(K)}$$

$$A = TBE(NT)$$

$$B = -0.5 \cdot TBE(NT+2) + 2.0 \cdot TBE(NT+1) - 1.5 \cdot TBE(NT)$$

$$C = 0.5 \cdot TBE(NT+2) - TBE(NT+1) + 0.5 \cdot TBE(NT)$$

and the TBE(J) are the entries in the table.

In preparing the table, one must be sure that the increments DE(K) are small enough that the quadratic fit to three points will give a sufficiently accurate interpolation. Also, the E(1) and DE(1) values must be such that no efficiencies below E(1) + DE(1) will be needed.

3.2 Intensity Calculations

The intensity of a gamma-ray transition is given simply by the ratio of the peak area to the detector efficiency for that transition energy. In this program the peak area is taken to be the area AR of the Gaussian function; that is,

$$AR = \sqrt{\frac{\pi}{4 \ln 2}} W \cdot Y \quad (13a)$$

The variance of the area value is then, for a fit to a single Gaussian,

$$\text{var } AR = \epsilon^2 \left(\frac{\pi}{4 \ln 2} \right) (Y^2 \cdot (M^{-1})_{33} + W^2 \cdot (M^{-1})_{11} + 2 \cdot Y \cdot W \cdot (M^{-1})_{13}) \quad (13b)$$

where the $(M^{-1})_{jk}$ are the matrix elements from Equation (10).

As discussed in Section 3.1, the efficiency is determined by interpolation from a table for the specific energy of this transition. The program also allows the user to provide an estimated uncertainty in the efficiency EF in the form of a constant fractional error, F. This is commonly 5% in our case; that is, $F = 0.05$. The intensity is then

$$I = AR/EF \quad (14a)$$

with the estimated error of

$$\sigma(I) = \left[(\text{var } AR)/EF^2 + (AR \cdot F/EF)^2 \right]^{1/2} \quad (14b)$$

The program also provides a set of relative gamma-ray intensities and uncertainties. With no input, the normalization is such that the largest intensity is set equal to 100. Other normalizations can be obtained by specifying the intensity of a particular peak to which the other intensities are to be normalized.

3.3 Gamma-Ray Energy Calculations

In order to compute the gamma-ray energies for the observed peaks in a particular spectrum, the program needs (a) the positions X_j of the peaks, (b) a table of the nonlinearity corrections for the spectrometer system used, and (c) information to allow the determination of the energy calibration. The latter information can be given either (1) by the energies of a set of calibration lines, or (2) by specifying the parameters of the $E(x)$ expression.

In the first and more common method, the known energies are provided for a set of peaks in the spectrum. From these calibration energies E_k and the associated peak positions X_k , the program computes the values of the parameters in the following manner.

- (1) The peak positions X_k of the calibration lines are corrected for the nonlinearity $L(x)$, so $X_k'' = X_k + L(X_k)$.
- (2) An unweighted, linear least-squares fit is carried out to the points E_k, X_k'' to determine the parameters a' and b' in the expression $E_k' = a' + b' \cdot X_k''$.
- (3) The "zero" correction is taken to be $\Delta = a'/b'$.
- (4) The nonlinearity corrections are recomputed for the peak positions

$$X_k' = X_k - \Delta + L(X_k - \Delta). \quad (15a)$$

(Steps 3 and 4 are necessary in order to make the method of evaluating the nonlinearity correction correspond to the method used to measure it.)

- (5) The peak positions X_k' and the energies E_k are used in weighted and unweighted least-squares fits to determine the values of

a, b, and c where

$$\bar{E}_k = a + b \cdot X_k' + c \cdot (X_k')^2 \quad (15b)$$

and c can be computed or set to zero (ie, a quadratic or linear function is used).

The computation of the parameters in Equation (15b) is carried out in the following manner. If E_k and $\sigma(E_k)$ are the energies and uncertainties of the calibration lines, the a, b, and c are determined such that they minimize the function

$$\phi = \sum_k w_k [E_k - \bar{E}(X_k')]^2 \quad (16a)$$

The function $\bar{E}$ is defined as in Equation (15b). The weights can be $w_k = 1$ (unweighted fit) or they can be functions of the $\sigma(E_k)$. Since there are errors $\sigma(X_k)$ in the peak positions X_k' as well as in the calibration energies it would be most proper to take these errors into account in the minimization by means of a bivariate fitting process. However, for simplicity a more qualitative method has been used. This error is taken into account by setting

$$1/w_k = \sigma(E_k)^2 + b'^2 \cdot \sigma(X_k')^2 \quad (16b)$$

The value of b' is taken from the same preliminary fit (item (2) above) used to determine the "zero" correction Δ . For either set of weights, ϕ is minimized by the same method as illustrated in Equations (4), (8), (9), and (10). The variances in the resulting parameter values are obtained in the manner analogous to Equation (11).

From the values of a, b, and c, the energies of all of the observed peaks can be obtained from Equation (15b). An estimate of the uncertainty in the computed energy is obtained from the expression

$$\sigma(E) = [\sigma_1^2 + \sigma_2^2]^{1/2} \quad (17a)$$

where σ_1 gives the contribution from the error in the peak location and σ_2 gives that from the uncertainties in a, b, and c. Here

$$\sigma_1 = (b + 2 \cdot c \cdot X') \cdot \sigma(X) \quad (17b)$$

and

$$\begin{aligned}\sigma_2^2 = & \text{var } a + (X')^2 \cdot \text{var } b + (X')^4 \cdot \text{var } c + 2 \cdot X' \cdot \text{covar}(a,b) \\ & + 2 \cdot (X')^2 \cdot \text{covar}(a,c) + 2 \cdot (X')^3 \cdot \text{covar}(b,c) .\end{aligned}\tag{17c}$$

In this computation, the nonlinearity correction $L(x)$ is assumed to be exact.

The second method of obtaining the gamma-ray energies is used if the parameters in Equation (15) are known to the accuracy desired. These parameters are then supplied in the input, and Equation (15) is used to determine the energies of all of the peaks. Since the errors in the parameters a , b , and c are not available when this option is used, Equation (17a) reduces to

$$\sigma(E) = \sigma_1 = (b + 2 \cdot c \cdot X') \cdot \sigma(X) .$$

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III. PROGRAM INPUT AND CONTROL OPTIONS

There are many control options in GAUSS V that the user may at times wish to exercise. These options are described in this section including a general description of the input deck and the card formats for each type of data (Section 1), a complete list of the input variables and their allowed values (Section 2), and a description of the input variables needed for each of the four input forms (Section 3).

GAUSS V operates on an IBM 360/75 computer and is dimensioned for the following data arrays:

- 4096 data points per spectrum,
- 50 energy calibration lines per spectrum, and
- 300 peaks per spectrum.

The execution region for the program is approximately 235K bytes. The program is written in FORTRAN IV and requires only one special system routine, DATE(D). This routine, which supplies the date, can be easily replaced.

1. INPUT DECK FORM AND CARD FORMATS

1.1 General Form of Input Deck

For each spectrum the GAUSS V input deck must consist of the following five or six groups of cards. The description of the data on these cards and the formats are given below.

- (1) Alphanumeric title card.
- (2) One or more fixed-point control information cards (the last card of this group must have a 1 in Column 3).
- (3) One or more floating-point control information cards (the last card of this group must have a 1 in Column 3).
- (4) Spectral data cards unless the spectral data are stored on an accessible magnetic tape library.
- (5a) Calibration energy table cards - when the peak location routine is used.
- (5b) Cards of type (2) and (3) for each peak to be fitted - when the peak location routine is not used.
- (6) A transfer card to mark the end of the analysis for the spectrum.

1.2 Card Formats

The formats for the various types of cards described in Section 1.1 are as follows.

- (1) Alphanumeric title card - format (8A8,A2,I8,A6)

This single card may contain any descriptive information in Columns 1-66. This information is used to identify the output. As noted below, Columns 67-80 contain the identification used to find the desired spectral data on a magnetic tape library.

- (2) and (3) Fixed-point and floating-point control cards

The fixed-point and floating-point control cards have the formats I2,I1,I3,I4I5 and I2,I1,I3,7E10.3, respectively, where

Columns

1-2	NPD	Number of items of control information on card.
3	NOC	0 (or blank), normal 1, this is the last fixed-point or floating-point information card
4-6	NAD	Address of the first item on the card (Tables 2 and 3 give lists of the addresses)
11-80		1 to 14 fixed-point words with I5 format or 1 to 7 floating-point words with E10.3 format. These numbers can be entered in F format whenever the field width allows.

The addresses of the control information must be consecutive starting with NAD and ending with NAD + NPD - 1. The options involved for the variables with the various addresses are discussed in Section 2 and are summarized in Tables 2 and 3.

- (4) Spectral data cards - I2,10I7,8X

If the spectral data are entered on cards, the format is as follows:

Columns

1-2	NOCARD	Card number (not used in program, but cannot be "-1")
-----	--------	---

Columns

3-72 YDATA Data in counts per channel, 10 channels per card. The first entry on the first card is called channel zero and is not stored.

The end of data is signalled by a "-1" card ("-1" in Columns 1-2). Alternatively, the spectral data may be on a magnetic tape library. The program to store the data on these libraries is described in Appendix B. The information in the last 14 columns of the "title" card is used to find the desired spectrum.

(5a) Calibration energy table cards - 10X,3E10.3

These cards contain the energy calibration information only if the peak location routine is used.

The cards must be entered in order of ascending energy. The maximum number of cards is 50.

Columns

11-20	Approximate channel (within 5 channels) location of calibration peak
21-30	Calibration energy (keV)
31-40	Uncertainty in energy (keV)

The last card in this group must be a "-1" card.

(5b) Fixed-point and floating-point control cards

These cards, which are present when the peak location routine is not used, have the same format and the same information as those described in (2) and (3) above. The various options and variables are discussed in Section 2.

(6) Transfer card - (A2)

The transfer card indicates the end of the deck associated with a spectrum and initiates the energy-intensity calculations and/or the summary output listing

Columns

1-2	The characters TR
-----	-------------------

2. LIST OF INPUT CONTROL VARIABLES AND OPTIONS

The list of fixed-point control variables that can be modified in the input of the program is given in Table 2. Most of these have values assigned in the program, so that values are included in the input only when they need to be changed. It is a general feature of GAUSS that the value of a variable remains the same until it is changed. Therefore, one must be sure that if a variable is given a special value for a particular peak fit, or a particular spectrum, that it is returned to its normal value for the next fit, or spectrum in that same computer run.

The format of the cards on which the values of the variables are entered is given in Section 1.2. At least one card of fixed-point control information is needed for each problem; and if the peak location routine is not used, one such card is needed for each peak fit. Since the fixed-point variable values are read in an I5 format, they must be right-adjusted.

For completeness the fixed-and floating-point variables associated with the parameters α_1 and α_2 are included in Table 2 although they are not discussed in the text. These are the parameters used to fit slightly non-Gaussian peaks.

The floating-point control variables are listed in Table 3. Many of these variables also have stored values, so that values are read in only when they need to be changed.

3. INPUT FORMS AND OPTIONS

In order to allow flexibility and ease of operation, four different input options are available. These options are controlled by the fixed-point variable KPUT (Address 5). As noted in Section II, 1.2, the user may supply the initial parameters for the Gaussian function and the background, or these values will be generated by routines in the program. Similarly, the parameter limits and convergence criteria may be entered in the input or the values stored in the program can be used.

In the following four sections, the specific cards and variables required for each input form are noted. Examples of these input forms for particular cases are illustrated in Section IV, 1.

TABLE 2
FIXED-POINT CONTROL INFORMATION

Address Cols. 4-6	Mnemonic Name	Stored Value	Application
1	ISTART	---	First channel in fit, $1 \leq \text{ISTART}$
2	IEND	---	Last channel in fit, $\text{ISTART} < \text{IEND} < 4096$
3	IGAUSS	---	Number of Gaussians to be fitted, $1 \leq \text{IGAUSS} \leq 5$
4	ITPUT	---	Source of spectrum input, 0, Card input 1, Library tape
5	KPUT	---	Control data input form, 0, Mini input form (automatic peak location option) 1, Short input form 2, Medium input form 3, Long form
6	KONST	---	Parameter which determines the set of coefficients to be used to compute the functional forms of α_1 , α_2 , and/or w_0 . The polynomial coefficients stored in the program are for the following cases: <u>KONST</u> 0 No relations needed 3 $w_0 = 1.5$ channels, $\alpha_1 = \alpha_2 = 0$ 4 $w_0 = 3.0$ channels, $\alpha_1 = \alpha_2 = 0$ 5 $w_0 = 8.0$ channels, $\alpha_1 = \alpha_2 = 0$ 6 $w_0 = \alpha + \beta x$ with α and β supplied as input.
7	IECAL	---	Parameter which indicates the type of energy computations required. It is of the form WX, where W Weighting option 0, Weighted fit 1, Unweighted fit 2, Both weighted and unweighted X Type of fit 0, Linear 1, Linear and parabolic
8	IYC	---	Identifies the analyzer linearity correction table to be used. If IYC is zero, no energy-intensity calculations will be made. If IYC is 3, no linearity correction is made.
9	IXC	---	Identifies the efficiency table to be used. If IXC is zero, no intensities are computed.
10	ILINE(1)	1	Line slope control option 0, No line used 1, Line slope is held constant 2, Vary line slope
11	ILINE(2)	1	Line intercept control option 0, No line used 1, Line intercept is held constant 2, Vary line intercept

FIXED-POINT CONTROL INFORMATION (cont'd)

Address Cols. 4-6	Mnemonic Name	Stored Value	Application
12	IPARIN(1,1)	2	Gaussian parameter control option y_0 of first Gaussian x_0 of first Gaussian w_0 of first Gaussian α_1 of first Gaussian α_2 of first Gaussian
13	IPARIN(1,2)	2	
14	IPARIN(1,3)	2	
15	IPARIN(1,4)	1	
16	IPARIN(1,5)	1	
17-21	IPARIN(2,1)		Same as above for second Gaussian
22-36	- - -		Control constants for Gaussians 3-5
37	M1ALF	4	Power of α_1 term (even, >0)
38	M2ALF	12	Power of α_2 term (even, >0)
39	IOUTPT	3	Parameter which determines the amount of output 1, Medium form 2, Diagnostic form 3, Short form
40	IWEIT	2	IWEIT determines the type of weighting to be used 1, $w_i = 1.0$ 2, $w_i = 1/y_i$ 4, $w_i = 1/y_i$ if $y_{\min} \leq y_i \leq y_{\max}$ $w_i = 1/y_{\min}$ if $y_i < y_{\min}$ $w_i = y_i/y_{\max}$ if $y_{\max} < y_i$
41	NOIT	10	Maximum number of iterations
42	ITEST	1	Number of after convergence iterations
43	ICON1	1	Lambda value is set to 1.0
44	NPPS	0	Indicates criteria for peaks in peak search option 0, Keep all peaks containing two or more points 1, Keep all peaks detected, including 1 point peaks
45	--	--	Not assigned
46	IPUN	0	Indicates whether punched card output is needed 0, No card output 1, Card output from energy-intensity calculations (see next item) 2, Card output from peak location routine
47	IOUTC	0	Indicates E(x) fit for which cards are punched (needed if IPUN > 1). 0, Set to 5 1, Weighted-linear 2, Weighted-quadratic 3, Unweighted-linear 4, Unweighted-quadratic 5, All of the above
48-80	--	--	Not assigned

TABLE 3

FLOATING-POINT CONTROL INFORMATION

Address Cols. 4-6	Mnemonic Name	Stored Value	Application
1	YMAX		Maximum y_1 value. This is required for weighting option 4 (IWEIT=4).
2	YMIN		Minimum y_1 value. This is required for weighting option 4 (IWEIT=4).
3	HCONT		Not assigned.
4	XLIN(1,1)		Line slope -- initial value upper limit lower limit convergence criterion
5	XLIN(1,2)		
6	XLIN(1,3)		
7	XLIN(1,4)		
8	XLIN(2,1)		Line intercept -- initial value (at channel ISTART) upper limit lower limit convergence criterion
9	XLIN(2,2)		
10	XLIN(2,3)		
11	XLIN(2,4)		
12	PARIN(1,1,1)		First Gaussian -- initial estimate of y_0 upper limit of y_0 lower limit of y_0 convergence criterion
13	PARIN(1,1,2)	10^9	
14	PARIN(1,1,3)	1	
15	PARIN(1,1,4)	1	
16	PARIN(1,2,1)		First Gaussian -- initial estimate of x_0 upper limit of x_0 lower limit of x_0 convergence criterion
17	PARIN(1,2,2)	10^4	
18	PARIN(1,2,3)	1	
19	PARIN(1,2,4)	10^{-3}	
20	PARIN(1,3,1)		First Gaussian -- initial estimate of w_0 upper limit of w_0 lower limit of w_0 convergence criterion
21	PARIN(1,3,2)	10^2	
22	PARIN(1,3,3)	10^{-1}	
23	PARIN(1,3,4)	10^{-3}	
24	PARIN(1,4,1)		First Gaussian -- initial estimate of α_1 upper limit of α_1 lower limit of α_1 convergence criterion
25	PARIN(1,4,2)	10^{-1}	
26	PARIN(1,4,3)	0.0	
27	PARIN(1,4,4)	10^{-10}	
28	PARIN(1,5,1)		First Gaussian -- initial estimate of α_2 upper limit of α_2 lower limit of α_2 convergence criterion
29	PARIN(1,5,2)	10^{-1}	
30	PARIN(1,5,3)	0.0	
31	PARIN(1,5,4)	10^{-19}	
32-51			Same as (12-31) for second Gaussian
52-111			Gaussian parameter information for Gaussian 3-5
112	D(1)	0.0	Coefficients for determining peak energies when no calibration lines are used. $E = D(1) + D(2) \cdot x + D(3) \cdot x^2$
113	D(2)	0.0	
114	D(3)	0.0	
115	DLX	0.0	Zero shift which must be supplied when using the previous option.
116-119			Not assigned

FLOATING POINT CONTROL INFORMATION (cont'd)

Address Cols. 4-6	Mnemonic Name	Stored Value	Application
120	ENGWT(1,1)		Energy value of calibration peak -- first Gaussian
121	ENGWT(1,2)		Uncertainty in energy value of calibration peak -- first Gaussian
122-129			Same as above for Gaussians 2-5
130	XWC1		Coefficients for determining w_0 . These are required input when KONST=6 $w_0 = XWC1 + x_0 \cdot XWC2$
131	XWC2		
132	TNOR		TNOR and ENOR are used in the normalized intensity calculations. Unless otherwise instructed the normalization is such that the largest intensity is 100. The user can have the results normalized to a given intensity (TNOR) for a peak of a given energy (ENOR).
133	ENOR		
134	FF1	0.5	FF1 and FF2 are constants which are used in determining the first channel of a peak detected by the peak search option.
135	FF2	1.5	
136	FF3	5.0	FF3 is a constant used in determining the background of the peak detected by the peak search option.
137	FF4	1.0	FF4 is a constant used to determine the width of the search Gaussian in the peak location routine.
138	FF5	1.0	FF5 is a constant used to determine the width of the search window in the peak location routine.
139-149	---		Not assigned
150	SCALE	10^{-5}	Scaling factor for matrix.

3.1 Mini Input and Peak Location Routine

This option (KPUT=0) is used when it is desired to have the peak location routine find the peaks in the spectrum. Under this option, the program generates all of the peak and line parameters and fitting limits. This option cannot be mixed with any of the other input forms ($KPUT \geq 1$).

The general form of the card deck for this case is given in Section III, 1.1. The fixed-point control information must contain values for the variables with Addresses 5 - 9 if one wishes the program to compute gamma-ray energies and intensities. If the intensities are not desired, the variable with Address 9 can be omitted; and if the energies and intensities are not needed, the variables No. 7 - 9 may be omitted, leaving only 5 and 6 to be entered. Other fixed-point variables may be modified by entering the new value as desired.

For a few cases, no floating-point information is needed, but even in this case a card of this type must be present.

For this input form, there are two methods of providing the energy calibration information. If the calibration is known with sufficient accuracy, the parameters a , b , c , and Δ in Equation (15) can be supplied (floating-point variables No. 112 - 115). However, in this case these parameters are assumed to be exact, so the computed uncertainties in the energies (Equation (17)) include only the contribution from the error in the peak position. The alternative, which is generally used, is to supply a table containing the energies and uncertainties for the calibration lines along with the approximate positions (to within 5 channels) of these peaks. (The format for this table is given in Section III, 1.2). The peak location routine then associates this energy with the first peak (ie, the one with the smallest channel number) within the 5 channel range. This table is concluded with a "-1" card, which is followed by a "TR" card. This completes the card deck for this input form.

3.2 Short Input Form

This input option (KPUT=1) is generally used when either the peak location routine does not give satisfactory results (eg, peaks on Compton edges, unresolved doublets, or for more precise intensity determinations), or only a few of the peaks in a spectrum need to be analyzed. For the fit to the first peak, the deck includes a title card, one or more fixed-point cards, and one or more floating-point cards (and the spectral data

if it is on cards). For each subsequent peak fit, one needs one or more fixed-point cards and one or more floating-point cards. The deck ends with the "TR" card.

For the first peak in the analysis, values must be given for the first nine fixed-point variables (except variables No. 7 - 9 can be omitted if no energies and intensities are desired). This is generally all of the fixed-point information needed on the first fit. On the subsequent fits, one usually enters only the values for the first two fixed-point variables (ie, the channel range used in the peak fit). Except for the energy calibration information which is discussed below, the only floating-point information that is normally needed is the intercept of the line which represents the spectral background (floating-point variable No. 8). In those cases where a sloping background is needed, the slope is also entered (floating-point variable No. 4). When a sloping background is used, two precautions must be taken. First, on the next peak fit the slope must be set back to zero (or else the nonzero value will be used on all subsequent fits). Second, the intercept A of the background line (Equation (7b)) is for the first channel FC in the particular peak fit (and not at channel zero).

For this input form, there are two methods of carrying out the energy calculations. First, as in the mini input, the calibration parameters a, b, c, and Δ in Equation (15) can be entered in the input. See comments in 3.1 about the resulting uncertainties. In the second method, a calibration energy and its uncertainty are entered (variables No. 120 and 121) along with the fitting limits and background value for each calibration peak. If the user does not wish to use weighted fits in the calculation of the calibration parameters in Equation (15), the uncertainties in the calibration energies are not needed.

3.3 Medium Input Form

This input (KPUT=2) is used primarily for multiplets. The input cards in this case are the same as in the short form, except that one must also supply an estimate of the positions of the components of the peak (variable No. 16 for the first component, No. 36 for the second, etc). This input form allows the user to provide good estimates of the initial positions when the components of a multiplet are not resolved. The energy computations are carried out in the same manner as in the short input form.

Peak fits using the medium input form can be carried out in the same analysis as fits using the short form (and the long form which follows). In order to change form, one need only enter the correct values for the fixed-point variables No. 3 and 5 which indicates the number of components in the fit and the input form.

3.4 Long Input Form

There are a few cases in which the convergence criteria or the parameter limits (see Section II, 2.1) stored in the program are unsatisfactory. An example would be a case where the parameters of the weaker component of a doublet will not converge to reasonable values, unless they are strongly constrained. In these cases the long input form (KPUT=3) can be used. Here all of the convergence criteria and parameter limits as well as the initial values must be supplied in the input. The energy calibration information can be entered in the same manner as in the short input form. This input form can be mixed with the above short and medium forms as long as the fixed-point variable No. 5 is properly entered.

4. COMPUTER SYSTEM REQUIREMENTS

The program makes use of the following files which can be located either on disc or tape.

File

2	Contains output from the peak location routine which is then used as input to the computational part of the program.
4	Contains the summary of the iterative output which is edited and listed at the end of a problem.
5	Standard input unit.
6	Standard output unit.
7	Standard punch file.
8	Standard library data tape. Required only when spectra are stored on tape.
9	Linearity - efficiency tables.

On the NRTS computer, these files are handled in the following manner. With the exception of file No. 8, all of these files are controlled within the program. For file No. 8, if the spectral data are on a magnetic tape library, the user must supply the library name and the tape number on a JOB Control Language (JCL) card. This card and the two JOB cards (which identify the user, the charge number, the limit on the computer time, etc) are the only system control cards needed at the front of the card deck. After the last problem, the system requires a /* card to terminate the job.

5. OUTPUT INFORMATION AND FORMS

GAUSS V provides several variations in the output to meet special needs. The printed output is controlled by the variable IOUTPT (fixed-point address No. 39). Certain information can also be punched on cards and this is controlled by fixed-point variables No. 46 and 47.

The printed output occurs in the following order. (Examples of the various portions of this output are given in figures in Section IV, 2.)

(a) Peak location routine

If the peak location routine is used (KPUT=0), the first portion of the output consists of the channel range to be used in each peak fit and the associated spectral background intensities. This output is printed in the same format as that of the short form input. At times this facilitates the use of the short form input for subsequent analyses of the spectrum.

(b) Iterations of parameters

If the medium or diagnostic output forms are requested (IOUTPT=1 or 2), the next portion of the printed output is a listing of the complete spectrum. Then, for each peak fit, the Gaussian and line parameters are given after each iteration. After convergence of the iteration process, the final parameters are listed along with a channel-by-channel comparison of the experimental data points and the Gaussian function.

(c) Summary of the final parameters

After all of the peak fits have been carried out, for all output forms a summary output list gives for each peak the

final Gaussian and line parameters and their uncertainties, the range of channels used in the fit, the quality of the fit, (ie, ϵ^2), and the peak area and its error.

(d) Energy and intensity results

If the user specifies a nonlinearity correction table, the next part of the output includes the energies of the observed peaks. If an efficiency table is also specified, the gamma-ray intensities are also printed. The program input allows the user to specify different combinations of weighting and functional form for the energy calibration function (ie, $E(x)$); these are,

weighted, linear
weighted, linear and quadratic
unweighted, linear
unweighted, linear and quadratic
all four.

For each of these possibilities, the first section consists of the energy calibration fit. This includes the identification of the linearity and efficiency tables used, the coefficients of the $E(x)$ function, and a comparison of the input and computed energies of the calibration lines. The second section for each case consists of the energies and intensities of each peak (in order of increasing energy).

(e) Diagnostic output

In addition to all of the above output, the diagnostic form lists the matrix M and its inverse M^{-1} (see Equations (8), (9), and (10)) for each iteration for each peak.

Provisions have been made in GAUSS V for punching two types of information on cards. The first is the energy and intensity information which can then be used as input to other analysis programs. These cards give the energy calibration function $E(x)$ and the results for each peak. The cards are punched if IPUN=1 (Address No. 46). The variable IOUTC (Address No. 47) controls which of the possible $E(x)$ functions are used (ie, weighted, linear, etc). These cards are punched in the following format.

<u>Card No.</u>	<u>Contents</u>
1	Title information
2	Calibration line coefficients
3	Variances
4	Covariances
≥5	Energy information cards which contain: Corrected channel number and its error Energy value and error Area and error.

If intensity calculations were made an additional set of cards are generated containing

Intensity and error

Normalized intensity and error.

The second set of cards that can be generated consist of the short input form cards. These can be used, with the necessary modifications, as input to the program to carry out the same analysis with the short input form. This option is used when it is known that a large number of the peaks in the spectrum will have to be reanalyzed with modified fitting limits or backgrounds. These cards are punched if the variable IPUN=2.

IV. EXAMPLES OF INPUT AND OUTPUT

1. INPUT FORMS

As can be observed from Section III, the complete input to GAUSS V can be very complex. However, in most cases the actual input is quite simple since most of the variables have stored values that are used. As discussed in Section III, 1.1, the input forms require at least the following: (1) a title card, (2) a card of fixed-point control information, (3) a floating-point control information card, and (4) a "TR" card. For some cases the complete input deck may consist of only four cards, while in others it may include two or more cards per peak.

Samples of the shortest and the most used input forms are given in the following sections, starting with examples that use the peak location routine. In all of these cases, the parameters of the line representing the spectral background (ie, A and B in Equation (7b)) are fixed at their initial values. The three parameters of each Gaussian (ie, X, Y, and W in Equation (7c)) are allowed to vary in the fitting process, except for one case in which the peak widths are fixed at their initial values.

1.1 Mini Input and Peak Location Routine

For simplicity a special keypunch form is generally used for the mini input. This form is shown in Figure 5. If one accepts the control variables as they are stored in the program, the only item that must be supplied to make the peak location routine operate is an estimate of the peak width (FWHM). This width can be a constant or a linear function of the channel number. If one wishes to obtain energies for the resulting peaks, the energy calibration information must be supplied in some form. If the calibration function $E(x)$ (see Equation (15)) is known it can be supplied directly. A sample of this minimum input is given in Figure 6 where the peak widths are taken to be 3 channels and the energy is $E = -0.065335 + 0.45632 (X' + 18.764) - 1.736 \times 10^{-8} (X' + 18.764)^2$.

An example of the most commonly used input form is given in Figure 7. Here the peak width is given as a linear function of the channel number ($W = 3.3 + 0.0006 \cdot x$). From the energies, their uncertainties, and the approximate peak positions (within 5 channels) of the calibration lines given in the table, the program determines the energy calibration curve $E(x)$.

GAUSS 5 MINI INPUT
TITLE CARD

LIBRARY ID

0000000000	1111111111	2222222222	3333333333	4444444444	5555555555	6666666666	7777777777	8888888888	9999999999
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

S	P	WX	L	E
1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1

FFS FFS

a	b	c	Δ
1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1

a β

x	E	σ
1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1

W = a + βX; Width For GAUSS & SEARCH

E = a + bx + cx² Δ = x' + Δ For Use If Gain Is Known
(set W=1 in 2nd Card)

Calibration Table

Put in Ascending Order

σ = Error in E Only

Put -1 Card at The End of Set

S - Spectrum
0 - Card
1 - Library

P - Peak Width
3 W = 1.5
4 W = 3
5 W = 6
6 W = a+βX

W - E vs x Weighting
0 - Weighted
1 - Unweighted
2 - Both

X - E vs x Fit
0 - Linear
1 - Quadratic & Linear

L - Linearity Table

E - Efficiency Table

Fig. 5. Special key punch form used for the mini input to GAUSS V.

GAUSS 5 MINI INPUT
TITLE CARD

LIBRARY ID

0000000000	1111111111	2222222222	3333333333	4444444444	5555555555	6666666666	7777777777	8888888888	9999999999
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

S	P	WX	L	E
1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1

a b c Δ

a	b	c	Δ
1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1	1,1,1,1,1,1,1,1,1,1

E = a + bx + cx² Δ = x' + Δ For Use If Gain Is Known
(set W=1 in 2nd Card)

Fig. 6. Sample of the minimum input to GAUSS V. In this case the energy calibration function is known and the peak location routine is used to find the peaks.

GAUSS 5 MINI INPUT

TITLE CARD

LIBRARY ID

SAMPLE, F, O, R, U, S, U, A, L, P, A, R, A, M, E, T, E, R, S, -, 3, 4, 5, 6, 7, 8, 9, 0										PEAKS, -, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0										SAME, DATA, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0										

S, P, W, X, L, E									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

a, b									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

X, E, σ									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

W = a + bX; Width For GAUSS B SEARCH

Calibration Table									
Put in Ascending Order									
σ = Error in E Only									
Put -1 Card at The End of Set									

Fig. 7. Example of the most commonly used input for use of the peak location program. The peaks widths are approximated by a linear function and the calibration lines are indicated in the table.

GAUSS 5 MINI INPUT

TITLE CARD

LIBRARY ID

SAMPLE, F, O, R, U, S, U, A, L, P, A, R, A, M, E, T, E, R, S, -, 3, 4, 5, 6, 7, 8, 9, 0										PEAKS, -, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0										SAME, DATA, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0	1 2 3 4 5 6 7 8 9 0										

S, P, W, X, L, E									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

FF4, FF5									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

a, b									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

W = a + bX; Width For GAUSS B SEARCH

X, E, σ									
0 0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1 1	2 2 2 2 2 2 2 2 2 2	3 3 3 3 3 3 3 3 3 3	4 4 4 4 4 4 4 4 4 4	5 5 5 5 5 5 5 5 5 5	6 6 6 6 6 6 6 6 6 6	7 7 7 7 7 7 7 7 7 7	8 8 8 8 8 8 8 8 8 8	9 9 9 9 9 9 9 9 9 9

Calibration Table

Put in Ascending Order

σ = Error in E Only

Put -1 Card at The End of Set

Fig. 8. An example of the mini input form showing the variations used to maximize the sensitivity of the peak search and with a sample of the deck giving the spectral data.

The sensitivity of the peak location routine is altered by means of the variables FF4 and FF5 which are included in the input example in Figure 8. These variables are related to the search Gaussian width and the search window as indicated in Equation (2). In this sample the peak location sensitivity is increased by carrying out fits for cases where there is only one positive point in the correlation function (ie, variable No. 44 is set to 1). A portion of the card deck which contains the spectral data is also given.

1.2 Short and Medium Input Forms

If in a particular case, the peak location routine cannot be used, the short and medium input forms are usually satisfactory. The keypunch form used in this case is shown in Figure 9. In the short form, the input includes for each peak the range of channels to be used and the spectral background. For each calibration peak, the gamma-ray energy and its uncertainty are also provided. For the medium input, the user provides, in addition, an estimate of the location of each peak. The short and medium input forms can be mixed in the same problem, although neither can be mixed with the mini input. Samples of these forms are given in Figure 10.

The most common reason for using the short form is that the peak location routine does not find a background that is satisfactory. This may occur when the background is sloping rather steeply, as on a Compton edge, or when there is a nearby peak. By use of this input form, the user can supply the desired background and especially its slope.

The principal use of the medium input is to analyze multiplets. In many cases the search routine will not identify a peak as having two components; or it does not obtain good enough initial estimates of the peak parameters to provide a convergent peak fit. With this input the user can provide more correct initial parameter values.

For the analysis of weak peaks, it is often desirable to fix the widths of the peaks. In this case the first step is to carry out the peak fits with variable widths (or a careful analysis of the peak widths is carried out by hand). From the widths of the strong, single peaks, the variation of the width with channel number is determined and entered into the subsequent analysis. (See floating-point variables No. 130 and 131 in Figure 7.) The peak widths are fixed at their initial values.

GAUSS V

SHORT & MEDIUM INPUT FORMS

ALPHANUMERIC TITLE CARD

<div style="display: flex; justify-content: space-between;"> 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 </div>																																																											
																																								<div style="display: flex; justify-content: space-between;"> 11A6 1B, A6 - Library Identification </div>																			
																																								<div style="display: flex; justify-content: space-between;"> 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 </div>																			

First Channel	Last Channel < 4096	# of Gaussians SS	Spectral Data 0. Cards 1. Library	Input Form 0. Mini 1. Short 2. Medium	Width 3. W ₀ = 1.5 4. W ₀ = 3 5. W ₀ = 8 6. Read α, β	IECAL (see below) W X	Linearity Table	Efficiency Table
9 1	1		1					

First Short - Form Fit

2	1	2	0
2	1	3	0
1	1	8	

Energy & Uncertainty
α & β of W₀ = α + β x₀
Line Intercept (at 1st channel)

For IECAL

Eva X₀ Fit
W = 0 Weighted
= 1 Unweighted
= 2 Both
X = 0 E = a + bx
= 1 E = a + bx and E = a + bx + cx²

Short-Form Calibration Fit

2	1	2	0
2	1	3	0
1	1	8	

First & Last Channel
Energy & Uncertain
Line Intercept

Short-Form Fit

2	1	2	0
2	1	3	0
1	1	8	

First & Last Channel
Line Intercept

Medium-Form Fit

5	1	1	
1	1	8	
1	1	6	
1	1	3	6

Line Intercept
1st Peak Channel
2nd Peak Channel

Triplets

5	1	1	
1	1	8	
1	1	6	
1	1	3	6
1	1	5	6
2	1	1	
1	1	8	
1	1	6	
1	1	3	6
1	1	5	6

Fig. 9. Special key punch form for short and medium input forms for GAUSS V.

GAUSS V

SHORT & MEDIUM INPUT FORMS

ALPHANUMERIC TITLE CARD

S A M P L E O F S H O R T F O R M P L U S O N E D O U B L E T - S A M E D A T A																																																											
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60

Library Identification									
4 4 4 4 2 5 5									
61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80									

First Channel	Last Channel < 4096	# of Gaussians ≤ 5	Spectral Data 0. Cords 1. Library	Input Form 0. Mini 1. Short 2. Medium	Width 3. W ₀ = 1.5 4. W ₀ = 3 5. W ₀ = 8 6. Read α, β	IECAL (see below) W X	Linearity Table	Efficiency Table
9 1	6 2 8	6 3 3	1	1	6	2 1	1 8	1 3

First Short - Form Fit

2 1 2 0	2 7 9	1 8 8	0 0 6
12 1 3 0	3	3	0 0 6
1 1 8	4 8 3 0 0		

Energy & Uncertainty
 $\alpha \pm \beta$ of $W_0 = \alpha + \beta x_0$
 Line Intercept (at 1st channel)

For IECAL

Evs X_0 Fit

W = 0 Weighted
 = 1 Unweighted
 = 2 Both

X = 0 $E = a + bx$
 = 1 $E = a + bx$ and $E = a + bx + cx^2$

Short-Form Calibration Fit

2 1 1	1 0 6 3	1 0 6 9
2 1 2 0	4 7 7	5 9 3
1 1 8	2 8 2 0 0	

2 1 1	1 4 6 6	1 4 7 2
2 1 2 0	6 6 1	6 4 6
1 1 8	2 3 0 0 0	

2 1 1	1 8 4 6	1 8 5 2
2 1 2 0	8 3 4	8 2 3
1 1 8	1 4 5 0 0	

Short-Form Fit

2 1 1	6 7 1	6 7 6
1 1 8	4 5 5 0 0	
2 1 1	1 3 3 7	1 3 4 3
1 1 8	2 4 8 0 0	
2 1 1	1 6 9 3	1 6 9 9
1 1 8	1 5 6 0 0	
2 1 1	2 2 1 2	2 2 1 8
1 1 8	7 9 0 0	
2 1 1	2 4 6 0	2 4 6 6
1 1 8	1 6 3 0	
2 1 1	2 7 1 4	2 7 2 0
1 1 8	5 4 0	
2 1 1		
1 1 8		
2 1 1		
1 1 8		
2 1 1		
1 1 8		

Medium-Form Fit

5 1 1	2	1	2
1 1 8	1 1 9 0 0		
1 1 6	2 1 2 8		
1 1 3 6	2 1 3 7		

Line Intercept
 1st Peak Channel
 2nd Peak Channel

Doublets

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35

Fig. 10. Samples of short and medium inputs to GAUSS V.

GAUSS V

SHORT & MEDIUM INPUT FORMS

ALPHANUMERIC TITLE CARD

SAMPLE OF SHORT FORM WITH FIXED WIDTHS & SLOPING BACKGROUND																																																											
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60

IIA6 - Library Identification									
D									
61	62	63	64	65	66	67	68	69	70
71	72	73	74	75	76	77	78	79	80

	First Channel	Last Channel <4096	# of Gaussians ≤5	Spectral Data 0. Cords 1. Library	Input Form 0. Mini 1. Short 2. Medium	Width 3. $W_0 = 1.5$ 4. $W_0 = 3$ 5. $W_0 = 8$ 6. $W_0 = \alpha, \beta$	IECAL (see below) W X	Linearity Table	Efficiency Table
First Short - Form Fit	9 0 1	6 2 8	6 3 3						
	1 1 4								
	1 1 9								
	2 1 2 0	2 7 9	1 8 8	0 0 6					
	2 1 3 0	3 3		0 0 0 6					
1 1 8	4 8 3 0 0								
				Line Intercept (at 1st channel)					
Short-Form Calibration Fit	2 1 1	1 0 6 3	1 0 6 9						
	2 1 2 0	4 7 7	5 9 3	0 1 2					
	1 1 8	2 8 2 0 0							
	2 1 1	1 4 6 6	1 4 7 2						
	2 1 2 0	6 6 1	6 4 6	0 1 9					
1 1 8	2 3 2 0 0								
Short-Form Fit	2 1 1	1 8 4 6	1 8 5 2						
	2 1 2 0	8 3 4	8 2 3	0 2 3					
	1 1 8	1 4 5 0 0							
	2 1 1	6 7 1	6 7 5						
	1 1 4		1 1 0 0						
Short-Form Calibration Fit	1 1 8	4 8 0 0 0							
	2 1 1	1 3 3 7	1 3 4 3						
	1 1 4		0						
	1 1 8	2 4 8 0 0							
	2 1 1	1 6 9 3	1 6 9 9						
Short-Form Fit	1 1 8	1 5 6 0 0							
	2 1 1	2 2 1 2	2 2 1 8						
	1 1 8	7 9 0 0 0							
	2 1 1								
	1 1 8								

Fixed Width 1st Gaussian
Fixed Width 2nd Gaussian
Energy & Uncertainty
 α & β of $W_0 = \alpha + \beta x_0$
For IECAL
Evs X_0 Fit
W = 0 Weighted
= 1 Unweighted
= 2 Both
X = 0 $E = a + bx$
= 1 $E = a + bx$ and $E = a + bx + cx^2$

Fig. 11. Example of short input with fixed peak widths and a sloping background for the first noncalibration peak.

by setting the fixed-point variable No. 14 to 1 (for singlets only) and variables No. 19, No. 24, . . . to 1 (for multiplets) as illustrated in Figure 11. (Fixed peak widths can also be used in the mini input form.)

The input for a sloping background is illustrated for the first noncalibration peak in Figure 11. The slope is given as floating-point variable No. 4 and the line intercept (at the first channel in the peak fit) is given as floating-point variable No. 8. Note that the slope is set back to 0.0 in the next peak fit (otherwise the nonzero value will continue to be used).

2. OUTPUT FORMS

As discussed in Section III, 5, there are several sections of the output, some of which are optional. These various sections are illustrated in Figures 12-15. The first section, Figure 12, which is printed only when the peak location routine is used, gives the information needed for possible subsequent runs with the short input. The listing is in a form that can be used as a keypunch sheet after the desired changes are made.

In Figure 13 the progress of the peak parameters toward convergence is shown for one peak. This output is provided only if $IOUPT \leq 2$.

For all output options, the program gives a summary listing of the final line and Gaussian parameters for each peak, along with the associated errors, the quality of the fit, etc, as illustrated in Figure 14. If the gamma-ray energies and intensities are computed, the results are given in a table (or tables) such as that shown in Figure 15. This table is for a weighted linear fit of the $E(x)$ function. If no detector efficiency table is identified, those columns related to the intensities and widths are omitted from this listing.

AG-110M

SN,BE,CS,OS,C058,MN,SC

10/7/70 P60,ND160

44444275

GAUSS INPUT GENERATED BY PEAK SEARCH OPTION

0000000001 111111112 222222223

1234567890 1234567890 1234567890

31	1	14	20	1	
11	8		0.		PEAK BYPASSED--BAD DATA
31	1	67	73	1	
11	8		46059.		PEAK BYPASSED--BAD DATA
31	1	252	257	1	
11	8		36477.		
31	1	264	269	1	
11	8		35485.		
31	1	272	277	1	
11	8		35291.		
31	1	305	311	1	
11	8		34282.		
31	1	314	320	1	
11	8		33734.		
31	1	432	438	1	
11	8		31922.		
31	1	444	449	1	
11	8		31644.		
31	1	482	487	1	
11	8		30748.		
31	1	572	577	1	
11	8		29335.		
31	1	618	623	1	
11	8		28971.		
31	1	816	821	1	
11	8		22164.		
31	1	887	893	1	
11	8		19303.		
31	1	970	975	1	
11	8		17489.		
31	1	1353	1360	1	
11	8		13828.		
31	1	1477	1483	1	
11	8		15072.		
31	1	1541	1548	1	
11	8		16193.		
31	1	1647	1653	1	
11	8		9705.		

Fig. 12. Illustration of the output from the peak location routine.

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STRAIGHT LINE PARAMETER INFORMATION				Y = AX+B			
PARAMETER	OPTN	INITIAL VALUE	UPPER	LIMIT	LOWER	LIMIT	CONVRG. CRIT.
A	FIXD	0.0		0.0		0.0	0.0
B	FIXD	36476.663		0.0		0.0	0.0

GAUSSIAN PARAMETER VALUES							
GAUSS	PARAMETER	OPTN	INITIAL VALUE	UPPER LIMIT	LOWER LIMIT	CONVRG. CRIT.	
1	HEIGHT	VARY	1733.3370	*****	1.0000	1.0000	
1	CHANNL	VARY	254.5003	10000.0000	1.0000	0.0010	
1	WIDTH	VARY	3.3782	100.0000	0.1000	0.0010	
1	ALPHA1	FIXD	0.0	1.0000 01	0.0	1.0000-10	
1	ALPHA2	FIXD	0.0	1.0000-01	0.0	1.0000-19	

ITR.	QUALITY OF FIT		GAUSSIAN PARAMETERS				AREA
	LAMBDA GAUSS	CHI**2 HEIGHT	CHI**2/NDF CHANNEL	WIDTH	ALPHA1	ALPHA2	
	0.0	6.00D 00	2.00D 00				
	1	1733.3	254.5003	3.3782	0.0	0.0	

1	1.00D 00	1.12D 00	3.74D-01				
	1	1751.8	254.3086	3.8433	0.0	0.0	7167.

2	1.00D 00	1.07D 00	3.57D-01				
	1	1764.0	254.2868	3.8751	0.0	0.0	7276.

3	1.00D 00	1.07D 00	3.57D-01				
	1	1763.5	254.2864	3.8777	0.0	0.0	7279.

4	1.00D 00	1.07D 00	3.57D-01				
	1	1763.5	254.2864	3.8778	0.0	0.0	7279.

				* CONVERGENCE CRITERION HAS BEEN MET. *			

4	1.00D 00	1.07D 00	3.57D-01				
	1	1763.5	254.2864	3.8778	0.0	0.0	7279.

ESTIMATED ERROR IN FITTED PARAMETERS						
	0.0	0.0				
1	145.3	0.1564	0.4191	0.0	0.0	631.

YDATA AND YBAR CALCULATIONS						
CHANNEL	YDATA	YBAR	DELT	SIG	DELT/SIG	(DELT/SIG) ²
252	37201.0	37149.3	51.7	192.876	0.268	0.1
253	37738.0	37776.4	-38.4	194.263	-0.198	0.0
254	38164.0	38213.7	-49.7	195.356	-0.254	0.1
255	38210.0	38082.1	127.9	195.474	0.654	0.4
256	37381.0	37502.9	-121.9	193.342	-0.630	0.4
257	36981.0	36930.3	50.7	192.304	0.263	0.1

NORMAL RETURN--PROBLEM COMPLETED

Fig. 13. Examples of the GAUSS V output showing the convergence of the peak parameters for a given peak.

AG-110M SN,RE,CS,OS,CO58,MN,SC 10/7/70 P60,ND160
 POWERS OF ALPHA TERMS 4,12 WEIGHTING = 1/Y

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FIRST CHAN	LAST CHAN	NO OF PEAKS	QUALITY OF FIT	HEIGHT	CHANNEL	WIDTH	AREA	ALPHA TERMS
252	257	1	0.36			LINE(AX+B)	A =	0.0 B = 36476.7
	PARAMETERS			1763.5	254.2864	3.878	7279.	0.0 0.0
	ERRORS			145.3	0.1564	0.419	631.	0.0 0.0
264	269	1	1.28			LINE(AX+B)	A =	0.0 B = 35485.3
	PARAMETERS			2125.0	266.2105	6.048	13681.	0.0 0.0
	ERRORS			147.5	0.2396	0.921	1598.	0.0 0.0
272	277	1	1.10			LINE(AX+B)	A =	0.0 B = 35291.3
	PARAMETERS			4428.7	274.0286	3.823	18020.	0.0 0.0
	ERRORS			155.8	0.0663	0.177	668.	0.0 0.0
305	311	1	0.70			LINE(AX+B)	A =	0.0 B = 34281.7
	PARAMETERS			3783.0	307.5309	4.767	19197.	0.0 0.0
	ERRORS			131.9	0.0828	0.229	727.	0.0 0.0
314	320	1	0.85			LINE(AX+B)	A =	0.0 B = 33734.0
	PARAMETERS			1950.9	316.3118	4.929	10235.	0.0 0.0
	ERRORS			126.8	0.1675	0.471	767.	0.0 0.0
432	438	1	2.22			LINE(AX+B)	A =	0.0 B = 31921.7
	PARAMETERS			9076.0	435.0142	3.633	35094.	0.0 0.0
	ERRORS			222.1	0.0418	0.100	828.	0.0 0.0
444	449	1	0.63			LINE(AX+B)	A =	0.0 B = 31644.0
	PARAMETERS			4108.1	446.2800	3.833	16763.	0.0 0.0
	ERRORS			140.5	0.0634	0.168	592.	0.0 0.0
482	487	1	1.03			LINE(AX+B)	A =	0.0 B = 30747.7
	PARAMETERS			1899.7	484.1637	4.346	8789.	0.0 0.0
	ERRORS			131.9	0.1519	0.439	690.	0.0 0.0
572	577	1	0.59			LINE(AX+B)	A =	0.0 B = 29335.3
	PARAMETERS			6780.1	574.4817	3.620	26128.	0.0 0.0
	ERRORS			142.9	0.0362	0.092	547.	0.0 0.0
618	623	1	0.52			LINE(AX+B)	A =	0.0 B = 28970.7
	PARAMETERS			1293.4	620.2326	3.057	4209.	0.0 0.0
	ERRORS			141.2	0.1624	0.393	460.	0.0 0.0
816	821	1	2.05			LINE(AX+B)	A =	0.0 B = 22164.3
	PARAMETERS			4258.8	817.9591	5.297	24011.	0.0 0.0
	ERRORS			158.2	0.1120	0.363	1264.	0.0 0.0
887	893	1	2.65			LINE(AX+B)	A =	0.0 B = 19303.0
	PARAMETERS			5262.3	889.6594	4.412	24712.	0.0 0.0
	ERRORS			175.5	0.0701	0.185	833.	0.0 0.0
970	975	1	2.64			LINE(AX+B)	A =	0.0 B = 17488.7
	PARAMETERS			1710.2	972.1005	5.650	10285.	0.0 0.0
	ERRORS			152.4	0.2849	1.008	1401.	0.0 0.0

Fig. 14. Summary output of the final peak parameters, their errors, the quality of the fit and other quantities.

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AG-110M 5N,8E,CS,OS,C058,MN,SC

10/7/70 P60,ND160

DATE COMPUTED 04/20/71
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WEIGHTED ENERGY CALCULATIONS

LINEARITY CORRECTION AT CHANNEL NUMBER PLUS -1.8462D 01

***LINEARITY TABLE = P60+NS626+ND160 1/70

***EFFICIENCY TABLE = P-60 FEP 5/1/70

ENERGY AND INTENSITY CALCULATIONS

ENERGY = 5.00357300-03 + 2.92818740-01(X)
ERRORS 5.3339488D-03 2.2337213D-06

CALIBRATION LINES

CHANNEL	CORRECTED CHANNEL	ENERGY	CALCULATED ENERGY	DELTA E	ERROR IN INPUT ENERGY	TOTAL CALIB ERROR
1356.119	1337.628	391.688	391.688	-0.000	0.010	0.013
1647.458	1631.001	477.593	477.593	-0.000	0.012	0.015
1964.030	1945.510	569.689	569.687	-0.002	0.013	0.016
2225.042	2206.490	646.111	646.107	-0.004	0.017	0.019
2278.081	2259.526	661.638	661.637	-0.001	0.019	0.021
2787.343	2768.796	810.757	810.760	0.003	0.020	0.022
2869.564	2851.025	834.830	834.839	0.009	0.025	0.026
3024.753	3006.231	880.282	880.286	0.004	0.019	0.022
3055.422	3036.904	889.259	889.267	0.009	0.018	0.020
3650.859	3632.361	1063.635	1063.628	-0.007	0.024	0.026
3845.153	3826.592	1120.516	1120.503	-0.013	0.025	0.026

ALL LINES

CHANNEL	CORRECTED CHANNEL	EFFIC (E-3)	CALC ENERGY	SIGMA(E)	INTENSITY (E+8)	SIGMA(I)	NORMALIZED INTENSITY	SIGMA(I)	WIDTH	SIG(W)
254.286	235.722	1.4854	69.029	0.0460	0.049006	0.004902	0.073	0.007	3.88	0.42
266.219	247.680	1.5666	72.530	0.0703	0.087330	0.011098	0.130	0.017	6.05	0.92
274.029	255.505	1.6084	74.827	0.0200	0.112042	0.006972	0.167	0.010	3.82	0.18
307.531	289.054	1.7103	84.645	0.0247	0.112240	0.007041	0.167	0.010	4.77	0.23
316.312	297.944	1.7183	87.219	0.0493	0.059566	0.005368	0.089	0.008	4.93	0.47
435.014	416.540	1.4533	121.776	0.0130	0.241487	0.013350	0.359	0.020	3.63	0.10
446.280	427.796	1.3861	125.272	0.0191	0.120935	0.007401	0.180	0.011	3.83	0.17
484.164	465.658	1.1948	136.358	0.0447	0.073564	0.006845	0.109	0.010	4.35	0.44
574.482	555.938	0.8462	162.794	0.0114	0.308791	0.016740	0.459	0.025	3.62	0.09
620.233	611.675	0.7469	176.187	0.0477	0.056203	0.006755	0.084	0.010	3.06	0.39
817.959	799.386	0.4033	234.080	0.0330	0.095317	0.043218	0.886	0.064	5.30	0.36
889.659	871.087	0.3287	255.076	0.0208	0.751791	0.045329	1.118	0.067	4.41	0.18
972.101	953.535	0.2736	279.718	0.0835	0.375927	0.054561	0.559	0.081	5.65	1.01
1356.119	1337.628	0.1349	391.688	0.0076	19.733359	1.025653	29.656	1.526	4.14	0.05
1479.488	1461.020	0.1125	427.819	0.0657	0.351564	0.042267	0.523	0.063	4.38	0.59
1544.439	1525.987	0.1025	446.841	0.0169	1.697037	0.097468	2.525	0.145	4.16	0.14
1649.458	1631.001	0.0889	477.593	0.0078	17.079449	0.876486	25.410	1.304	4.52	0.06
1763.400	1744.921	0.0768	510.951	0.0354	3.466935	0.235305	5.158	0.350	9.41	0.55
1964.030	1945.510	0.0617	569.687	0.0068	14.211263	0.724650	21.143	1.078	4.64	0.05
2040.331	2021.799	0.0575	592.026	0.0278	1.361563	0.086833	2.026	0.129	5.08	0.25
2069.169	2050.652	0.0560	600.474	0.1112	0.236225	0.055053	0.351	0.082	3.42	0.91
2136.947	2118.398	0.0529	620.317	0.0403	1.575328	0.140927	2.344	0.210	4.86	0.46
2225.042	2206.490	0.0498	646.107	0.0040	67.216234	3.380129	100.000	5.079	4.73	0.03
2264.773	2246.218	0.0483	657.740	0.0048	48.857470	2.464613	72.687	3.667	4.80	0.04
2278.081	2259.526	0.0479	661.637	0.0051	65.028597	3.284631	96.745	4.887	4.77	0.04
2332.586	2314.028	0.0460	677.596	0.0089	6.487293	0.334415	9.651	0.498	5.28	0.09
2364.598	2346.039	0.0450	686.969	0.0143	5.451308	0.305049	8.110	0.454	6.01	0.20
2431.822	2413.261	0.0429	706.653	0.0058	8.823711	0.447169	13.127	0.665	4.76	0.05
2468.564	2450.023	0.0418	717.418	0.0162	3.562737	0.197642	5.300	0.294	4.92	0.15
2560.239	2541.677	0.0394	744.256	0.0181	2.829152	0.157383	4.209	0.234	5.40	0.17
2627.412	2608.852	0.0377	763.926	0.0049	11.638395	0.586499	17.315	0.873	5.10	0.04
2787.343	2768.796	0.0342	810.760	0.0043	9.691595	0.496818	14.419	0.739	5.10	0.07
2812.179	2793.634	0.0336	818.033	0.0136	3.898874	0.207730	5.800	0.309	5.26	0.12
2869.564	2851.025	0.0324	834.839	0.0051	22.158193	1.116873	32.966	1.662	5.19	0.04
3006.166	2987.642	0.0299	874.042	0.0114	5.571814	0.290744	8.289	0.433	5.39	0.10
3024.753	3006.231	0.0296	880.286	0.0119	4.226233	0.222039	6.288	0.330	5.07	0.10
3039.742	3021.222	0.0293	884.675	0.0047	38.919900	1.957341	57.903	2.912	5.35	0.03
3055.422	3036.904	0.0291	889.267	0.0066	25.966130	1.316075	38.631	1.958	5.30	0.05
3220.055	3201.563	0.0275	937.483	0.0089	18.018763	0.922872	26.807	1.373	5.43	0.08
3650.859	3632.361	0.0223	1063.628	0.0073	11.079437	0.560717	16.483	0.834	5.85	0.06
3845.153	3826.592	0.0206	1120.503	0.0059	25.613652	1.288789	38.106	1.917	5.77	0.04
4025.095	4006.469	0.0191	1173.174	0.0283	1.730710	0.105041	2.575	0.156	6.22	0.28
4087.777	4069.126	0.0186	1191.521	0.2264	1.109156	0.269695	1.650	0.401	5.37	1.03

Fig. 15. Portion of the output giving the energy calibration fit information and the computed energies and intensities for all peaks. This result is for a weighted, quadratic energy fit.

V. COMMENTS ON ENERGY AND INTENSITY DETERMINATIONS

Often one wishes to obtain both the gamma-ray energies and intensities from a spectrum. However, the fitting methods needed to get the best intensities may be somewhat different from those needed to obtain the best energies. Since it is difficult to determine the efficiency of a Ge(Li) detector to better than ~2% over an extended range (ie, a few hundred keV) and the energy calibration is generally accurate to better than 0.01%, this program has been designed to obtain the best possible energies with some possible loss in the quality of the intensities.

The quality of the gamma-ray energies and intensities obtained with this computer program will generally depend to a large extent on the performance of the Ge(Li) spectrometer as well as on the experimental techniques used. It is clear that since the program uses a symmetric function (ie, a Gaussian) to fit the points in the peak, the quality of the results will degenerate rapidly as the amount of asymmetry (ie, the tailing) increases. For spectrometers that have a significant amount of asymmetry, one should consider the use of a fitting function which takes this asymmetry into account.^[10]

There are three features of the program that should be considered if one wishes to obtain the best possible intensities (or relative peak areas). Probably the most important is the choice of the background. If the background generally slopes downward, by the nature of the method used, the peak location routine will normally pick a background that is too low. Therefore, it is generally necessary to do the peak analysis with the short input form to obtain the best intensities. The second problem is the choice of the channel fitting range. It may be desirable to include more channels in the peak fit than those selected by the peak location routine. This question can only be resolved by the comparison of different choices for the particular spectrometer. (For the determination of absolute intensities, the choice also depends on the method which was used to determine the detector efficiency curve.) And finally, especially for weak peaks it may be desirable to fix the widths of the peaks. This prevents the large variations in widths that may otherwise occur for small neighboring peaks. There is also at least one instrumental effect that may produce errors in the computed intensities. The

shape of the experimental peaks may change with counting rate: that is, low-energy tails may develop on the peaks. If this change cannot be accounted for with the Gaussian function, errors will result.

The analysis of the data in Reference 5 on precise gamma-ray energy measurements below 420 keV with Ge(Li) detectors was carried out with a version of this program which did not have the automatic peak location routine. During the course of that work, extensive tests were made to determine a satisfactory procedure for choosing the range of data to be used in a peak fit. From the results of that study, the rules for the fitting limits (Equation (13)) used in the peak location routine were developed.

An example of the variation in the computed energy for various choices of the fitting limits is given in Table 4 for some typical strong peaks. The various fitting limits are shown in Figure 16 where the fits

Fig. 16. Channels ranges used to determine the variation in the computed gamma-ray energy.

labeled No. 1 are those selected by the peak location routine. From Table 4 it is seen that as more of the peak is included in the fit, the calculated energy decreases due to the inclusion of more low-energy tailing. As fewer points are used in the fit, the counting statistics begin to cause a more random variation in the computed energy.

If the energy computations involve peaks distributed over a large fraction of the total channel range, the quality of the results may be very dependent on the accuracy of the determination of the nonlinearity correction.

This problem might be reduced somewhat by fitting over only a

TABLE 4

The effect of the fitting limits on the computed energy for the peaks in Figure 16.

Fit No.	308-keV			316-keV			320-keV		
	Computed (keV)	E_γ	$E_\gamma(n) - E_\gamma(1)$ (eV)	Computed (keV)	E_γ	$E_\gamma(n) - E_\gamma(1)$ (eV)	Computed (keV)	E_γ	$E_\gamma(n) - E_\gamma(1)$ (eV)
6							320.073		0
4	308.447		7	316.492		-1	320.074		1
2	308.441		1	316.495		2	320.073		0
1	308.440			316.493			320.073		
3	308.437		-3	316.491		-2	320.072		-1
5	308.435		-5	316.489		-4	320.070		-3
7							320.068		-5

having an insufficient number of calibration lines to show the deviations that are present. Therefore, it is our practice to use as many calibration lines as is feasible, often from 6 to 15, and thereby verify for each calibration run that the linearity correction is essentially correct.

It is, of course, true that the quadratic term in $E(x)$ can be used to account for some of the nonlinearity. But, even in this case, the correction must account for all of the nonlinearity that shows a higher order dependence on x .

Samples of the quality of the fits to the calibration lines are given in Tables 5 and 6 for two typical good fits. In Table 5, the linear fit is good; the root-mean-square energy difference is 5.6 eV. The results in Table 6 are for the spectrum in Figure 1. In this case, the quadratic fit is somewhat better than the linear fit.

One of the most accurate methods of determining the energy of a transition is to measure the difference between its energy and that of a close lying calibration line. The formulas for the energy difference and its uncertainty are given in Reference 6 along with the results from over fifty energy difference measurements. Most of these differences have uncertainties of ≤ 5 eV. The consistency shown by values from different spectrometers indicates that the nonlinearity corrections are not affecting the results adversely.

TABLE 5

Results of an Energy Calibration with a Linear E(x) Function

Peak Location (channel)	Calibration Energy (keV)	Calculated Energy ^a (keV)	Energy Difference (eV)
735.945	84.678±0.004	84.684	6
868.889	100.103±0.004	100.101	-2
985.893	113.671±0.004	113.670	-1
1009.647	116.416±0.005	116.425	9
1319.980	152.432±0.004	152.425	-7
1354.084	156.385±0.004	156.382	-3
1435.642	165.854±0.011	165.845	-9
1552.426	179.390±0.004	179.397	7
1715.745	198.353±0.005	198.349	-4
1920.355	222.106±0.004	222.100	-6
1982.488	229.318±0.008	229.315	-2
2281.772	264.068±0.008	264.077	9
2411.855	279.190±0.007	279.189	-1
2556.091	295.945±0.008	295.946	1
2663.625	308.437±0.009	308.440	3
2732.941	316.496±0.009	316.493	-3
2763.758	320.080±0.013	320.074	-6
3552.965	411.795±0.007	411.802	7

$$^a E(x) = (0.0015 \pm 0.0029) + (0.1161010 \pm 0.0000019)x$$

An attempt has been made to make the uncertainties quoted by GAUSS V in the calculated gamma-ray energies as accurate as possible. As noted in Section II, 3.3, the uncertainties in the peak positions of the calibration lines are taken into account in an approximate manner, instead of neglecting them as would be done in a normal weighted least-squares fit. However, in many cases the uncertainties in the energies calculated in the program may be too small. This is because in carrying out the least-squares fit, the standard mathematical procedure assumes that the uncertainties of the calibration energies are independent. As a result, the procedure tends to average out these uncertainties and can quote smaller errors on the calculated energies. This result would be valid if the calibration energies and their errors were truly independent. In most cases, however, the errors on the calibration lines are related and, in fact, generally most of the uncertainty is common to all of them. (This results from the fact that the calibration errors are often all based on the same reference energy.)

TABLE 6

Results from Analysis of Spectrum in Figure 1

Peak Location (Channel) ^a	Calibration Energy (keV)	Calculated γ -Ray Energy			
		Linear E(x) ^b		Quadratic E(x) ^c	
		Energy (keV)	ΔE^d (eV)	Energy (keV)	ΔE^d (eV)
471.015 $\pm$ 0.018	145.440 $\pm$ 0.003	145.455 $\pm$ 0.008	15	145.442 $\pm$ 0.006	2
537.207 $\pm$ 0.012	165.853 $\pm$ 0.007	165.864 $\pm$ 0.006	11	165.854 $\pm$ 0.004	1
958.960 $\pm$ 0.006	295.949 $\pm$ 0.006	295.940 $\pm$ 0.004	-9	295.944 $\pm$ 0.002	-5
999.482 $\pm$ 0.006	308.445 $\pm$ 0.007	308.440 $\pm$ 0.004	-5	308.444 $\pm$ 0.002	-1
1025.577 $\pm$ 0.007	316.497 $\pm$ 0.007	316.489 $\pm$ 0.004	-8	316.495 $\pm$ 0.002	-2
1269.348 $\pm$ 0.009	391.688 $\pm$ 0.010	391.683 $\pm$ 0.004	-5	391.693 $\pm$ 0.003	5
1516.923 $\pm$ 0.010	468.062 $\pm$ 0.010	468.048 $\pm$ 0.005	-14	468.060 $\pm$ 0.003	-2
1570.416 $\pm$ 0.035		484.547 $\pm$ 0.011		484.559 $\pm$ 0.011	
1886.525 $\pm$ 0.009	582.063 $\pm$ 0.013	582.049 $\pm$ 0.005	-14	582.061 $\pm$ 0.003	-2
1907.596 $\pm$ 0.051		588.546 $\pm$ 0.016		588.558 $\pm$ 0.016	
1958.942 $\pm$ 0.037	604.396 $\pm$ 0.012	604.385 $\pm$ 0.012	-11	604.396 $\pm$ 0.012	0
1985.084 $\pm$ 0.032		612.445 $\pm$ 0.010		612.458 $\pm$ 0.010	
2144.553 $\pm$ 0.013	661.643 $\pm$ 0.020	661.640 $\pm$ 0.007	-3	661.650 $\pm$ 0.005	7
2277.382 $\pm$ 0.013		702.617 $\pm$ 0.007		702.624 $\pm$ 0.004	
2347.268 $\pm$ 0.017		724.176 $\pm$ 0.008		724.181 $\pm$ 0.006	
2452.753 $\pm$ 0.021		756.716 $\pm$ 0.009		756.718 $\pm$ 0.007	
2482.153 $\pm$ 0.012		765.785 $\pm$ 0.007		765.787 $\pm$ 0.004	
2548.261 $\pm$ 0.016	786.180 $\pm$ 0.016	786.178 $\pm$ 0.008	-2	786.178 $\pm$ 0.005	-2
2659.866 $\pm$ 0.013		820.606 $\pm$ 0.008		820.603 $\pm$ 0.005	
2706.970 $\pm$ 0.013	835.129 $\pm$ 0.016	835.137 $\pm$ 0.008	8	835.132 $\pm$ 0.005	3
2823.552 $\pm$ 0.015		871.099 $\pm$ 0.009		871.089 $\pm$ 0.005	
2882.462 $\pm$ 0.021	889.249 $\pm$ 0.021	889.271 $\pm$ 0.010	22	889.259 $\pm$ 0.007	10
3368.720 $\pm$ 0.020	1039.246 $\pm$ 0.019	1039.274 $\pm$ 0.012	28	1039.237 $\pm$ 0.022	-9

a. Peak location before correction for nonlinearity.

b. $E(x) = (-0.009 \pm 0.007) + (0.3084503 \pm 0.0000044)X'$ where X' has been corrected for the nonlinearity.c. $E(x) = (-0.046 \pm 0.004) + (0.3085097 \pm 0.0000060)X' + (-1.76 \pm 0.17) \times 10^{-8}X'^2$.d. ΔE = calculated energy minus the calibration energy.

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VI. REFERENCES

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APPENDIX A

GENERATION OF DATA SET OF LINEARITY AND EFFICIENCY TABLES

Several methods for measuring linearity corrections^[6,11,12] and efficiencies^[12,13] have been described. Here it is assumed that the linearity and efficiency functions can be represented by smooth curves. From these curves, it is necessary to determine groups of equally spaced points to describe the function. From this table of values, GAUSS V interpolates the function at the desired energy or channel.

Specifically, a table is made up in the following manner as illustrated for a linearity correction function in Figure 17. Over the first portion of the curve, where the function varies rapidly, values of the function are determined every 20 channels as indicated. It should be noted that the function will not be evaluated for an argument (ie, channel) smaller than that of the second entry in the table. Therefore, it is necessary to provide an extra (or dummy) point before the first channel for which the data are valid. This extra point does not need to lie on the function; it should rather, lie on the smooth extension of the second and third points of the section. (Since a parabolic interpolation method is used, "smooth" means that the curvature should be about constant.)

Fig. 17. Illustration of data used to define nonlinearity correction in table form in GAUSS.

Only the functional values (ie, linearity correction) are entered in the table. The arguments (ie, the channel) are given by specifying the argument of the first point, the increment in the argument, and the number of points in the group.

In the second section of the curve in Figure 17, the function is represented by points every 50 channels. To get the proper overlap of the two sections, the second point of the second section should be the same as the next-to-last point of the first section. Similarly, the subsequent sections are added to the table with the proper overlap.

The information for each table is stored on either magnetic tape or disc by means of the program LCTAPE. The following is a description of the card formats required to store a table.

Card Number

1	Format (15,18A4)	
	Columns 1-5 IDNT	Identification number of the table. This number is used in GAUSS to find the proper table (see IXC and IYC in Table 2).
	Columns 6-78 ITLABL	Alphanumeric identification. This is printed by GAUSS V.
2	Format (6I10)	
	Columns 1-10 NSECT	Number of sections in table ($NSECT \leq 5$)
	Columns 11-20 NVAL	Number of values in section No. 1
	21-30	Number of values in section No. 2
	.	etc.
	.	
	.	
	51-60	Total number ≤ 99
3	Format (5E10.0)	
	Columns 1-10	Starting channel or energy for section No. 1
	11-20	Starting channel or energy for section No. 2
	.	etc.
	.	
	.	
	41-50	
4	Format (6E10.0)	
	Columns 1-10	Increment size in section No. 1
	11-20	Increment size in section No. 2
	.	etc.
	.	
	.	
	51-60	

Card Number

5 to n Format (8E10.0)

Columns 1-10

Table values of linearity correction or
efficiency

11-20

.

.

.

71-80

When a new data set is created, all of the desired linearity and efficiency tables must be present in the deck. All of the linearity tables are first in order of increasing IDNT and followed by all of the efficiency tables (also in order of increasing IDNT). (The same values of IDNT may be used for an efficiency and a linearity table.) All of the tables are preceded by the following card.

Format (2I5, 8A8, A2)

Columns 1-5

NLT

Number of linearity tables present

Columns 6-10

NET

Number of efficiency tables present

Columns 11-77

TITLE

Alphanumeric identification - used only
on the output of this program.

The output of the program consists of a list of the tables and the data set on either a disc or a magnetic tape.

APPENDIX B

LIBRARY STORAGE OF SPECTRAL DATA

LIBRARY STORE is a general data editing and storage program. The data are stored in the form counts/channel for up to 4096 channels. The program accepts spectral data from cards, from three types of analyzer magnetic tapes, and from another library. The analyzer tapes are seven track tapes which are written at 200 bpi. They are (1) a 36 bit binary (each 36 bit word consists of two packed 18 bit words), (2) a 24 bit binary, and (3) a 36 bit BCD. The output consists of a new library tape.

The editing capabilities of this program include:

1. Creating a new library
2. Adding to existing library
3. Replacing a section of the data
4. Replacing the title section
5. Changing the identification (ID,IA) attached to the data
6. Overflow correcting data
7. Merging two libraries.

A maximum of five tape drives can be utilized

FT04 - An analyzer magnetic tape	} If only one analyzer tape is present, it can be on either unit.
FT08 - An analyzer magnetic tape	
FT09 - Old library (created on a previous job) - all spectra transferred to new library	
FT10 - New library (created this job)	
FT11 - Secondary old library - some or all spectra transferred to the new library.	

1. LIBRARY CONTROL CARD (1 per job)

<u>Card</u> <u>Columns</u>	<u>Name</u>	<u>Description</u>
10	NLIB	0 - Create a new library
		1 - Add data to old library
		2 - Put part of secondary old library on new library
		3 - Put all of secondary old library on new library - no analyzer tapes present
		4 - Read data off old library

<u>Card Columns</u>	<u>Name</u>	<u>Description</u>
20	IPRNT	0 - No list except ID numbers 1 - Gives a second list of ID numbers 2 - List all data on library 3 - Read specific ID's for list, punch or plot of those particular spectra 4 - List and plot all data on library 5 - Plot all data on library

2. DATA CONTROL CARD (1 for each spectrum added or modified)

<u>Card Columns</u>	<u>Name</u>	<u>Description</u>
1-8	ID	Number identification
9-16	IA	Alphanumeric identification
20	ILIB	0 - Creating a new library 1 - Adding to old library (from either analyzer. tape or old secondary library) 2 - Replace section of data (cards of Type IV needed) 3 - Replace title(s) (cards of Type III needed) 4 - Delete spectrum 5 - Change identification number(s) 6 - Overflow correct data (cards of Type V needed)
25	INOP	Data input from: 0 - Cards 1 - 160/161 analyzer (36 bit binary magnetic tape) 2 - 50/50 analyzer (24 bit binary magnetic tape) 3 - Library tape 4 - ND 2200 analyzer (BCD magnetic tape)
30	NALF	Number of alphanumeric title cards for this particular spectrum (is blank for ILIB=2, 4, 5, or 6)
45	IOFL	Overflow description 0 - Binary tape (overflow at 262,144 counts) 1 - BCD tape (overflow at 1,000,000 counts)

<u>Card Columns</u>	<u>Name</u>	<u>Description</u>
50	NTP	Number of tape to be read 0 - analyzer magnetic tape identified (ie, type and reel number) on JCL card FT08 1 - analyzer magnetic tape identified on JCL card FT04
55	NDMP	Sequence number of the dump wanted off analyzer magnetic tape
65-72	IDD	Numeric ID } for ILIB=5 replacing ID on library Alphanumeric ID }
73-80	IDDA	

3. TITLE CARD If NALF > 0 and/or ILIB=3
(Read 'NALF' number of Title Card)

1-80	TITLE	Any alphanumeric information (allowed up to 8 cards)
------	-------	---

4. AUXILIARY CARDS TO REPLACE SECTIONS OF DATA
(Needed if ILIB=2)

4.1 Correction Range

1-5	ICH1	First channel to be corrected
6-10	ICH2	Last channel to be corrected

4.2 Corrected Data (format 2X,10I7,8X)

3-9	IDAT(1)	Corrected data for first channel
10-16	IDAT(2)	Corrected data for second channel
17-23	IDAT(3)	Corrected data for third channel
.		
.		
.		
etc	etc	etc

A "-1" card must follow last correction card; the program then cycles back to read another correction range card (to 4.1). If the "-1" is followed by a blank card, the program goes back to read another data control card.

5. AUXILIARY CARD FOR OVERFLOW CORRECTIONS

(Needed if ILIB=6)

<u>Card Columns</u>	<u>Name</u>	<u>Description</u>
1-10	NOLF	Number of times overflowed
11-20	ISTA	First channel to be corrected
21-30	ISTP	Last channel to be corrected

A blank card follows the last overflow correction card.

6. END OF JOB CARD (one card per job)

9-11	END	"END" punched in Cols. 9-11 stops the reading of data control cards and sends the program to the output area.
------	-----	---

7. AUXILIARY CARD FOR OUTPUT FOR SPECIFIC SPECTRA

(Needed if IPRNT=3)

1-8	IDD	Numeric ID
9-16	IDDA	Alphanumeric ID
20	NPRNT	Output option for this identification 2 - List 3 - List and punch 4 - List and plot 5 - Plot only

A blank card must follow the last card of this set.

It should be noted that when creating a library, the last ID number must be a 99999999 and this card must be followed by a "-1" card. This is the END OF LIBRARY ID CODE for the tape.

APPENDIX C

SUBROUTINE DESCRIPTION

Following is a brief description of the subroutine which comprise the GAUSS program. All are coded in FORTRAN IV except where noted:

ALPHA1	Evaluates the functional form $\alpha_1(x_0)$
ALPHA2	Evaluates the functional form $\alpha_2(x_0)$
BOUND	Tests parameters to determine if they are within the specified upper and lower limits
COEFF	Storage area for the coefficients for the functional forms $\alpha_1(x_0)$, $\alpha_2(x_0)$, and $w_0(x_0)$.
EFFCN	Calculates the efficiency corrections.
ENTENT	Performs the energy and intensity calculations and lists the results.
ERREA	Calculates the photopeak areas and errors in the areas.
ERRSET	IBM system routine which modifies the error monitor. In GAUSS V this routine was used to allow an unlimited number of floating point overflows and divide checks (division by zero) without terminating execution.
ESORT	Sorting routine used to sort energies in order of increasing value. Uses shell-sort algorithm
EXTRA	Generates the summary output by editing data written on unit 4.
FCN	Evaluates the modified-Gaussian function to determine the y values.
GAUSS	Performs the iterations and tests for convergence. The calculation of the partial derivatives and formation of the partial derivative matrix is accomplished here.

INPUT	Entry point for the GAUSS V program. All fixed point data, floating point data, and the spectrum are read and stored. The execution of the fit is initiated unless the peak search option is requested, in which case, INPUT2 is called.
INPUT2	Control program for the peak search option. It initiates the peak location procedure and then the fit procedure.
LINEAR	Calculates the linearity corrections.
LINFIT	Linear least-square routine which is used in fitting the calibration curve in the efficiency-intensity calculations.
MAIND	Double precision matrix inversion routine.
OMEGA	Evaluates the functional form $w_0(x_0)$.
OUTPUT	Output routine which prints iteration results and calculates the estimated errors in the fitted parameters.
PARMTR	Calculates the Gaussian parameters, upper and lower limits and convergence criteria.
PART1 PART2 PART3	Evaluates $\partial\alpha_1/\partial x_0$, $\partial\alpha_2/\partial x_0$, and $\partial w_0/\partial x_0$, respectively.
PKSRCH	Locates the peaks and determines the fitting parameters (ie, the data points to be used in the fit and the background values). The information is written on Unit 2 and used as input to the fitting portion of the program.
TABLKUP	Searches linearity-efficiency table tape for requested tables and stores them on tape or disc.
XOVARI	A composite routine which evaluates the functional forms $\alpha_1(x_0)$, $\alpha_2(x_0)$, and $w_0(x_0)$ by calling the ALPHA1, ALPHA2, and OMEGA routines.