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SAMPO, A Fortran IV Program for Computer Analysis of Gamma Spectra from Ge(Li) Detectors,
and for Other Spectra with Peaks

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Publication Date

1969-10-20

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UC-34 Physics
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SAMPO, A FORTRAN IV PROGRAM FOR COMPUTER ANALYSIS OF GAMMA SPECTRA FROM Ge(Li) DETECTORS, AND FOR OTHER SPECTRA WITH PEAKS

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SAMPO

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UCRL-19452

SAMPO, A FORTRAN IV PROGRAM FOR COMPUTER ANALYSIS OF GAMMA SPECTRA FROM Ge(Li) DETECTORS, AND FOR OTHER SPECTRA WITH PEAKS

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ABSTRACT

SAMPO is a Fortran IV program written to perform the data-reduction analysis described by J. T. Routti and S. G. Prussin in Photopeak Method for the Computer Analysis of Gamma-Ray Spectra from Semiconductor Detectors, Nuclear Instruments and Methods 72, 125-142 (1969). The code has also been used to analyze other spectra with peaks and continua.

Program SAMPO can be used for an automatic off-line or an interactive on-line analysis. It includes algorithms for line-shape, energy, and efficiency calibrations, and peak-search and peak-fitting routines. Different options are available to make the code applicable to accurate nuclear spectroscopic work as well as to routine data reduction. The mathematical methods and their coding are briefly described. Instructions for using the program and for preparing input data are given and the optimal strategies for running the code are discussed. Instructions are given for using the LRL program library version of SAMPO and for obtaining source decks.

1. INTRODUCTION

In earlier reports we described a "Photopeak Method for the Computer Analysis of Gamma-Ray Spectra from Semiconductor Detectors."[1,2] Simultaneously with the development of the analysis methods we wrote a Fortran IV program SAMPO* to perform the computations. The code includes algorithms for automatic peak-search and peak-fitting routines, as well as for line-shape, energy, and efficiency calibrations. Many options have been included to make the code applicable to accurate nuclear spectroscopy work or to routine data reduction. The program has been designed primarily for an off-line analysis, but can be also run in an interactive on-line mode employing cathode-ray-tube (CRT) display and teletype input and output.

Program SAMPO has been used extensively at the Lawrence Radiation Laboratory in Berkeley for the last few years to analyze gamma-spectral data, including some of great complexity.[3-5] The code was developed with CDC-6600 computers, but has been successfully run also at other centers with different computers.

The present version of the code includes adequate options for most tasks in spectrum

analysis. Some of the options for constrained fitting have not yet been incorporated in the general purpose version; similarly, improvements in speed may be obtained through further optimization of the algorithms. Because of wide interest expressed in the analysis methods and the program, this report is prepared at this time to serve the users of the code not only at LRL but also at other laboratories.

For detailed explanations of the mathematical methods employed the reader is referred to the original reports by Routti and Prussin.[2] A brief summary of these is given in Section 2. The structure of the code is discussed in Section 3, where we also include comments on restrictions and possible modifications of the program. The uniform format data input is explained in Section 4. Optimal ways of running the code are discussed in Section 5 and input examples are given. Finally, instructions for using the LRL program library version of SAMPO and information for obtaining the source decks are given in Section 6.

The functional form used to describe the peak shape has been designed primarily for the analysis of γ-ray spectra measured with Ge(Li) detectors. The analysis method has been found applicable also to electron spectra[4] and simple γ-ray spectra measured with NaI(Tl) detectors. As such, or with a modified representation of the line-shape function, the method and program SAMPO should be applicable to a wide range of spectroscopy problems in which the interpretation is based on the analysis of single or multiple peaks.

2. ANALYSIS METHODS

The purpose of the analysis is to determine in a γ-ray spectrum, measured with a Ge(Li) detector and a multichannel pulse-height analyzer, the exact channel locations and areas of photopeaks, the energies and intensities of the corresponding γ rays, and the statistical and calibration uncertainties of these quantities. The analysis is based upon the study of photopeaks in the spectrum. These may be single peaks or clusters of peaks (called multiplets) on the continuum due to the Compton continua of higher-energy lines and the general counting background. There is no difference between the analyses of full-energy and escape peaks. In Fig. 1 we show a γ-ray spectrum used in input and output examples that follow; it is a partial spectrum of a ^{177m}Lu source, characterized generally by good statistics and several multiplets of varying complexity.

The essential quantities of each peak--that is, the exact channel location and peak area together with their statistical uncertainties-- are determined by fitting the section of measured spectrum in the least-squares sense by using internally calibrated analytical functions to represent the peak shapes. This approach gives much better stability and accuracy of the results than fitting the data with Gaussian functions, especially with poor statistics and complex multiplets, and reduces the computing time significantly. In the following we briefly summarize the formalism for the line-shape calibrations and peak fitting, as well as for automatic peak search and selection of fitting intervals, and energy and efficiency calibrations.

The input of program SAMPO is designed around special data-control cards which are identified by English code words. The program input is discussed in detail in Sections 4 and 5; however, to initially familiarize the reader with these input options we refer briefly to the appropriate code words when describing different parts of the analysis in this section.

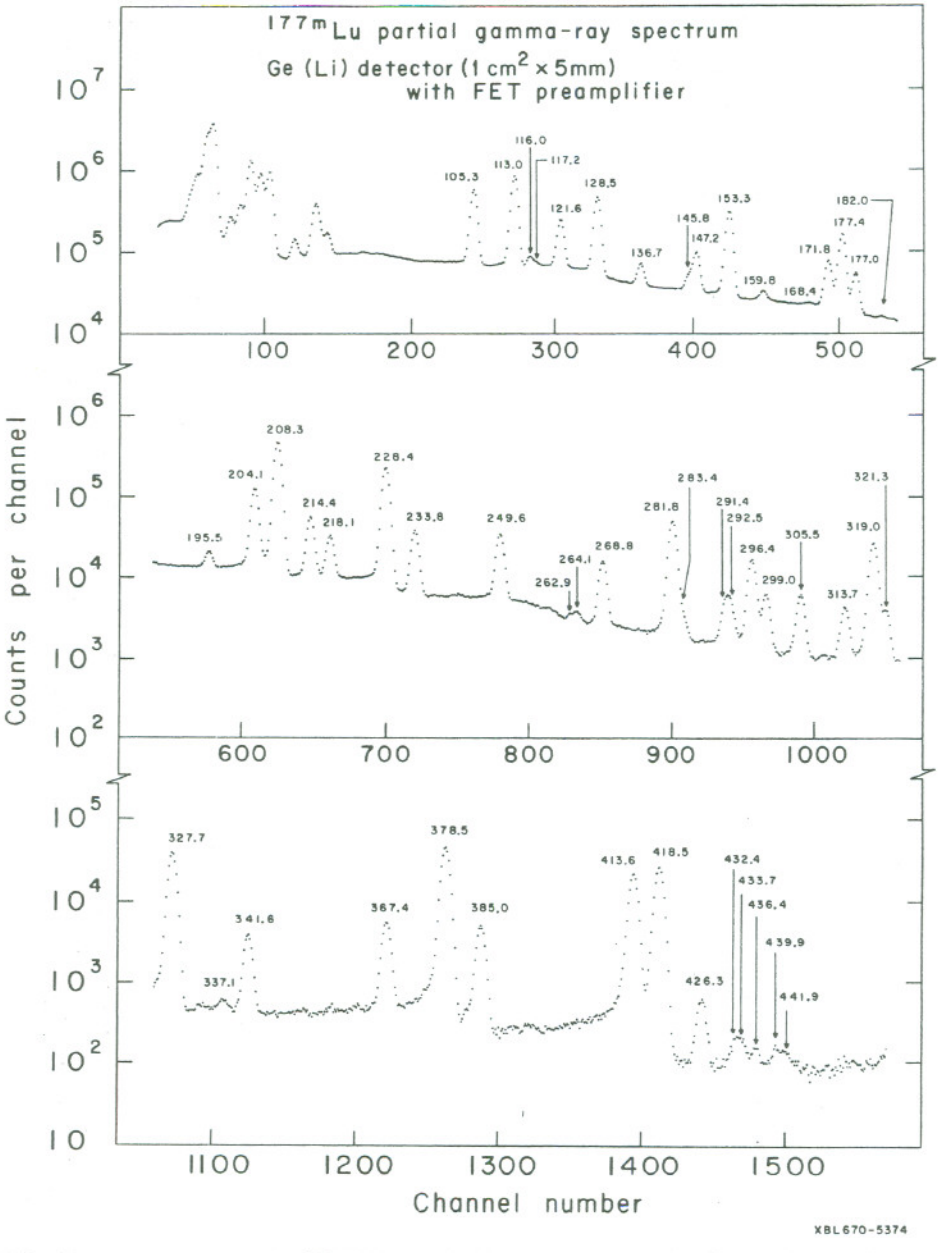


Fig. 1. Partial γ-ray spectrum of ^{177m}Lu counted with 1 cm^2 × 0.5 cm Ge(Li) detector with field-effect-transistor preamplifier. This spectrum is used in examples of the subsequent analysis.

Data Plotting — Code words DATAGRAPH, DATAPLOT, DATATV

In the analysis of complex γ-ray spectra it is mandatory to have some means of presenting the spectral data in a graphical way. In the following analysis with program SAMPO we display also the results in a graphical form, either as printer plots, computer drawings, or CRT pictures. The graphical representation is particularly useful in an interactive analysis where the user may exercise his judgment and aid the program with difficult cases, if required.

To start the analysis, a plot of the spectrum (if not already available) can be obtained as a computer plot as shown (with some elaboration) in Fig. 1 (DATAPLOT). A less precise printer graph of the spectrum or a part of it is often sufficient. SAMPO code includes options for logarithmic or linear printer graphs of the spectral data, such as shown in Fig. 2 (DATAGRAPH). In the on-line analysis, plots (similar to Fig. 1) of sections of the spectrum under analysis are displayed on a CRT (DATATV).

Peak-Shape Calibrations — Code words SHAPEDO, SHAPEIN, CALDATA, OPTIONS

The peak shape is approximated by an analytical function that consists of a Gaussian with provisions for tailing on both low- and high energy-energy sides. The degree of tailing is defined by the distance from the peak centroid to a point at which the Gaussian is extended by a simple exponential so that the function and its first derivative are continuous. In this representation the peak shape is defined by three parameters--the width of the Gaussian, and the distances from the centroid to the junction points, all in units of channels. Figure 3 shows a number of such peak shapes on a constant continuum. The width parameter is the same for all curves and only the tailing parameter is varied; the same curves are drawn on both semilogarithmic and linear scales.

The Gaussian-plus-exponential representation of the shape function for photopeaks has the characteristic that the defining shape parameters vary smoothly with energy and therefore the values of these parameters for any line in a spectrum may be found by interpolation between neighboring lines. For this purpose, intense and well-isolated lines are used as internal calibrations, and their shape parameters are defined by fitting with the function described and a straight-line approximation for the background continua. This is performed by minimizing the weighted sum of the squares,

$$\chi^2 = \sum_{i=k-\ell}^{k+m} \frac{(n_i - f_i)^2}{n_i}, \qquad (1)$$

where i = channel number,

n_i = counts in channel i,

k = approximate center channel of the peak,

ℓ, m = channels specifying the fitting interval,

$$f_i = p_1 + p_2(i-p_4) + p_3 \exp\left[-\frac{(i-p_4)^2}{2p_5^2}\right],$$

for $p_4 - p_6^2 \le i \le p_4 + p_7^2$,

$$f_i = p_1 + p_2(i-p_4) + p_3 \exp\left[\frac{p_6^2(2i-2p_4+p_6^2)}{2p_5^2}\right],$$

for $i < p_4 - p_6^2$,

$$f_i = p_1 + p_2(i-p_4) + p_3 \exp\left[\frac{p_7^2(2p_4-2i+p_7^2)}{2p_5^2}\right],$$

for $i > p_4 + p_7^2$.

The minimization is performed with respect to the parameters p_j, $j = 1$ through 7, which have the following interpretations:

p_1 = constant in the continuum approximation,

p_2 = slope in the continuum approximation,

p_3 = height of the Gaussian,

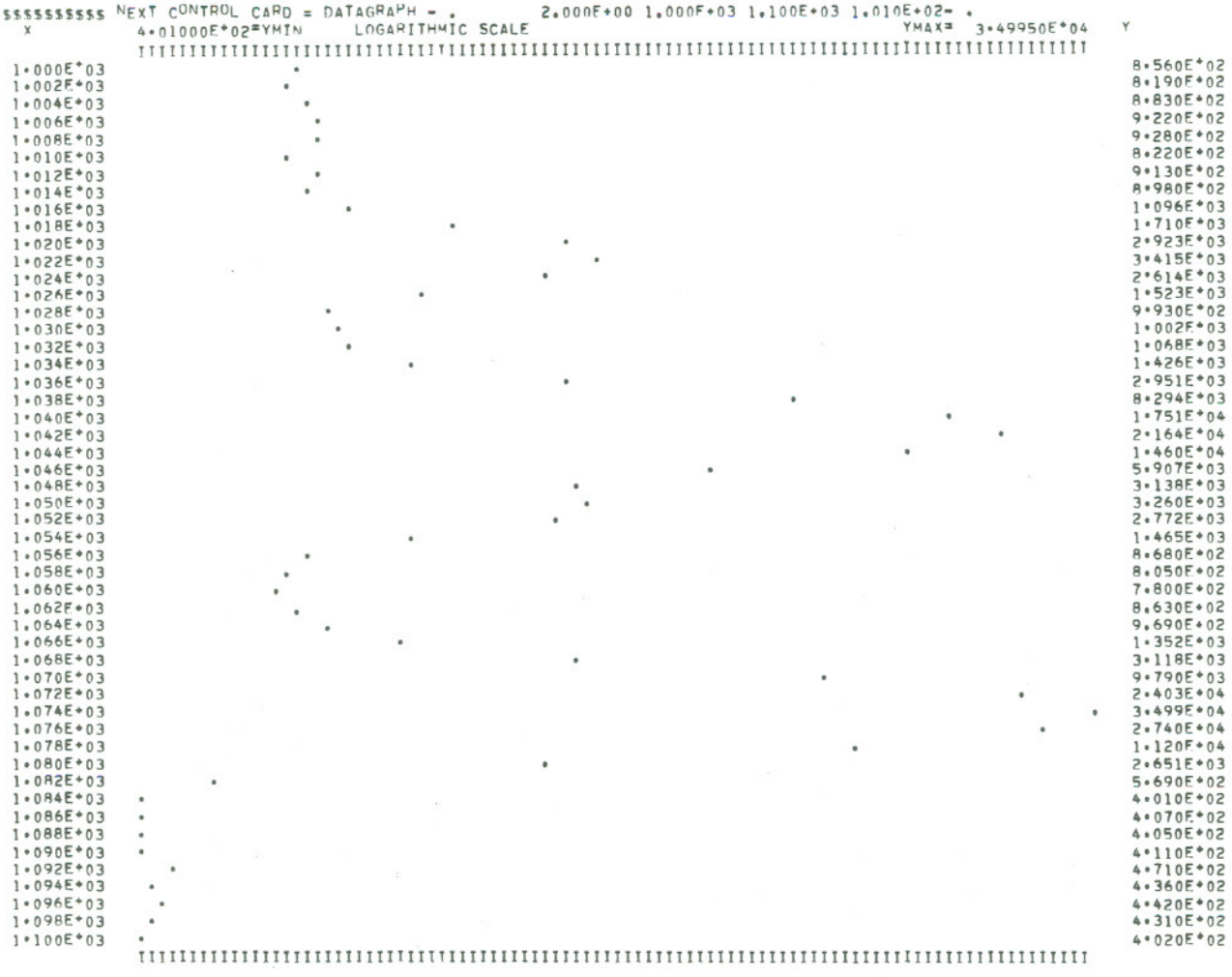


Fig. 2. Printer graph of spectrum shown in Fig. 1, showing every second channel between 1000 and 1100 on a semilogarithmic scale.

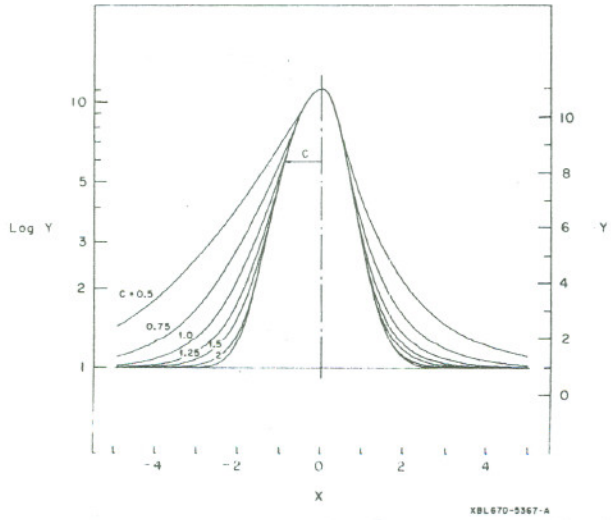


Fig. 3. Line-shape functions with various degrees of tailing. The Gaussian is extended with an exponential at c so that the function and the slope are continuous. The same curves are drawn on logarithmic and linear scales.

p_4 = centroid of the Gaussian,
p_5 = width of the Gaussian (FWHM = 2.355 p_5),
p_6^2 = distance in channels to lower junction point,
p_7^2 = distance in channels to higher junction point.

The straight-line approximation for the continuum under the peak is chosen to stabilize the solution of tailing parameters, and for the same reason these parameters are forced to be positive by being squared.

The minimization of the sum in Eq. (1) is performed by subprogram VARMIT, which is an iterative gradient algorithm with variable metric.[6] This routine uses χ^2, its gradient in the parameter space, and the inverse of its second-derivative matrix. The first two quantities are calculated for each iteration step and the third is constructed during the minimization by the method of successive approximations. All this information is used to predict the size and direction of the next iteration step. In addition to the best values for χ^2 and the parameters, the results include a good approximation to the complete error matrix for calculating errors in different parameters. The minimization is terminated when all the components of the next step are less than 10^{-8}, or if four succeeding values of χ^2 are the same, or if 100 iterations have been completed. To obtain good initial guesses for the tailed fit, the data are first fitted with a Gaussian with no tailing options.

Figure 4 shows the results as printed out by SAMPO for a peak-shape calibration fit (SHAPEDO). The upper part of the figure shows numerical information of the initial Gaussian and the subsequent fit with the tailing options. The final fit is also shown as a semilogarithmic printer graph displaying the original data points, the fitted function, and the fitted continuum. These functions are also listed as a function of the channel number, together with the residuals in the fit. The residuals are the differences between the data and the calculated points measured in units of standard deviations of the data, $r_i=(n_i-f_i)/\sqrt{n_i}$. Below the graph are printed the sum of the data points and the sum of calculated points above the fitted continuum. The shape-calibration parameters obtained are also shown below the graph; these are related to the parameters in the fit as the channel location CP = p_4, the lower tailing parameter CL = p_6^2, the higher tailing parameter CH = p_7^2, and the width parameter CW = p_5. These parameters are stored from each shape-calibration fit. The line shape in any part of the spectrum is then defined by interpolating the shape parameters linearly with respect to the channel numbers. The number of calibration fits required depends on the total energy range of the spectrum. When enough strong single lines are available we generally use one for each interval of about 100 to 200 keV in the spectrum. It is strongly recommended that the user check the behavior of the shape parameters by plotting them as a function of channel numbers.

Note that the fitting interval needs to be wide enough to include the tails; however, it should not be so wide as to make the assumption of linearity of the continuum unreasonable. Note also that when a tailing parameter gets large compared with the width parameter it indicates a small degree of tailing and the accuracy of the value is of small significance. It should also be remembered that some peaks, such as the positron annihilation peak at 511 keV, have shapes which do not follow the generally smooth variation of the shape parameters as a function of the channel number. The linear interpolation between adjacent calibration points enables us to use proper values for these peaks as well, whenever their locations in the spectrum are known.

```
$$$$$$$$$$ NEXT CONTROL CARD = SHAPEDO     7.020E+02 6.880F+02 7.130E+02- .          1.000E+00- .


CALIBRATION FIT GAUSSIAN WITH EXPONENTIAL TAILS       RUN NUMBER=GE-E    CHANNEL NUMBER=    702
RUN NUMBER AND INDICATIVE DATA                                                    -0         -0       1550
GE-E   LU-177M 0-500 KEV 1550 CH 4/20/66
GAUSSIAN FIT PARAM.= PEAK HEIGHT PEAK CENTR. GAUS.WIDTH  CONT.CONST. CONT.SLOPE
INITIAL GUESSES     =   1.828E+05   7.020E+02   1.800E+00   6.868E+03  -1.167E+02
INITIAL F OR CHISQR=   9.766E+04
INITIAL GRADIENT    =  -1.150E+00   6.365E+04  -2.877E+05  -1.066E+01   2.480E+01
FINAL F OR CHISQR   =  1.0102E+03+0R-  8.0035E-11
FINAL PARAMETERS    =   1.824E+05   7.016E+02   2.305E+00   7.267E+03  -1.583E+02
FINAL GRADIENT      =  -1.501F-09   9.589E-05   3.109E-05   4.233E-09  -3.754F-07
TAILED GAUSS.PARAM.= CONT.CONST. CONT.SLOPE  PEAK HEIGHT GAUSS.WIDTH LOWW TAIL   HIGH TAIL   PEAK CENTROID
INITIAL GUESSES     =   7.267E+03  -1.583E+02   1.824E+05   2.305E+00   2.147E+00   2.147E+00   7.016E+02

INITIAL F OR CHISQR=   1.363E+03
INITIAL GRADIENT    =   1.866F+00   2.753E+00   2.953E-02   1.703E+04   8.977E+02  -7.293E+03   1.103E+03

FINAL F OR CHISQR   =  1.73914E+02+0R-  3.34513E-11
FINAL PARAMETERS    =   6.938E+03  -1.275E+02   1.838E+05   2.286E+00   1.979E+00   7.780E+00   7.016E+02

FINAL GRADIENT      =   1.648F-08  -1.292E-08   2.018E-09   3.045E-05  -4.775E-05    .         -7.009E-05

CHAN. DEV. CONTINUUM YMIN= 5.491E+03  IIIIIIIIIIIIII SEMILOGARITHMIC SCALE IIIIIIIIIIIIII  YMAX= 1.896E+05     DATA      FIT
 688  -2.2 8.68E+03            $                                                                              8.502E+03 8.707E+03
 689  -1.2 8.55E+03            $                                                                              8.501F+03 8.612E+03
 690   1.3 8.42E+03            $                                                                              8.674F+03 8.552E+03
 691   1.9 8.30E+03           I*.                                                                             8.742F+03 8.568E+03
 692   2.6 8.17E+03           I *                                                                             8.991E+03 8.744E+03
 693   1.5 8.04E+03           I  *                                                                            9.406E+03 9.260E+03
 694  -1.6 7.91E+03          I     .*                                                                         1.033E+04 1.049E+04
 695  -4.2 7.79E+03          I        *                                                                       1.276E+04 1.324E+04
 696    .3 7.66E+03         I            *                                                                   1.924E+04 1.921E+04
 697   4.6 7.53E+03         I              *.                                                                3.281E+04 3.198E+04
 698   4.8 7.40E+03         I                 *                                                              5.996F+04 5.878E+04
 699  -2.4 7.28E+03        I                    .*                                                          1.004E+05 1.012E+05
 700  -3.1 7.15E+03        I                      *                                                         1.477E+05 1.488E+05
 701  -4.6 7.02E+03       I                       .*                                                        1.816F+05 1.836E+05
 702   2.4 6.89E+03       I                        *                                                        1.896F+05 1.886E+05
 703   3.1 6.77E+03      I                          *                                                      1.624E+05 1.612E+05
 704   2.3 6.64E+03      I                           *                                                     1.158E+05 1.150E+05
 705   -.1 6.51E+03      I                             *                                                   6.927E+04 6.929E+04
 706   -.7 6.38E+03     I                               *                                                 3.628F+04 3.642E+04
 707  -4.6 6.26E+03     I                    .*                                                           1.752E+04 1.812E+04
 708  -1.9 6.13E+03    I           .*                                                                     9.815E+03 1.000E+04
 709   -.4 6.00E+03    I  *                                                                             7.008E+03 7.044E+03
 710  -1.0 5.87E+03    I*                                                                               6.026E+03 6.105E+03
 711    .6 5.75E+03    $                                                                                5.831E+03 5.788E+03
 712   1.9 5.62E+03    (.                                                                               5.769E+03 5.625E+03
 713   1.2 5.49E+03    $                                                                                5.584F+03 5.492E+03
       SYMBOLS   I = CONTINUUM  . = DATA   * = FIT    @ = .AND+   ( = IAND+   ) = IAND.   $ = IAND+AND.
SUMDATA=   1.064355E+06SUMCALC=   1.064181E+06


SHAPE CALIBRATION RESULTS
CHI/DEG.FREE =   9.153E+00 SIGMA=     3.025
CP =   701.649  +0R-       .006
CL =     3.916  +0R-       .034
CH =    60.521  +0R-      2.381
CW =     2.286  +0R-       .005
```

Fig. 4. Printed results of a shape-calibration fit. The upper part shows numerical results of the Gaussian and the tailed function, and the lower part a printer graph of the fit and the resulting shape parameters.

The results of a shape-calibration fit can be used directly for energy and efficiency calibrations as well; for the required data cards consult Section 4.

The shape-calibration results can normally be obtained from the spectrum to be analyzed. This calibration needs to be done only once for each experimental setup, and for later runs the parameters may be read into the program (SHAPEIN). The ease of these internal calibration procedures and the fact that no special calibration data are normally needed makes the analysis well suited for different detector systems and experimental situations.

Fitting of Single and Multiple Peaks

Code words FITS
FITDO
FITREPEAT
DATATV

The accurate channel locations and peak areas are determined by fitting, in the least-squares sense, the original data points with the predetermined line shapes and a polynomial approximation for the continuum. For each fit

an interval in the spectrum needs to be specified. This can be done either by the user (FITS, FITREPEAT, DATATV) or by an automatic algorithm (FITDO) described later. The actual fitting procedures are identical in both cases.

The program SAMPO minimizes the weighted sum of squares,

$$\chi^2 = \sum_{i=k-\ell}^{k+m} \frac{\left(n_i - b_i - \sum_{j=1}^{np} f_{ij}\right)^2}{n_i} \qquad (2)$$

where i = channel number,

n_i = counts in channel i,

k = reference channel for background polynomial,

ℓ, m specify the fitting interval,

$b_i = p_1 + p_2(i-k) + p_3(i-k)^2$, background function,

np = number of peaks in the fitting interval,

$$f_{ij} = p_{2+2j} \exp\left[-\frac{(i-p_{3+2j})^2}{2\,w_j^2}\right],$$

for $p_{3+2j} - \ell_j \le i \le p_{3+2} + h_j$,

$$f_{ij} = p_{2+2j} \exp\left[\frac{\ell_j(2i-2p_{3+2j}+\ell_j)}{2\,w_j^2}\right],$$

for $i < p_{3+2j} - \ell_j$,

$$f_{ij} = p_{2+2j} \exp\left[\frac{h_j(2p_{3+2j}-2i+h_j)}{2\,w_j^2}\right],$$

for $i > p_{3+2j} + h_j$.

Here parameters p_1, p_2, and p_3 define the continuum, p_{2+2j} and p_{3+2j} are the height and the centroid of the jth peak, and w_j, ℓ_j, and h_j are the parameters defining the line shape obtained by interpolating linearly the results of the shape analysis of the calibration peaks.

The minimization is again performed by the VARMIT routine. The initial guess required by this algorithm is obtained from a fast, linear least-squares routine (GLSQ) that fits the data with the background approximation plus the correct shape functions, corresponding to the approximate channel locations specified by the user or the search algorithm. The convergence criteria are the same as in the shape analysis.

This computation yields the best values of χ^2 and the parameters, the partial derivatives of χ^2 with respect to parameters calculated, and the error matrix. The channel locations are directly expressed by the best values of p_{3+2j}, and the peak areas are obtained by integrating the shape functions. The final fit is also displayed as a graphical printer plot, showing the original spectral points, the continuum, the sum of the continuum and the shape functions, and the residuals in units of standard deviations of the data points, as represented for a multiplet in Fig. 5. The numerical and graphical information similar to that from a shape calibration fit makes it convenient to establish the goodness of the fit and the presence of previously unobserved photopeaks. In an on-line run the results are also shown on the CRT, as represented for an incomplete and a complete fit in Fig. 6. Each line of a multiplet is drawn separately and the residuals are plotted in the lower part of the plot on a linear scale; the missing component is clearly evident in the upper part of Fig. 6.

From the final value of χ^2 and the error matrix we also get estimates for the uncertainties of the parameters computed. The standard deviation of the channel location of the jth peak, p_{3+2j}, is expressed as

$$\sigma_{3+2j} = (\chi^2 d_{3+2j,\ 3+2j}/nf)^{1/2}, \qquad (3)$$

where nf is the number of degrees of freedom in the fit and $d_{3+2j,\ 3+2j}$ is the corresponding diagonal element of the error matrix. The standard deviation of the peak height, $(\chi^2 d_{2+2j,\ 2+2j}/nf)^{1/2}$ expressed in per cent

```
FITTING INTERVAL   =  1003 (  1033 )  1063          PEAK CHANNELS =   1022   1042   1050
LINEAR LSQ PARAM.  =  CHISQUARE   CONT.CONST.  CONT.SLOPE  CONT.PARAB.  PEAK HEIGHTS
                      2.499E+03   9.161E+02  -1.078E+00  -9.953E-02   2.558E+03   2.063E+04   2.117E+03

FITTING PARAMETERS = CONT.CONST.  CONT.SLOPE  CONT.PARAB.  PEAK HEIGHT PEAK CENTR.  PEAK HEIGHT PEAK CENTR.
INITIAL GUESSES    =  9.161E+02  -1.078E+00  -9.953E-02   2.558E+03   1.022E+03   2.063E+04   1.042E+03
                                                          2.117E+03   1.050E+03
INITIAL F OR CHISQR=  2.499E+03
INITIAL GRADIENT   = -2.091E-12  -1.450E-11  -5.912E-10   8.647E-14   6.278E+02  -7.055E-13   1.110E+04
                                                         -7.128E-13  -8.579E+02
FINAL F OR CHISQR  =  1.75229E+02+08-  7.2759GE-12
FINAL PARAMETERS   =  8.474E+02  -1.442E+00  -1.322E-02   2.664E+03   1.022E+03   2.103E+04   1.042E+03
                                                          2.384E+03   1.050E+03
FINAL GRADIENT     = -1.201E-08   1.372E-06   9.663E-06   1.225E-08   1.534E-05  -6.079E-09  -7.636E-05
                                                          7.295E-09  -1.117E-05

CHAN. DEV. CONTINUUM YMIN= 7.760E+02  IIIIIIIIIIIIII SEMILOGARITHMIC SCALE IIIIIIIIIIIIII  YMAX= 2.166E+04     DATA      FIT
1003  -1.1 8.79E+02      .(                                                                              8.470E+02 8.795E+02
1004    .1 8.79E+02       $                                                                              8.830E+02 8.788E+02
1005   1.0 8.78E+02       $                                                                              9.070E+02 8.782E+02
1006   1.5 8.77E+02       (.                                                                             9.220E+02 8.777E+02
1007   1.4 8.76E+02       (.                                                                             9.210E+02 8.774E+02
1008   1.7 8.76E+02       (.                                                                             9.280E+02 8.774E+02
1009   1.2 8.75E+02       (.                                                                             9.140E+02 8.780E+02
1010  -2.0 8.74E+02     . (                                                                              8.220E+02 8.798E+02
1011  -1.6 8.73E+02     .I+                                                                              8.370E+02 8.839E+02
1012    .7 8.72E+02      I+.                                                                             9.130E+02 8.924E+02
1013  -1.0 8.71E+02      I*                                                                             8.790E+02 9.088E+02
1014  -1.4 8.70E+02      I.*                                                                            8.980E+02 9.401E+02
1015  -4.7 8.69E+02      )   +                                                                          8.610E+02 9.994E+02
1016   -.4 8.68E+02      I     .*                                                                       1.096E+03 1.111E+03
1017   1.4 8.67E+02      I        *.                                                                    1.371E+03 1.319E+03
1018    .1 8.66E+02      I             *                                                               1.710E+03 1.708E+03
1019    .8 8.65E+02      I                 *                                                           2.340E+03 2.300E+03
1020   -.3 8.64E+02      I                    *                                                        2.923E+03 2.940E+03
1021   1.3 8.63E+02      I                       *                                                     3.489E+03 3.409E+03
1022  -1.6 8.62E+02      I                       .+                                                    3.415E+03 3.511E+03
1023   -.2 8.61E+02      I                          *                                                  3.188E+03 3.198E+03
1024    .1 8.60E+02      I                             *                                               2.614E+03 2.609E+03
1025    .2 8.58E+02      I                                *                                            1.979E+03 1.970E+03
1026   1.7 8.57E+02      I                                * .                                          1.523E+03 1.458E+03
1027  -1.8 8.56E+02      I                                  .*                                         1.078E+03 1.136E+03
1028    .6 8.54E+02      I                                  *.                                         9.930E+02 9.747E+02
1029    .2 8.53E+02      I                                  * .                                        9.220E+02 9.153E+02
1030   2.8 8.52E+02      I                                  * .                                        1.002E+03 9.126E+02
1031   1.8 8.50E+02      I                                  *.                                         1.006E+03 9.478E+02
1032   1.3 8.49E+02      I                                    *.                                       1.068E+03 1.026E+03
1033   -.3 8.47E+02      I                                       *                                     1.166E+03 1.176E+03
1034   -.8 8.46E+02      I                                        *                                    1.426E+03 1.455E+03
1035    .2 8.44E+02      I                                           *                                 1.985E+03 1.976E+03
1036    .2 8.43E+02      I                                              *                              2.951E+03 2.943E+03
1037   3.4 8.41E+02      I                                                 *.                          4.977E+03 4.739E+03
1038   2.6 8.40E+02      I                                                    *                        8.294E+03 8.059E+03
1039  -1.2 8.38E+02      I                                                       *                     1.273E+04 1.286E+04
1040  -2.4 8.37E+02      I                                                          .*                 1.751E+04 1.783E+04
1041  -1.4 8.35E+02      I                                                             *               2.104E+04 2.124E+04
1042   -.1 8.33E+02      I                                                             *               2.164E+04 2.166E+04
1043   -.5 8.31E+02      I                                                                *            1.885E+04 1.892E+04
1044   3.1 8.30E+02      I                                                                   *.        1.460E+04 1.473E+04
1045   -.7 8.28E+02      I                                                                      *      9.338E+03 9.403E+03
1046   1.6 8.26E+02      I                                                                       *.    5.907E+03 5.788E+03
1047  -1.5 8.24E+02      I                                                                         .*  3.748E+03 3.841E+03
1048  -1.0 8.23E+02      I                                                                          *  3.138E+03 3.192E+03
1049   -.4 8.21E+02      I                                                                          *  3.168E+03 3.191E+03
1050   -.1 8.19E+02      I                                                                          *  3.260E+03 3.264E+03
1051    .5 8.17E+02      I                                                                         *.  3.121E+03 3.092E+03
1052   2.5 8.15E+02      I                                                                      * .    2.772E+03 2.642E+03
1053   1.2 8.13E+02      I                                                                        *.   2.121E+03 2.065E+03
1054  -2.0 8.11E+02      I                                                                  .*         1.465E+03 1.541E+03
1055  -1.9 8.09E+02      I                                                                    . *      1.108E+03 1.171E+03
1056  -3.1 8.07E+02    I .  +                                                                         8.680E+02 9.591E+02
1057  -2.9 8.05E+02    ) +                                                                            7.790E+02 8.592E+02
1058   -.5 8.03E+02    )+                                                                             8.050E+02 8.192E+02
1059   -.2 8.00E+02    $                                                                              7.980E+02 8.047E+02
1060   -.7 7.98E+02    $                                                                              7.800E+02 7.992E+02
1061   -.7 7.96E+02    $                                                                              7.760E+02 7.963E+02
1062   2.4 7.94E+02    ( .                                                                            8.630E+02 7.979E+02
1063   4.7 7.92E+02    (  .                                                                           9.340E+02 7.917E+02
        SYMBOLS   I = CONTINUUM  . = DATA   + = FIT    * = .AND+   ( = IAND+   ) = IAND.   $ = IAND+AND.
SUMDATA=     1.64729E+05 SUMCALC=     1.64554E+05

    RESULTS FROM THE ABOVE FIT. BE CRITICAL WITH THE  ERROR ESTIMATES
    REJECT IF CHISQUARE =  1.7523E+02   OR  SIGMA =     1.436     IS UNACCEPTABLE. CHECK PLOT FOR MISSING PEAKS
    CHANNEL      FIT-ERR-CH  ENERGY-KEV  CAL-ERR-KEV EN-ERR-KEV   AREA-COUNTS FIT-ERR-PC  INTENS-COUNT CAL-ERR-PC INT-ERR-PC

  1021.7397        .0381     313.7274       .1000       .1005  1.6737E+04      1.4203  5.4304E+07      5.0000      5.1978

  1041.6185        .0123     319.0109       .1000       .1001  1.3274E+05       .3960  4.4771E+08      5.0000      5.0157

  1050.1874        .0494     321.2884       .1000       .1009  1.5077E+04      1.5976  5.1701E+07      5.0000      5.2490
TIMES IN SECONDS=        .062    1.592      .800     8.489    DATE=  12/17/69.
RUN NUMBER AND INDICATIVE DATA
    GF-E   LU-177M 0-500 KEV 1550 CH 6/20/66                                          -0        -0      1550
COMMENTS = 3RD RUN OF GF-E ANALYSIS. CORRECTED FITS AND FINAL TABULATION OF RESULTS.
```

Fig. 5. Printed results of a fit of a multiplet consisting of three components. The upper part shows numerical results of the linear and nonlinear least-squares computations, the lower part the resulting graph and quantities of interest for each line.

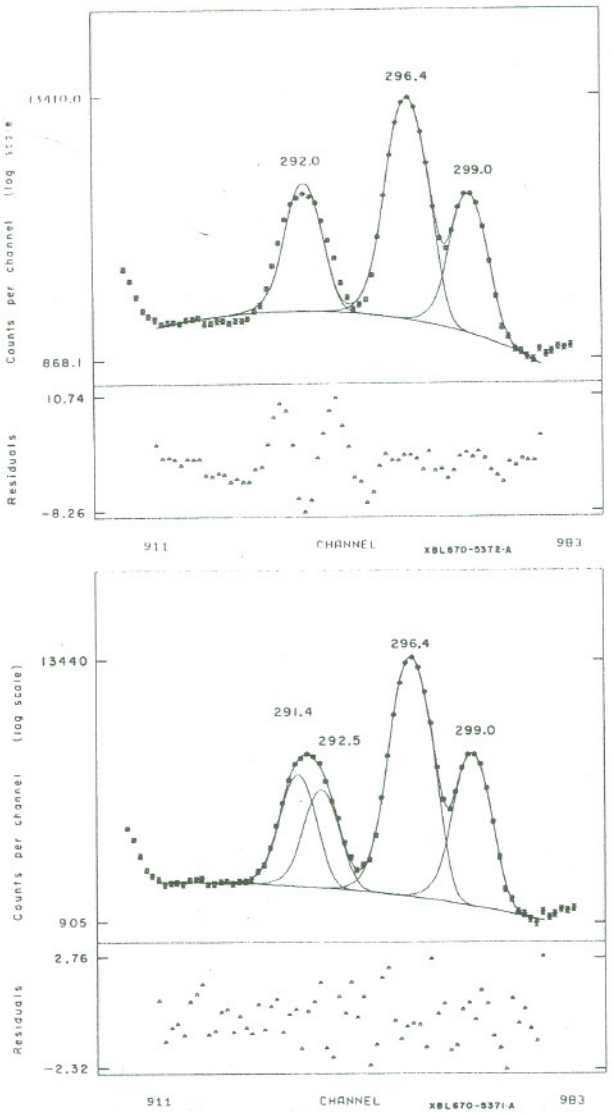


Fig. 6. Two fits to the same region of data in the ^{177m}Lu spectrum. The upper fit has clear indications of a missing component, both in the fit and in the residuals. The complete fit below has small random deviations. Graphs like these are drawn on the CRT display screen with on-line runs.

of the peak height, is taken to be the uncertainty in the peak area.

Automatic Peak Search and Selection of Fitting Intervals	Code words	PEAKFIND PEAKADD PEAKDROP PEAKLIST FITTEST FITDO

SAMPO program is provided with an algorithm which automatically locates the statistically significant peaks in the spectra (PEAKFIND). The significance of a potential peak in channel i is measured as

$$ss_i = dd_i / sd_i, \qquad (4)$$

where the generalized second-difference expression

$$dd_i = \sum_{j=-k}^{k} c_j \, n_{i+j}$$

is divided by its standard deviation,

$$sd_i = \left[\sum_{j=-k}^{k} c_j^2 \, n_{i+j} \right]^{\frac{1}{2}} .$$

The expressions of dd_i and sd_i are obtained by summing over 2k+1 channels the counts per channel, n_i, multiplied by coefficients c_j. These coefficients define a weighting function which is designed to enhance the detection of real photopeaks and to discriminate against statistical fluctuations and spurious peaks. The weighting function is of the form of the second derivative of a Gaussian,

$$c_j = \frac{\sigma^2 - j^2}{\sigma^4} \exp\left(-\frac{j^2}{2\sigma^2} \right), \qquad (5)$$

where σ is the average Gaussian width obtained from the shape-calibration table or provided by the user.

In addition to computing the statistical significance of a potential peak, one uses additional tests based on the expected line shape. Normally two different threshold levels are used to test the significance of the peak. In order to be accepted the peak has to exceed the higher significance level and pass the shape test. Listed but unaccepted peaks provide information on photopeaks that may have to be included in the fitting for a complete analysis. The results from a peak-search computation are illustrated by the printout shown in Table I.

The printout has special columns for editing the list of peaks accepted. Peaks can be added to this list (PEAKADD) or dropped

Table I. Printed results from the peak search computations. Columns for editing these results are provided on the right.

```
$$$$$$$$$$ NEXT CONTROL CARD = PEAKFIND   2.000E+02- .       - .       - .       - .       - .

 PEAK SEARCH     RUN GE-E          1550  CHANNELS
 SEARCH BETWEEN CHANNELS          190       1539
RUN NUMBER AND INDICATIVE DATA
GE-E    LU-177M 0-500 KEV 1550 CH 4/20/66                                        -0        -0       1550

 AVERAGE PEAK WIDTH (SIGMA) =  2.27  AND THE COEFFICIENTS OF THE GENERALIZED SECOND DIFFERENCE ARE
  -100.00     -72.46     -15.24      31.13      44.57      34.09      18.24       7.35       2.31

 SIGNIFICANCE LIMIT FOR THE SEARCH =     2.00     AND FOR FITTING =     4.00
```

I	APPROXIMATE CHANNEL	APPROXIMATE ENERGY	SIGNIFICANCE OF PEAK	CHECK-1 SIGNIF	CHECK-2 SHAPE	ACCEPTED CHANNELS	NUMBER	ADD CHANNEL	DROP CHANNEL
1	242	105.4	832.121			242	1		
2	270	112.9	1074.972			270	2		
3	282	116.1	48.818			282	3		
4	302	121.5	429.690			302	4		
5	328	128.5	760.861			328	5		
6	359	136.8	139.500			359	6		
7	398	147.3	215.779			398	7		
8	420	153.2	627.243			420	8		
9	445	159.9	44.263			445	9		
10	476	168.1	5.583			476	10		
11	489	171.6	198.314			489	11		
12	499	174.3	420.820			499	12		
13	510	177.2	149.277			510	13		
14	528	182.0	7.742			528	14		
15	536	184.2	2.418	SMALL	REJECT				
16	578	195.4	56.326			578	15		
17	610	204.0	368.949			610	16		
18	626	208.2	809.768			626	17		
19	649	214.4	230.805			649	18		
20	663	218.1	146.104			663	19		
21	702	228.5	554.797			702	20		
22	722	233.9	192.862			722	21		
23	736	237.6	2.317	SMALL	REJECT				
24	753	242.1	3.576	SMALL	CHECK				
25	781	249.6	181.928			781	22		
26	816	258.9	4.695		CHECK	816	23		
27	835	264.0	10.832			835	24		
28	853	268.8	120.850			853	25		
29	878	275.5	2.299	SMALL	REJECT				
30	902	281.8	245.352			902	26		
31	940	292.0	48.428			940	27		
32	957	296.5	126.371			957	28		
33	967	299.2	52.416		REJECT				
34	991	305.6	71.329			991	29		
35	1007	309.8	3.681	SMALL	REJECT				
36	1022	313.8	53.448			1022	30		
37	1042	319.1	169.255			1042	31		
38	1052	321.8	3.492	SMALL	REJECT				
39	1074	327.6	228.510			1074	32		
40	1093	332.7	3.030	SMALL					
41	1109	337.0	6.029			1109	33		
42	1127	341.8	61.605			1127	34		
43	1166	352.2	2.697	SMALL	CHECK				
44	1184	357.0	3.932	SMALL	CHECK				
45	1202	361.8	3.195	SMALL	CHECK				
46	1223	367.4	74.050			1223	35		
47	1265	378.6	233.143			1265	36		
48	1289	385.0	71.479			1289	37		
49	1321	393.6	2.423	SMALL					
50	1396	413.8	151.397			1396	38		
51	1414	418.6	169.140			1414	39		
52	1443	426.4	21.515			1443	40		
53	1467	432.8	4.615			1467	41		
54	1481	436.6	4.321		CHECK	1481	42		
55	1494	440.1	3.786	SMALL	REJECT				
56	1529	449.5	2.011	SMALL	REJECT				

from it (PEAKDROP) to ensure its completeness before the more time-consuming fitting procedures. This can be done either by using the on-line facilities with CRT display and light-pen input by using plots such as shown in Fig. 7, or by performing the analysis in two runs. The first run produces a plot of the spectrum and a list of peaks found. This list can then be corrected in the second run on the basis of careful inspection of the spectrum. Some of the smallest components in multiplets may become evident only after fitting of the data. These cases can conveniently be accounted for in the on-line runs or in follow-up runs off-line.

The selection of the fitting intervals can also be done automatically by the code (FITTEST, FITDO). Depending on the closeness of adjacent peaks, one or more lines are included in each fitting interval. The selection algorithm uses information on the peak widths, too. Up to six peaks are normally included in a single interval. If more than six peaks are clustered together the interval is broken at the widest separation between adjacent peaks. If the final interval remains narrower than a specified lower limit, typically 15 $CW_{average}$ (OPTIONS), then no parabolic correction is applied for the continuum. This is done to avoid grossly erroneous background approximations when not enough data are available for determination of the parabolic correction.

Energy Calibrations — Code words: ENDO, ENIN, ENFITDO, ENFITIN, CALDATA, OPTIONS, RESULT

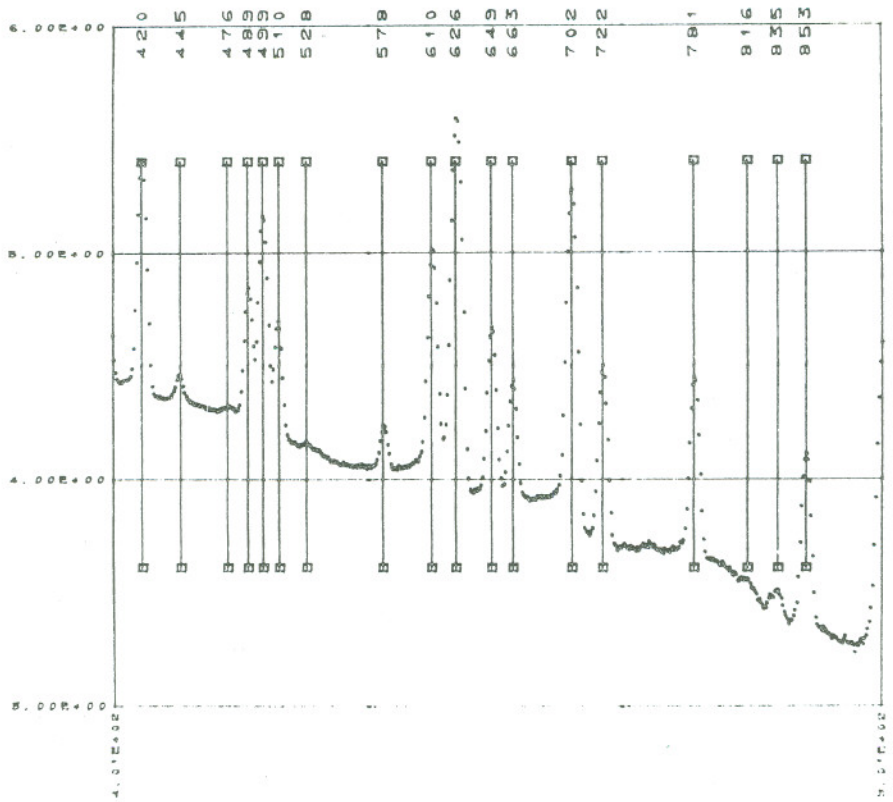
The high resolution of the Ge(Li) systems and the accurate procedures for determination of the centroids and the areas of the photopeaks set stringent requirements for the calibration techniques. Within the computer code we also want a high degree of flexibility in the calibration procedures, for instance, in order to use some fitting results as calibrations for the others.

We have incorporated into program SAMPO two methods of energy calibration. The first routine uses a number of energy-calibration points and interpolates linearly between these points. In the second method a polynomial least-squares fit is made to these points by minimizing the expression

$$\chi^2 = \sum_{i=1}^{n} \frac{1}{D_i}\left[E_i - \sum_{j=1}^{m} p_j C_i^{j-1}\right]^2 \qquad (6)$$

with respect to parameters p_j (ENFITDO). Here C_i, E_i, and D_i are the channel numbers, the corresponding energies, and the calibration uncertainties read in or generated for the linear interpolation scheme (ENDO, ENIN). The minimization is performed by a linear least-squares algorithm, GLSQ. The resulting calibration curve, which is defined by parameters p_j, can then be used for energy determinations (ENFITDO, ENFITIN, OPTIONS, RESULT). In both approaches an estimate of the errors associated with the energy calibration is also needed. These uncertainties reflect inaccuracies in the energies and channel locations of the energy-calibration peaks and expected drifts in the detector system. These uncertainties are expressed as a band around the energy calibration curve, the width of which is specified at different energies and interpolated linearly between them.

The upper part of Fig. 8 summarizes the energy calibration results, as shown on the CRT with on-line runs, which were obtained with a system of very good linearity.[5] The graph shows the integral nonlinearity of the response and the corresponding polynomial fit of fifth order. The linear interpolation and the polynomial expansion give consistent results, and either one may be used. The lower

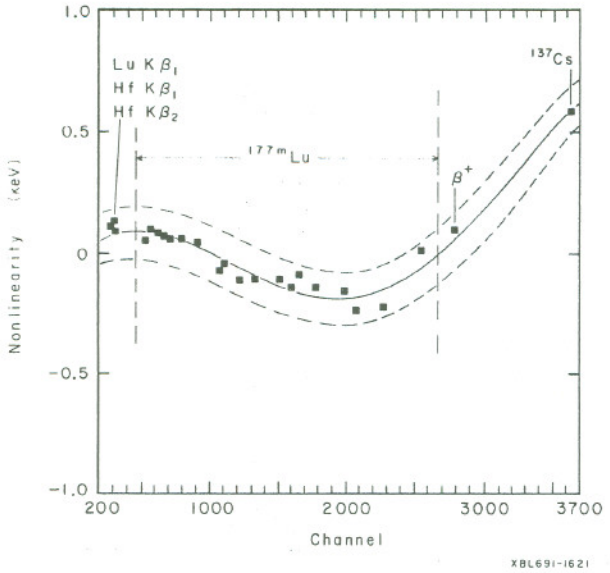


XBL 702-369

Fig. 7. A section of ^{177m}Lu spectrum as shown on the CRT display with indications of peaks found by the search algorithm. With on-line runs corrections can be conveniently made with a light pen.

part of Fig. 8 shows a more significant nonlinearity of a system employing a biased amplifier. Here strong lines of a complex spectrum of ^{176}Ta have been used as internal energy standards.[4] In this case a polynomial of a high order is required to obtain a good fit; however, such a polynomial introduces nonrealistic oscillations between the calibration points. That the polynomial expansion should not be used beyond the extreme data-calibration points is well exemplified by this case.

The energies of the photopeaks are assigned by using either one of the two procedures. The uncertainty in the energy is obtained by adding in root-mean-square sense the calibration error at that energy and the statistical uncertainty in the peak centroid translated into the energy units. In most cases the calibration errors dominate the total uncertainties, and depending on how stable the system is and how much effort is spent in the calibration procedures, the energies of strong lines may be determined with an accuracy up to 0.02 to 0.2 keV or 0.01%.



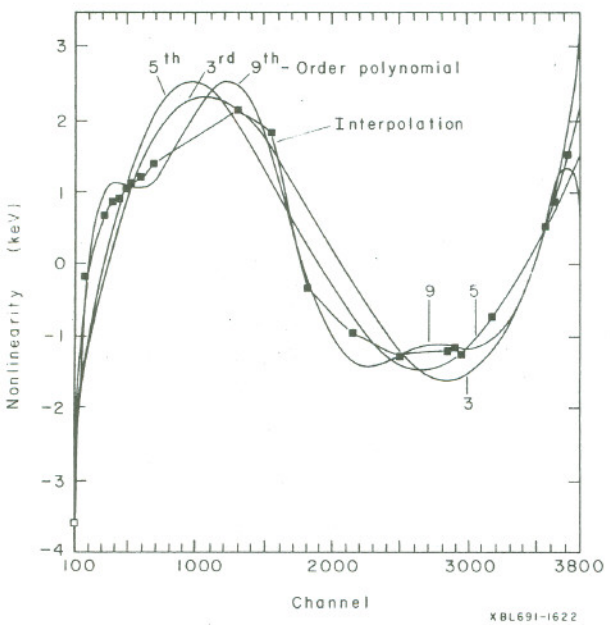


Fig. 8. The result of the energy calibrations of two detector systems. The upper graph shows the calibration points and fifth-order polynomial fit with assigned uncertainties to these points in a system with small nonlinearity. The lower graph shows results with a system with significant nonlinearity; the results caution against the use of polynomial fits in this case.

Efficiency Calibrations

Code words EFDO
EFIN
EFFITDO
EFFITIN
CALDATA
OPTIONS
RESULT

Two methods of efficiency calibrations have been incorporated into program SAMPO. The first scheme uses a number of calibration points and interpolates logarithmically between these points (EFDO, EFIN). The second method (EFFITDO, EFFITIN) employs an approximate functional representation of the efficiency curve expressed as

$$F = p_1\left[E^{p_2} + p_3 \exp(p_4 E)\right] \qquad (7)$$

The parameters p_1, p_2, p_3, and p_4 are determined by using VARMIT routine to minimize the expression

$$\chi^2 = \sum_{i=1}^{m} \left\{ \frac{F_i - p_1\left[E_i^{p_2} + p_3 \exp(p_4 E_i)\right]}{F_i} \right\}^2, \qquad (8)$$

where F_i and E_i are the efficiency and energy points generated or read in for the interpolation scheme.

As with energy calibrations, the calibration uncertainties are expressed as a band around the efficiency curve, the width of which is obtained by interpolating between given values. The overall accuracy obtained depends largely on the stability of the system and on the quality of the calibration data. At best, accuracies approaching the statistical uncertainties--that is, about 1 to 3% --can be obtained with relative intensities of strong lines. The uncertainty in the intensity calculation is again obtained by adding in the root-mean-square sense the calibration and statistical uncertainties.

Tabulation of Results Code words CALDATA
FITIN
RESET
RESULT

The results from the peak-shape, energy, and efficiency calibrations and from peak-search and editing routines, as well as from fitting procedures, are stored in special arrays. These arrays may be modified, erased, or printed out at any time. In general the calibration results remain unchanged until altered. The peak-search and fitting arrays are reset by reading in a new spectrum, or by the user at any time (RESET). The calibration data can be printed also at any time (CALDATA). The fitting results obtained (FITS, FITDO, FITREPEAT) are summarized in a table, such as Table II, which also includes relative intensity and decay-rate computations (RESULT). The shape-calibration and fitting results can be punched on cards to be used in further analysis. These cards can be read back into the program (FITIN), and thus the fitting results can be subjected to new energy and efficiency computations. Thus the more time-consuming fitting procedures need not be repeated to complete the analysis in cases in which not all calibration data were initially available. Similarily these cards can be used for half-life determinations and corrections.

3. STRUCTURE OF THE PROGRAM

SAMPO is written in Fortran IV language and consists of the main program and some 23 subroutines. Additional subroutines may be loaded for on-line displays, for computer plotting, and for reading data on magnetic tapes. The source deck is about 3000 cards long and requires about 28 000 (decimal) core locations to run on a CDC-6600 machine. A schematic block diagram of SAMPO is shown in Fig. 9.

In structuring the code special emphasis has been placed on maintaining a high degree of flexibility and ease in input options to make the code applicable to a wide range of different spectroscopy problems. In the following we make a few comments on some of the design features. These comments concentrate on points that should help the user to make best use of the code or to adapt it with a minimum of difficulty to his computer and his needs.

Input and Output Files

Several disk and tape files are used by program SAMPO for various input and output operations. The names of these files appear on the program card. Not all these files are always necessary; for instance, if the on-line facilities are not used. The complete list of these files is

INPUT, TAPE2=INPUT	for card input data,
OUTPUT, TAPE3=OUTPUT	for printed output,
TAPE14	for punch output,
TAPE5	for spectral data on magnetic tape,
TAPE7	for duplicate result tables,
TAPETTY, TAPE6=TAPETTY	for teletype input and output with on-line runs,
TAPE98	for auxiliary operations with CalComp and CRT plotting,
FILM	for CRT input and output,
PLOT, TAPE99=PLOT	for CalComp plotting of the spectral data.

The input file INTAPE can be changed between card reader and teletype input at any time during an on-line run. This makes it convenient to use the same read statements and input formatting for both devices; see Section 4.

Common Blocks and Dimensions of Arrays

The input and output as well as the calibration data are handled through special common blocks and arrays. These arrays are automatically reset by certain operations or

Table II. The fitting results summarized from the analysis of the spectrum of ^{177m}Lu source. The energies and the intensities of the γ-ray lines were recomputed during the tabulation by using the polynomial and functional fits to the energy and efficiency calibration points.

```
$$$$$$$$$$ NEXT CONTROL CARD = RESULT      2.420E+02 4.000E+00 4.000E+00- .        - .        - .

 RUN NUMBER AND INDICATIVE DATA
GE-E   LU-177M 0-500 KEV 1550 CH 4/20/66                                          -0         -0      1550
COMMENTS = 3RD RUN OF GE-E ANALYSIS. CORRECTED FITS AND FINAL TABULATION OF RESULTS.          DATE =   12/17/69.

ENERGIES RECOMPUTED USING OPTION  4

INTENSITIES RECOMPUTED USING OPTION  4

TABLE OF RESULTS
```

NUMBER	CHANNEL	CHANNEL ERROR	ENERGY IN KEV	ENERGY ERROR	AREA COUNTS	PC-AREA ERROR	INTENSITY	INTENSITY ERROR PC	RELATIVE INTENSITY	REL.INT. ERROR PC	INTENSITY PER TIME
1	241.834	.001	105.317	.100	2.079E+06	.17	5.6171E+08	5.00	1.000E+02	7.075	5.6171E+08
2	270.119	.002	112.920	.100	3.271E+06	.23	1.0077E+09	5.01	1.794E+02	7.077	1.0077E+09
3	281.581	.108	116.001	.104	7.993E+04	3.80	2.5962E+07	6.28	4.622E+00	8.029	2.5962E+07
4	286.699	.394	117.376	.146	2.187E+04	15.18	7.2718E+06	15.98	1.295E+00	16.747	7.2718E+06
5	302.448	.008	121.607	.100	7.837E+05	.56	2.7998E+08	5.03	4.984E+01	7.095	2.7998E+08
6	328.084	.004	128.492	.100	1.793E+06	.18	7.1878E+08	5.00	1.280E+02	7.075	7.1878E+08
7	358.745	.008	136.722	.100	1.438E+05	.35	6.5893E+07	5.01	1.173E+01	7.082	6.5893E+07
8	392.390	.034	145.748	.100	7.767E+04	1.34	4.1003E+07	5.18	7.300E+00	7.199	4.1003E+07
9	397.630	.006	147.153	.100	2.943E+05	.41	1.5875E+08	5.02	2.826E+01	7.085	1.5875E+08
10	420.456	.005	153.273	.100	1.301E+06	.23	7.6983E+08	5.01	1.371E+02	7.077	7.6983E+08
11	444.658	.044	159.759	.101	3.599E+04	1.86	2.3413E+07	5.33	4.168E+00	7.314	2.3413E+07
12	477.660	.326	168.598	.133	9.992E+03	9.04	7.3642E+06	10.33	1.311E+00	11.478	7.3642E+06
13	489.782	.013	171.844	.100	2.819E+05	.50	2.1718E+08	5.02	3.866E+01	7.091	2.1718E+08
14	499.288	.007	174.388	.100	7.080E+05	.27	5.6459E+08	5.01	1.005E+02	7.078	5.6459E+08
15	508.976	.017	176.981	.100	1.831E+05	.68	1.5112E+08	5.05	2.690E+01	7.106	1.5112E+08
16	527.844	.226	182.029	.117	3.781E+03	9.28	3.3349E+06	10.54	5.937E-01	11.668	3.3349E+06
17	578.397	.004	195.546	.100	3.586E+04	1.17	3.7452E+07	5.14	6.668E+00	7.169	3.7452E+07
18	610.419	.012	204.102	.100	5.255E+05	.52	6.0750E+08	5.03	1.082E+02	7.092	6.0750E+08
19	626.358	.001	208.359	.100	2.183E+06	.22	2.6502E+09	5.00	4.718E+02	7.077	2.6502E+09
20	649.079	.007	214.426	.100	2.192E+05	.47	2.8492E+08	5.02	5.072E+01	7.089	2.8492E+08
21	662.815	.008	218.092	.100	1.100E+05	.77	1.4883E+08	5.06	2.650E+01	7.115	1.4883E+08
22	701.645	.002	228.452	.100	1.068E+06	.25	1.6140E+09	5.01	2.873E+02	7.078	1.6140E+09
23	721.812	.019	233.831	.100	1.529E+05	.80	2.4427E+08	5.06	4.349E+01	7.118	2.4427E+08
24	781.119	.003	249.640	.100	1.428E+05	.31	2.6668E+08	5.01	4.748E+01	7.080	2.6668E+08
25	830.729	.407	262.856	.147	2.094E+03	14.52	4.4209E+06	15.36	7.870E-01	16.151	4.4209E+06
26	835.321	.227	264.079	.117	3.898E+03	7.59	8.3230E+06	9.09	1.482E+00	10.375	8.3230E+06
27	852.890	.013	268.758	.100	6.614E+04	.53	1.4726E+08	5.03	2.622E+01	7.093	1.4726E+08
28	901.712	.008	281.758	.100	2.441E+05	.30	6.0820E+08	5.01	1.083E+02	7.080	6.0820E+08
29	908.910	.120	283.674	.105	7.287E+03	4.25	1.8454E+07	6.56	3.285E+00	8.250	1.8454E+07
30	938.479	.093	291.546	.103	1.742E+04	3.93	4.7089E+07	6.36	8.383E+00	8.092	4.7089E+07
31	942.369	.120	292.582	.105	1.376E+04	4.78	3.7521E+07	6.92	6.680E+00	8.537	3.7521E+07
32	956.829	.014	296.431	.100	7.633E+04	.54	2.1472E+08	5.03	3.823E+01	7.094	2.1472E+08
33	966.586	.028	299.029	.100	2.445E+04	1.08	7.0225E+07	5.12	1.250E+01	7.155	7.0225E+07
34	990.855	.023	305.490	.100	2.584E+04	.93	7.8107E+07	5.09	1.391E+01	7.134	7.8107E+07
35	1021.740	.038	313.713	.101	1.674E+04	1.42	5.3893E+07	5.20	9.594E+00	7.214	5.3893E+07
36	1041.619	.012	319.007	.100	1.327E+05	.40	4.4483E+08	5.02	7.919E+01	7.084	4.4483E+08
37	1050.187	.049	321.289	.101	1.508E+04	1.60	5.1392E+07	5.25	9.149E+00	7.252	5.1392E+07
38	1074.161	.010	327.675	.100	2.212E+05	.39	7.9024E+08	5.02	1.407E+02	7.084	7.9024E+08
39	1109.346	.148	337.050	.107	9.711E+02	4.90	3.7108E+06	7.00	6.606E-01	8.605	3.7108E+06
40	1126.598	.013	341.648	.100	1.918E+04	.49	7.5684E+07	5.02	1.347E+01	7.090	7.5684E+07
41	1223.195	.002	367.424	.100	2.866E+04	.63	1.3453E+08	5.04	2.395E+01	7.101	1.3453E+08
42	1264.699	.012	378.518	.100	2.549E+05	.46	1.2846E+09	5.02	2.287E+02	7.088	1.2846E+09
43	1289.063	.051	385.037	.101	2.677E+04	1.91	1.4053E+08	5.35	2.502E+01	7.326	1.4053E+08
44	1395.533	.014	413.598	.100	1.226E+05	.51	7.6356E+08	5.03	1.359E+02	7.091	7.6356E+08
45	1413.489	.012	418.429	.100	1.469E+05	.46	9.4038E+08	5.02	1.674E+02	7.088	9.4038E+08
46	1442.663	.036	426.287	.100	3.071E+03	1.86	2.0554E+07	5.33	3.659E+00	7.314	2.0554E+07
47	1466.055	.467	432.597	.161	5.018E+02	15.00	3.4780E+06	15.81	6.192E-01	16.584	3.4780E+06
48	1470.844	.494	433.889	.167	4.822E+02	15.48	3.3664E+06	16.27	5.993E-01	17.019	3.3664E+06
49	1480.275	.309	436.437	.130	3.454E+02	12.08	2.4453E+06	13.07	4.353E-01	13.998	2.4453E+06
50	1494.453	.375	440.269	.142	3.589E+02	11.68	2.5943E+06	12.71	4.619E-01	13.655	2.5943E+06
51	1501.532	.482	442.183	.164	2.885E+02	13.11	2.1072E+06	14.03	3.751E-01	14.896	2.1072E+06

```
COUNTING TIME =  1.0000E+00
```

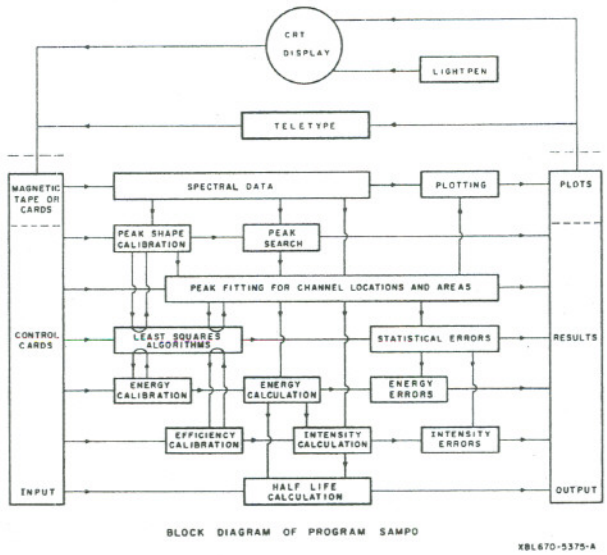


Fig. 9. Schematic block diagram of program SAMPO.

can be reset by the user at any time. For an efficient use of the program it is important to consider the following arrays and blocks of arrays:

COMM / 1 / SPEC(1600), LABEL(20) contains the spectral data in the array SPEC and the indicative data in the array LABEL. These arrays are read in either on cards or input tape 5 (DATAIN). When required by the number of channels in the spectra to be analyzed, the length of the SPEC array can be changed--for instance, to 4100. The indicative data array contains an alphanumeric spectrum number LABEL(1), alphanumeric information on the spectrum in LABEL(2) through LABEL(13), integer labels LABEL(14) and LABEL(15), not used by the general-purpose version, and the number of channels in the spectrum LABEL(16). The LABEL array is printed out under FORMAT(13A6, 3I10) at various places in the printout.

COMMON/ 2 /XDATA(150), YDATA(150), WEIGHT(150), YCALC(150), YCONT(150), HMATR(20, 20), CMATR(20, 20), HDIAGO(20), BUF(400): These arrays are used for temporary working storage in the least-squares, tape-reading, and data-display routines. This space is sometimes overlayed by other temporary arrays in some subroutines. The present dimensions, which can be changed (although not very easily), limit the maximum width of a fitting interval to 150 channels and the number of lines in one fit to six.

COMMON/ 3 / contains the following result arrays:

NPEAK(100) approximate peak centroids as specified by the search routine or by the user,

FITCH(100) accurate peak centroids as computed in the fitting,

CHER(100) statistical uncertainties in the

channel locations,
PEAK(100) areas of photopeaks as computed in the fitting,
PKER(100) statistical uncertainties in peak areas,
ENERG(100) energies of the fitted photopeaks,
ENER(100) photopeak energy uncertainties,
EFFSUM(100) intensities of fitted photopeaks,
EFER(100) uncertainties in photopeak intensities.

Depending on the complexity of the spectra and considerations of field length requirements, the dimensions of these arrays can be changed--for instance, up to 200.

COMMON/IOTAPE/INTAPE, IOUTAP, KOUT specifies input and output files. These are initially specified as INTAPE = 2 and IOUTAP = 3 corresponding to the standard file names at LRL. Furthermore the input file name can be changed between card and teletype input, as discussed in the section on input and output files.

Arrays CPREAD(20), CLREAD(20), CHREAD(20), CWREAD(20), which are stored in subroutine SHAPE, contain the shape calibration results generated (SHAPEDO) or read in (SHAPEIN). The shape parameters for fitting are obtained by interpolating these values linearly with respect to the channel numbers.

Arrays CHREAD(50), ENREAD(50), ERREAD(50) in subroutine ENERGY contain the energy calibration points generated (ENDO) or read in (ENIN) for the energy determinations through linear interpolation. Similarily the arrays PLREAD(10), ERENER(50), ERVALU(50) contain the coefficients generated (ENFITDO) or read in (ENFITIN) for a polynomial energy curve and the associated calibration error arrays which are interpolated linearly.

Arrays ENREAD(50), EFREAD(50), ERREAD(50) in subroutine EFF contain the efficiency calibration points generated (EFDO) or read in (EFIN) for logarithmic interpolation. Similarily the arrays PRREAD(4), ERENER(50), ERVALU(50) have the parameters generated (EFFITDO) or read in (EFFITIN) for the functional efficiency curve and the associated calibration uncertainties.

Reading Spectral and Indicative Data on Input Tape

If large numbers of spectra are handled, the spectral and indicative data can be conveniently stored on and read from high-density magnetic tapes. In SAMPO a reference is made to such input tape, tape 5, on the program card. Since no uniform standards exist for writing such data tapes, even within the same laboratory, separate tape-reading routines are needed for different tape formats. SAMPO library at LRL–Berkeley contains several such routines, of which the user needs to load an appropriate one; see information on SAMPO library in Section 6.

The main program has a call statement to the tape-reading routine (DATAIN) of the form CALL DATAT1 (KERROR, SPEC, LABEL, WHAT, NAME, XDATA). Here KERROR is an error flag which should be returned as KERROR = 0 when the spectrum specified is successfully read, and as KERROR = 1 when the spectrum is not found or read properly. If KERROR = 1 is returned, the main program will skip operations where the spectral data would be needed, normally up to the next data read. The spectral data are read into array SPEC, the maximum dimension of which is specified in the main program. The indicative data are read into the array LABEL in the format specified in the section on common blocks and arrays. Up to six numbers and one alphanumeric word are transferred through WHAT and NAME to the tape-reading routine to identify the spectrum to be searched and to perform spectral additions or subtrac-

tions if required; see Section 4. The array XDATA marks the beginning of temporary arrays of total length of 1970 words; this space can be used by the tape-reading routine for temporary working space.

Except for a possible tape-reading routine, program SAMPO is self-contained. The user needs only supply data and indicate which options and calculations are desired.

4. PROGRAM OPTIONS AND DATA INPUT

In the earlier sections references have been made to different SAMPO execution options and input cards. These options and cards are discussed in detail in this section.

The large number of options can be controlled and specified by SAMPO input cards. These cards are processed by the main program and they may be sequenced in any logical fashion. Illegal input cards are generally rejected, similarily data cards following an unsuccessful data-tape reading are ignored if the presence of the spectral data would be required for the operation requested. In general all the program parameters have been initially set, and remain unchanged until altered. The altered value will remain in effect until further changed. The same applies to the different calibration data.

The logical sequencing of the input cards simply means that the spectral and calibration data must be read in or generated before they are used for computations. Thus, for instance, the energy determination can be done during fitting if data for this are known in advance. If the energy calibration is performed by using the fitting results, then the energy determinations need to be postponed until tabulation of the results. Illustrations with examples of possible input card sequencing are given in Section 5.

For uniformity all SAMPO input cards have the same format, namely FORMAT(A10, 6E10.0, A10). The first word is a left-adjusted code word, CODEW, which identifies the function of the input card. Up to six numbers (WHAT(I), I = 1,6) follow the code word; the interpretation of these numbers depends on the CODEW. The last word is an alphanumeric word, NAME, which can be used to identify the data or computation it belongs to; it is not used by the program, except possibly to specify spectrum numbers for input tape-reading routines. The uniformity of the input cards also requires that the parameters that ordinarily are integers be read in as decimal (floating-point) numbers; they will be converted into integers by the program.

Although the code words can be up to ten letters long, the first six letters suffice to identify them; this is of advantage with those computers for which the maximum length of words is six letters. The teletype input sometimes requires an additional word to indicate the end of the line, and thus the input card format may be also written as FORMAT(A6, A4, 6E10.0, A6, A4, I1). This change does not cause any changes in the use of the input cards.

An alphabetic list of the code words was given in the beginning of this report. The explanation of their functions and associated parameters is given in the rest of this chapter. In general the default option of a parameter is specified by a blank or zero number; this minimizes the amount of numerical input data required. The result and calibration arrays will be automatically ordered, so that the order of inputting calibration data dards is not crucial.

Chapter 5 contains illustrative examples and useful comments on the use of the code words which are described in detail in the rest of this Chapter 4. The reader may find it easier to go directly to Chapter 5 in the first reading and look up the code words in this chapter, only as they appear in the examples used. Later he can use the rest of this chapter as the basic handbook for running program SAMPO.

DATAIN reads indicative and spectral data.

WHAT(1) = 0. searches and reads the spectrum specified on input tape 5;

= 1. specifies that the indicative and spectral data are on cards, spectral data in FORMAT(10F7.0). The indicative data are on one card between DATAIN and the spectrum as follows: alphanumeric run number in columns 1–6, alphanumeric indicative data in columns 7–66, and an integral number of channels in columns 76–80.

= 2. reads data on cards as with WHAT(1) = 1., except that the spectral data are in format specified on a card between DATAIN and indicative data card, for example (5(5X, F8.0)). The variable format also allows the user to shift the spectrum or delete channels, if desired.

WHAT(2) $\neq$ 0. adds previous spectrum multiplied by WHAT(2) to the new spectrum.

WHAT(3) $\neq$ 0. multiplies the new spectrum by WHAT(3) before the addition. Normally WHAT(2) and WHAT(3) would be blank.

DATAGRAPH makes a printer graph of the spectrum.

WHAT(1) = 0. for semilogarithmic scale,

= 1. for linear scale.

WHAT(2) every WHAT(2) channel is plotted; if blank, every channel;

WHAT(3) is the starting channel; if blank, the first channel;

WHAT(4) is the termination channel; if blank, the last channel;

WHAT(5) channels in each subdivision; if blank, 100 channels.

DATAPLOT makes a CalComp point plot of the spectrum. If the peak search is done before the plotting then the peaks found are also plotted. For standard plots specify four-cycle semilogarithmic paper, No. 40, and liquid ink pen.

WHAT(1) = 0. specifies four-cycle semilogarithmic paper,

= 1. specifies plain paper.

WHAT(2) is the starting channel; if blank, the first channel;

WHAT(3) is the termination channel; if blank, the last channel;

WHAT(4) is the upper bound of the counts-per-channel scale; if blank, this is set and re-scaled, if required, automatically;

WHAT(5) is the lower bound of the count scale; if blank, set automatically;

WHAT(6) specifies channels per inch; if blank, set automatically, normally 40 channels to an inch.

SHAPEDO performs a shape-calibration fit. This should be done by using strong single lines. In specifying the fitting interval include enough channels to cover both tails, but do not overextend to include fluctuations due to neighboring peaks. The resulting parameters will be stored and used in the fitting analysis. The shape parameters need to be computed only once for each experimental setup; the values will remain unchanged until altered, and can be read in for later runs with SHAPEIN cards. The resulting shape parameters are also written on tape 14 for getting SHAPEIN cards punched.

WHAT(1) is the approximate center channel of the calibration peak,
WHAT(2) specifies the lower limit of the fitting interval,
WHAT(3) is the upper limit of the fitting interval.
WHAT(4) = 0. for no energy or efficiency calibrations;
= 1. for using the fitted peak centroid for the energy calibration, place ENDO card with the energy and the calibration error after SHAPEDO card;
= 2. for using the fitted peak area for the efficiency calibration, place EFDO card with the correct peak intensity and calibration error after SHAPEDO card.
= 3. if both energy and efficiency calibrations are performed as instructed above,
WHAT(5) = 0. adds the resulting parameters to the present table of shape parameters,
= 1. starts a new shape parameter table with the resulting values.
WHAT(6) is the initial guess for the CW-parameter; if blank, set to 1.8.

SHAPEIN reads in and stores the shape parameters computed previously. This should be preferred over SHAPEDO, whenever possible, to minimize the computing required; the user may also check and correct the shape parameters before reading them in.
WHAT(1) is the peak centroid in channels;
WHAT(2) is the CL parameter specifying the lower tailing,
WHAT(3) is the CH parameter specifying the higher tailing;
WHAT(4) is the CW parameter specifying the peak width;
WHAT(5) = 0. adds the values to the existing shape parameter table,
= 1. starts a new shape parameter table.

PEAKFIND searches and lists statistically significant peaks; this must be performed before PEAKADD, PEAKDROP, or FITDO commands.
WHAT(1) is the starting channel for the search; if blank, channel 50;
WHAT(2) is the termination channel; if blank the last channel;
WHAT(3) is the significance limit for listing peaks; if blank, the existing value, initialized 2., is used;
WHAT(4) is the significance limit for fitting peaks with FITDO; if blank, the existing value, initialized 4., is used;
WHAT(5) is the average value for the CW parameter; if blank, the average value obtained from the shape-parameter table is used.
WHAT(6) = 0. rejects the peaks which do not pass the shape test,
= 1. does not reject such peaks.

PEAKADD adds peaks to the list of peaks to be fitted. Use this option to correct the list of found peaks before peak fitting. The search routine should be executed (PEAKFIND) before this.
WHAT(I), I = 1,6 are the approximate channel numbers of the peaks to be added, in any order.

PEAKDROP drops peaks from the list of found peaks. See comments regarding PEAKADD;
WHAT(I), I = 1,6 are the channel numbers of the peaks to be dropped.

PEAKLIST prints the corrected list of peaks found.

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

FITDO performs complete nonlinear fits of peaks found by the search algorithm. Selection of the fitting intervals and the peaks included in each fit is done automatically as in FITTEST. The peak search and editing has to be performed before FITDO, similarily the shape parameters have to be generated or read in before this, as well as energy and efficiency calibrations, if specified on OPTIONS card.

FITS performs complete nonlinear fits of intervals specified on the following cards. The computation is the same as performed with FITDO, only complete control over the selection of the fitting intervals is possible. Up to 200 numbers read on the following cards are stored to be used with FITREPEAT, if desired.

WHAT(1) is the number of fitting intervals specified on following WHAT(1) cards.

WHAT(3) = 0. specifies automatic initial guesses,

= 1. if the initial guesses are read in for each peak amplitude in FORMAT(8E10.0) after each card specifying the fitting interval,

WHAT(5) = 0. adds the results to the existing list of fitted peaks,

= 1. starts a new list of fitted peaks.

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

Column 1-5 the number of peaks in the interval, up to six allowed.

6-10 the channel defining the lower limit of the interval;

11-15 the upper limit of the fitting interval;

16-20 the centroid of the parabolic correction in the background polynomial; if blank, assigned automatically;

21-25 the approximate centroid of the first peak in the interval,

26-30 the centroid of the second peak in the interval;

31-35 etc., up to the specified number of peaks.

36-40 number of peaks.

FITREPEAT repeats the cases specified by last FITS card. Only channel numbers read in under FORMAT (16 I 5) were stored, not the special initial guesses. WHAT(5) has the same meaning as with FITS.

FITIN reads in the fitting results on punched cards. The format is the same as used in punching results.

WHAT(1) is the number of peaks to be read in,

WHAT(5) = 0. adds the results to the existing list of fitted peaks,

= 1. starts a new list of fitted peaks.

FITIN card is followed by WHAT(1) cards each as follows,

Columns	Format	
2- 9	F8.3	the exact centroid of the peak expressed in channels,
10-14	F5.3	the statistical uncertainty of the centroid.
15-23	F9.3	the exact energy in keV,
24-29	F6.3	the uncertainty in energy in keV.
30-40	E11.4	the photopeak area, from the fitting,
41-46	F6.2	the statistical uncertainty of peak area.
47-57	E11.4	the photopeak intensity,
58-63	F6.2	the uncertainty in peak intensity in per cent,
64-74	E11.4	the photopeak intensity per time unit.
75-80	A6	the spectrum number.

ENDO — assigns an energy calibration point for the linear interpolation by using a fitted peak centroid obtained previously with FITDO or FITS. The energy determinations can then be performed by using some of the fitted lines as internal energy standards. See OPTIONS and RESULT cards.

WHAT(1) — is the approximate channel location for the calibration line; it has to be correct within 3 channels, or as specified by WHAT(4).

WHAT(2) — is the energy in keV,

WHAT(3) — is the calibration uncertainty in keV.

WHAT(4) $\neq$ 0. — changes the accuracy tolerance of peak centroid to WHAT(4),

WHAT(5) = 0. — adds the values to the existing energy-calibration table,

= 1. — starts a new energy-calibration table.

ENIN — reads in an energy-calibration point to be used in the linear interpolation. See OPTIONS and RESULT cards,

WHAT(1) — is the exact channel location of the calibration line.

WHAT(2) — is the energy in keV,

WHAT(3) — is the calibration uncertainty in keV,

WHAT(5) = 0. — adds the values to the existing energy-calibration table,

= 1. — starts a new energy-calibration table.

ENFITDO — performs a polynomial fit to the points generated or read in for the linear interpolation with ENDO or ENIN. The resulting curve may be used for the subsequent energy determinations. See OPTIONS and RESULT cards. The calibration uncertainties will be the same as specified for the linear interpolation.

WHAT(1) — is the number of terms in the polynomial fit, that is, one plus the degree of the polynomial. If enough energy-calibration points are available, polynomials up to 8th degree can be used,

WHAT(2) = 0. — specifies no CRT display of the results,

= 1. — displays on the CRT the nonlinearity of the polynomial and the interpolation table between the first and the last calibration points,

= 2. — displays the nonlinearity over the whole range of the spectrum.

ENFITIN reads in a coefficient for the polynomial curve computed before,

WHAT(1) is the value of the polynomial coefficient,

WHAT(2) is the energy in keV for the calibration uncertainty point,

WHAT(3) is the calibration uncertainty in keV.

WHAT(4) is the number of the coefficient, that is, one plus the degree of the term. Value 1. starts a new coefficient list,

WHAT(5) = 0. adds the energy-calibration uncertainty to the existing list,

= 1. starts a new energy-calibration uncertainty table.

EFDO assigns an efficiency calibration point for the logarithmic interpolation by using a fitted peak area obtained previously with FITDO or FITS. The intensity determinations can then be performed by using some of the fitted lines as internal intensity standards. See OPTIONS and RESULT cards.

WHAT(1) is the approximate energy of the calibration point; it has to be correct within 3 keV or as specified by WHAT(4).

WHAT(2) is the intensity of the peak at the energy WHAT(1).

WHAT(3) is the calibration uncertainty in per cent.

WHAT(5) = 0. adds the values to the existing efficiency-calibration table,

= 1. starts a new efficiency-calibration table.

EFIN reads in an efficiency-calibration point to be used in the logarithmic interpolation. See OPTIONS and RESULT cards.

WHAT(1) is the energy of the calibration point,

WHAT(2) is the corresponding efficiency,

WHAT(3) is the calibration uncertainty in per cent.

WHAT(5) = 0. adds the values to the existing efficiency calibration table,

= 1. starts a new efficiency-calibration table.

EFFITDO performs a functional fit to the points generated or read in with EFDO or EFIN. The resulting curve may be used for the subsequent intensity determinations. See OPTIONS and RESULT cards. The calibration uncertainties will be the same as with the logarithmic interpolation. The function used is of the form

$$F = p_1 (E^{p_2} + p_3 \exp(p_4 E)),$$

where F is the efficiency, p_1, p_2, p_3, and p_4 are the parameters to be determined, and E is the energy in keV.

WHAT(1) is the initial guess for parameter p_1; if blank, set to 1000.

EFFITIN reads in a parameter computed before for the functional fit of the above form, plus a point for the calibration uncertainty.

WHAT(1) is the energy for the calibration uncertainty point,

WHAT(2) is the value of the parameter,

WHAT(3) is the calibration uncertainty in per cent,

WHAT(4) is the index of the parameter, that is 1., 2., 3., or 4.,

WHAT(5) = 0. adds the calibration uncertainty point to the existing table,

= 1. starts a new calibration uncertainty table.

EFFITADJ adjusts the functional form of the efficiency calibration curve by changing the parameter p_1,

WHAT(1) is the energy of the adjustment point,

WHAT(2) is the efficiency at that energy,

WHAT(4) = 1. adjusts the parameter stored in the program,

= 2. adjusts the parameter generated or read in with EFFITDO or EFFITIN.

CALDATA prints the calibration data for the shape, energy, and efficiency determinations.

WHAT (1) specifies the shape calibration to be printed,

= 0. prints no data,

= 1. prints the arrays permanently stored in the program,

= 2. prints the arrays generated or read in with SHAPEDO or SHAPEIN.

WHAT(2) specifies the energy calibration to be printed,

= 0. prints no data,

= 1. prints the arrays permanently stored in the program for the linear interpolation,

= 2. prints the arrays generated or read in with ENDO or ENIN for the linear interpolation.

= 3. prints the coefficients permanently stored for the polynomial curve,

= 4. prints the coefficients generated or read in with ENFITDO or ENFITIN for the polynomial curve.

WHAT(3) specifies the efficiency calibration to be printed,

= 0. prints no data,

= 1. prints the arrays permanently stored for the logarithmic interpolation,

= 2. prints the arrays generated or read in with EFDO or EFIN for the logarithmic interpolation,

= 3. prints the coefficients permanently stored for the functional efficiency curve,

= 4. prints the coefficients generated or read in with EFFITDO or EFFITIN for the functional curve.

OPTIONS specifies the calibrations and other options for the program; these options should be specified before the computations, and they can be changed at any time.

WHAT(1) specifies the shape calibration option for the fitting,

= 1. specifies the arrays permanently stored in the program,

= 2. specifies the arrays generated or read in with SHAPEDO or SHAPEIN. This is the initially specified value.

WHAT(2) specifies the energy calibration for the peak fitting,

= 0. for no energy determinations, this is the initially specified value.

= 1. specifies the linear interpolation stored permanently,

= 2. specifies the linear interpolation generated or read in with ENDO or ENIN,

= 3. specifies the polynomial curve permanently stored,

= 4. specifies the polynomial curve generated or read in with ENFITDO or ENFITIN.

WHAT(3) specifies the efficiency calibration for the peak fitting,

= 0. for no intensity determinations, this is the initially specified value.

= 1. specifies the logarithmic interpolation permanently stored,

= 2. specifies the logarithmic interpolation generated or read in with EFDO or EFIN,

= 3. specifies the functional curve permanently stored,

= 4. specifies the functional curve generated or read in with EFFITDO or EFFITIN.

WHAT(4) specifies when only linear background approximation instead of the parabolic curve is used. Whenever the fitting interval measured in units of the CW parameter remains smaller than a specified parameter, initially 15, then only linear background is used.

$\neq 0.$ changes the parameter to WHAT(4).

WHAT(6) specifies the display of the fitting results on the CRT. See comments on on-line runs.

= 0. for no display of the fitting results, this is the initially specified value,

= 1. for the display with interactive on-line runs with VISTA console,

= 2. for the CRT camera pictures with off-line runs.

RESULT tabulates the fitting results accumulated, recomputes energies and intensities, if desired, and computes relative intensities and decay rates.

WHAT(1) specifies the reference peak for the relative intensity computations,

= 0. specifies the strongest peak as the reference peak,

$\neq 0.$ specifies the peak approximately in channel WHAT(1) as the reference peak.

WHAT(2) $\neq 0.$ specifies that the energies should be recomputed by using the option as specified by WHAT(2). See OPTIONS card.

WHAT(3) $\neq 0.$ specifies that the intensities should be recomputed by using the option as specified by WHAT(3). See OPTIONS card.

WHAT(4) = 0. for no punching of the results,

= 1. for punching one card for each line fitted; these cards can be read back to SAMPO for additional energy and intensity computations without repeating the fitting procedures.

WHAT(5) is the counting time for the decay rate computations; if blank, taken to be one time unit.

COMMENTS reads alphanumeric comments on the following card to be printed with fitting results and tables. Comments are initially blank.

RESET resets the arrays for peak search and fitting results; this can be used to break up the analysis of very complex spectra into smaller parts. The arrays are automatically reset by reading in a new spectrum.

CPTIME prints the central processor time elapsed in seconds.

STOP terminates the computations and endfiles the disk files used.

On-line usage

At LRL–Berkeley program SAMPO can be run in an interactive fashion by using the VISTA display system and teletype input and output. With on-line runs most of the input data should, however, be read on cards and only corrective statements made through the slow teletype input. The spectral data, the results from the peak-search routines as well as peak fitting, and energy calibrations can be displayed. The display can also be used in off-line runs to get high-resolution CRT pictures of the spectra and the fitting results. For these options see OPTIONS and ENFITDO

cards, also check the control cards required in Section 6. The specific control cards and VISTA keyboard options for on-line runs are listed below.

DAYFILE — displays the current dayfile of SAMPO run on the CRT. Put this card in the beginning of the data input deck for on-line runs; the dayfile is useful with the automatic recovery procedure described in SAMPO information in Chapter 6; push red I button to proceed from dayfile.

IOFILE — switches the input between the card reader and the teletype. The input formatting is identical with both devices, and all the SAMPO control cards listed before can be read in through the teletype also.

WHAT(1) = 2. specifies the card input; this is the initially specified value;

= 6. specifies the teletype input; following this card up to next IOFILE, WHAT(1) = 2., the SAMPO control statements are read through the teletype.

DATATV — displays the spectrum on the CRT screen. If the peak search has been done before DATATV then the peaks found are also marked in the display.

WHAT(2) every WHAT(2) channel is plotted; if blank, every channel;

WHAT(3) is the starting channel of the display; if blank, the first channel;

WHAT(4) is the termination channel; if blank, the last channel;

WHAT(5) channels in each subdivision; if blank, 500 channels, with an overlap of 100 channels between subdivisions.

If the interactive mode of on-line run has been specified--that is OPTIONS, WHAT(6) = 1. -- then the following keyboard options of the VISTA console are available after the spectrum has appeared on the screen following DATATV statement. The light pen and the latching R buttons are used; pushing the red I button executes the command specified.

R I — advances to the next frame;

R 2 I — replots the present frame.

R123 5 I — displays the channel number at the light-pen hit;

R123 I — adds a peak to the list of peaks to be fitted at the light-pen hit, this can be used to edit the list of peaks found;

R1234 I — drops a peak from the list of peaks found closest to the light-pen hit.

R 3 I — changes the background approximation from parabolic to linear;

R 4 I — changes the background approximation from linear to parabolic, as specified on OPTIONS card.

R12345 I — specifies the fitting interval and approximate peak centroids for the peak fitting. First specify with the light pen the lower and upper limit of the interval. Then you can optionally specify all the peaks in the interval or let the code pick up the peaks found by the search routine in this interval; the latter mode is executed if no peaks are specified by the light pen.

R1 I — performs the fit of the interval specified by R12345 I commands. The results will be displayed on the screen, after which the user has the following options available:

R I — accepts the fit and enters the results in the result arrays;

R 2 I — rejects the fit and does not store the results.

The CRT display of the fitting results is also available in the automatic mode under FITDO, and the last two options listed above can be executed for each fit. The request for the display of the fitting results must be made before FITDO by specifying WHAT(6) = 1. on OPTIONS control card. The value WHAT(6)= 2. on the same card will photograph each fit on the CRT camera when the program is run off-line. Please avoid producing large quantities of film this way.

The energy calibration results may also be displayed on CRT. The nonlinear parts of both the linear interpolation scheme (see OPTIONS) and the polynomial fitting are displayed, see Fig. 8. To obtain the display in ENFITDO set WHAT(2) = 1. to get the curves between the first and the last calibration points or WHAT(2) = 2. for the graphs over the whole range of the spectrum. These results may also be photographed in off-line run; see comment on OPTIONS above.

5. COMMENTS ON ANALYSIS STRATEGIES WITH INPUT EXAMPLES

The large number of internal options and the flexibility in inputting data enable the user to run SAMPO in a variety of different ways. The optimal running strategies depend on the complexity of the spectral data, the requirements on the accuracy and completeness of the results, and whether facilities are available for running the code on-line.

Since the analysis requires a certain amount of calibration data it is generally recomened that the user try to limit the number of pulse-height analyzer settings and experimental situations to as few cases as possible, in order that adequate calibration data can be maintained and be kept readily available. The shape-calibration data, for instance, can be fairly easily generated from the spectra to be analyzed; however, significant savings in time and effort can be realized if such data are already available from earlier computations.

The program data input has been designed so that the user can in principle complete the analysis of any number of spectra in a single computer run. For analyzing complex spectra without the on-line facilities this approach is, however, not the most efficient one. Because of limitations in the peak-search and peak-fitting routines some peaks are likely to be missed or poorly fitted.

The efficiency of the analysis can in such cases be improved by performing it in a few steps. Thus the user may check and possibly correct the intermediate results. In particular, since the fitting procedures are the most time-consuming part of the analysis, one should make an effort to obtain good fitting results with a minimum number of recomputations. It is therefore important to check the correctness of the shape-calibration results and the performance of the peak-search routines before the final fitting.

As an example let us consider the complete analysis of the spectrum shown in Fig. 1. We assume that a plot of the spectrum and the efficiency calibration of the detector system are available; the energy calibration is to be performed by using a few strong lines in the spectrum as internal standards. The peak shape calibration is also going to be done by using the data in the spectrum to be analyzed. The complete analysis is performed in three computer runs as explained below.

In the first run the objective is to obtain peak shape parameters and results from the peak search routine. For a rough energy calibration the energies of the first and the last shape-calibration peaks are also given. If desired one could perform a more complete energy calibration with all shape-calibration lines, or leave the more complete energy calibrations to later runs, as is done here.

The fitting intervals that will later be selected by the program can also be listed so that the user may foresee possible problems that may arise when the actual fitting is performed in the second run. The data cards appropriate to the first run are given in the first part of Table III.

We now have obtained standard peak shapes for the spectrum as well as a list of peaks found by the search routine and a list of fitting intervals chosen. For the second run we have to check the consistency of the shape parameters and select the appropriate cards from the SHAPEIN cards punched by the program; no correction of these cards is necessary in this case. We also need to check the results of the peak search routine and to edit the list of peaks to be fitted. We also want to prepare energy and efficiency calibration data for the second run, in which most of the actual fitting is performed. Appropriate data cards for the second run are listed under that heading on the first half of Table III.

The data are now fitted, and may be inspected for regions where the analysis may not be satisfactory. The only obvious difficulties in the fitting were: (a) the small peak around channel 528 was not properly fitted, because of the presence of several much more intense lines in the same interval; (b) from the fitting of the peak about channel 902 it is clear that a small component was missed on the high-energy side of that peak. In the next run these deficiencies can be easily corrected through fitting just these regions with FITS card. These results are then included in the final tabulation together with the earlier results.

In the second run the more complete energy calibrations are performed, with the fitting results used as internal standards. The energies and intensities are recomputed during the tabulation (after the fitting), since the complete calibration data are not available before fitting. If it were available, then the energy and intensity determinations could be done during the fitting, as is shown in the next run. We also produce a few polynomial energy calibration curves to select an appropriate one for an alternative energy determination in the next (final) run.

In the third run the regions of data where satisfactory results were not obtained in the second run are refitted. We also read in the results from the previous run to obtain complete result tables, by using different options of energy and efficiency calibrations. Since the peak around channel 902 will be recomputed, it should be deleted from the cards punched in the second run that will now be read into SAMPO for tabulation of the results.

A polynomial curve with five terms is selected to perform energy determinations alternative to the linear interpolation scheme; similarly, the results from the functional fit of the efficiency curve are read for an alternative intensity determination. The data cards appropriate for the third run are listed on the second half of Table III.

The analysis is now complete. The results with the interpolating calibration procedures are summarized, except for the peaks around channels 528 and 902, by the cards read into SAMPO in the third run after FITIN cards. The complete results with polynomial energy calibration and functional efficiency curve were shown in Table II in Section 3.

If on-line facilities such as at LRL Berkeley are available, then the corrections to peak-search and peak-fitting results can be made immediately and the analysis can be completed without corrective reruns. The on-line facilities have been quite successfully used for the analysis of spectra more complex than that of ^{177m}Lu. As an example, Fig. 10 shows a resolved multiplet in the spectrum of ^{176}Hf from Ref. 4.

6. SOURCE AND BINARY DECKS

The Fortran source deck of SAMPO is about 3000 cards long. The core requirements depend partly on the options used and the length of the spectral and result arrays. The basic program for 1600 channel spectra and up to 100 peaks in the spectrum can be compiled and executed in about 28 000 (decimal) core locations on a CDC-6600 machine. The lengths of these arrays can be easily modified; all the cards that need to be changed in the deck have been marked for this.

The source decks and listings for the basic program required for off-line running are available from the author at Lawrence Radiation Laboratory in Berkeley. It should be noted, when running the code on other computers, that different compilers produce slightly different execution modes of the program. Because of this and the differences in word lengths and similar effects the results may differ. The discrepancies may be fairly large in results of iterative calculations, especially if these results are not very well defined, like the error estimates of various parameters.

The subroutines required for on-line runs and computer plotting are generally not included in the distribution version of SAMPO decks. These subroutines require special system routines and hardware which are generally not compatible between different systems. These decks, however, can be sent also, if requested. The basic program contains some call statements for these routines. These call statements have been marked in the deck and can be deleted or changed to comment statements.

Table III. Detailed input example for the complete analysis of ^{177m}Lu spectrum. The analysis consists of three separate runs in which results of the previous steps are used in the later runs. The card images also show the input formatting in detail.

TABLE III. 30A

```
COLUMN
1         11        21        31        41        51        61        71
12345678901234567890123456789012345678901234567890123456789012345678901234567890

CODEW     WHAT(1)   WHAT(2)   WHAT(3)   WHAT(4)   WHAT(5)   WHAT(6)   NAME

DATA CARDS FOR SAMPO FOLLOW THE NEXT LINE
--------------------------------------------------------------------------------


COMMENTS
 1ST RUN OF THE ANALYSIS OF GE-E SPECTRUM. SHAPE CALIBRATIONS AND PEAK SEARCH.
DATAIN    2.
(5X,F8.0,5X,F8.0,5X,F8.0,5X,F8.0,5X,F8.0)
GE-E   LU-177M 0-500 KEV 1550 CH 4/20/66                                  1550
   0.    198.   1.    607.   2.   1203.   3.   3189.   4.  19797.
   5. 666434.   6. 110088.   7. 105435.   8. 102552.   9.  51216.
  10.  23092.  11.  12260.  12.   7499.  13.   5493.  14.   4099.
  15.   2907.  16.   4614.  17.  58671.  18. 170774.  19. 156013.
  20. 141481.  21. 153775.  22. 159024.  23. 165053.  24. 168163.

          MORE SPECTRAL DATA CARDS

1535.     71.1536.     64.1537.     89.1538.     75.1539.     61.
1540.     70.1541.     98.1542.     84.1543.     71.1544.     80.
1545.     71.1546.     83.1547.     86.1548.     82.1549.     80.
OPTIONS   2.         2.                                          GE-E 1ST
SHAPEDO   242.       229.       254.       1.         1.        GE-E 1ST
ENDO      242.       105.31     1.                    1.        GE-E 1ST
SHAPEDO   328.       316.       339.                           GE-E 1ST
SHAPEDO   420.       409.       432.                           GE-E 1ST
SHAPEDO   702.       688.       713.                           GE-E 1ST
SHAPEDO   781.       768.       794.                           GE-E 1ST
SHAPEDO   1074.      1059.      1088.                          GE-E 1ST
SHAPEDO   1264.      1247.      1277.                          GE-E 1ST
SHAPEDO   1443.      1430.      1456.      1.                  GE-E 1ST
ENDO      1443.      426.29     1.5                            GE-E 1ST
CALDATA   2.         2.
PEAKFIND  200.
FITTEST
STOP


COMMENTS
2ND RUN OF GE-E ANALYSIS. PEAK FITTING WITH ALL CALIBRATIONS.
DATAIN    2.
(5X,F8.0,5X,F8.0,5X,F8.0,5X,F8.0,5X,F8.0)
GE-E   LU-177M 0-500 KEV 1550 CH 4/20/66                                  1550
   0.    198.   1.    607.   2.   1203.   3.   3189.   4.  19797.
   5. 666434.   6. 110088.   7. 105435.   8. 102552.   9.  51216.

          MORE SPECTRAL DATA CARDS

1545.     71.1546.     83.1547.     86.1548.     82.1549.     80.
OPTIONS   2.         2.         2.                          GE-E 2ND
SHAPEIN    2.418E+02 3.798E+00 2.809E+01 2.041E+001.       GE-E
SHAPEIN    3.281E+02 3.987E+00 3.008E+01 2.092E+00         GE-E
SHAPEIN    4.205E+02 3.844E+00 3.382E+01 2.129E+00         GE-E
SHAPEIN    7.016E+02 3.916E+00 6.052E+01 2.286E+00         GE-E
SHAPEIN    7.811E+02 3.684E+00 7.765E+01 2.334E+00         GE-E
SHAPEIN    1.074E+03 3.798E+00 1.396E+01 2.491E+00         GE-E
SHAPEIN    1.265E+03 3.889E+00 9.232E+00 2.589E+00         GE-E
SHAPEIN    1.443E+03 3.747E+00 6.955E+00 2.701E+00         GE-E
```

TABLE III continued

ENIN	241.84	105.31	.1		1.	GE-E
ENIN	1442.66	426.29	.1			GE-E
EFIN	70.	6.38	E-035.		1.	GE-E
EFIN	80.	5.91	E-035.			GE-E
EFIN	90.	4.94	E-035.			GE-E
EFIN	100.	4.12	E-035.			GE-E
EFIN	120.	2.87	E-035.			GE-E
EFIN	150.	1.73	E-035.			GE-E
EFIN	200.	8.84	E-045.			GE-E
EFIN	250.	5.23	E-045.			GE-E
EFIN	300.	3.42	E-045.			GE-E
EFIN	350.	2.39	E-045.			GE-E
EFIN	400.	1.77	E-045.			GE-E
EFIN	450.	1.34	E-045.			GE-E
EFIN	500.	1.05	E-045.			GE-E
CALDATA	2.	2.	2.			
PEAKFIND	200.					GE-E
PEAKADD	285.	392.	830.	937.	943.	GE-E
PEAKADD	967.	1050.	1471.	1494.	1501.	GE-E
PEAKDROP	816.	940.				GE-E
PEAKLIST						GE-E
FITDO						
ENDO	242.	105.31	0.1		1.	GE-E
ENDO	328.	128.50	0.1			GE-E
ENDO	420.	153.29	0.1			GE-E
ENDO	626.	208.34	0.1			
ENDO	702.	228.44	0.1			GE-E
ENDO	781.	249.65	0.1			GE-E
ENDO	991.	305.52	0.1			
ENDO	1074.	327.66	0.1			GE-E
ENDO	1264.	378.51	0.1			GE-E
ENDO	1443.	426.29	0.1			GE-E
CALDATA		2.				
RESULT	242.	2.	2.	1.		GE-E 2ND
ENFITDO	3.					
ENFITDO	4.					
ENFITDO	5.					
ENFITDO	6.					
ENFITDO	7.					
STOP						

TABLE III continued

```
COMMENTS
3RD RUN OF GE-E ANALYSIS. CORRECTED FITS AND FINAL TABULATION OF RESULTS.
DATAIN    2.
(5X,F8.0,5X,F8.0,5X,F8.0,5X,F8.0,5X,F6.0)
GE-E   LU-177M 0-500 KEV 1550 CH 4/20/66                                    1550
   0.     199.    1.     607.    2.    1203.    3.    3189.    4.   19797.
   5. 666434.    6. 110088.    7. 105435.    8. 102552.    9.   51216.

          MORE SPECTRAL DATA CARDS

1545.      71.1546.      83.1547.      86.1548.      82.1549.      80.
OPTIONS    2.          2.          2.                                      GE-E 3RD
SHAPEIN    2.418E+02 3.798E+00 2.809E+01 2.041E+001.                       GE-E
SHAPEIN    3.281E+02 3.987E+00 3.008E+01 2.092E+00                         GE-E
SHAPEIN    4.205E+02 3.844E+00 3.382E+01 2.129E+00                         GE-E
SHAPEIN    7.016E+02 3.916E+00 6.052E+01 2.286E+00                         GE-E
SHAPEIN    7.811E+02 3.684E+00 7.765E+01 2.334E+00                         GE-E
SHAPEIN    1.074E+03 3.798E+00 1.396E+01 2.491E+00                         GE-E
SHAPEIN    1.265E+03 3.889E+00 9.232E+00 2.589E+00                         GE-E
SHAPEIN    1.443E+03 3.747E+00 6.955E+00 2.701E+00                         GE-E
ENIN       241.84     105.31     .1                  1.                    GE-E
ENIN       328.09     128.50     .1                                        GE-E
ENIN       420.46     153.29     .1                                        GE-E
ENIN       626.36     208.34     .1                                        GE-E
ENIN       701.65     228.44     .1                                        GE-E
ENIN       781.12     249.65     .1                                        GE-E
ENIN       990.86     305.52     .1                                        GE-E
ENIN       1074.16    327.66     .1                                        GE-E
ENIN       1264.70    378.51     .1                                        GE-E
ENIN       1442.66    426.29     .1                                        GE-E
EFIN       70.        6.38  E-035.          1.                            GE-E
EFIN       80.        5.91  E-035.                                        GE-E
EFIN       90.        4.94  E-035.                                        GE-E
EFIN       100.       4.12  E-035.                                        GE-E
EFIN       120.       2.87  E-035.                                        GE-E
EFIN       150.       1.73  E-035.                                        GE-E
EFIN       200.       8.84  E-045.                                        GE-E
EFIN       250.       5.23  E-045.                                        GE-E
EFIN       300.       3.42  E-045.                                        GE-E
EFIN       350.       2.39  E-045.                                        GE-E
EFIN       400.       1.77  E-045.                                        GE-E
EFIN       450.       1.34  E-045.                                        GE-E
EFIN       500.       1.05  E-045.                                        GE-E
CALDATA    2.         2.          2.
FITIN      48.                                 1.
  241.834 .001  105.308 .100 2.0791E+06   .17 5.5914E+08   5.00 5.5914E+08GE-E
  270.119 .002  112.913 .100 3.2708E+06   .23 1.0101E+09   5.01 1.0101E+09GE-E
  281.581 .108  115.995 .104 7.9933E+04  3.80 2.6038E+07   6.28 2.6038E+07GE-E
  286.699 .394  117.371 .146 2.1869E+04 15.18 7.2924E+06  15.98 7.2924E+06GE-E
  302.448 .008  121.606 .100 7.8369E+05   .56 2.8142E+08   5.03 2.8142E+08GE-E
  328.084 .004  128.498 .100 1.7935E+06   .18 7.2984E+08   5.00 7.2984E+08GE-E
  358.745 .008  136.727 .100 1.4382E+05   .35 6.7375E+07   5.01 6.7375E+07GE-E
  392.390 .034  145.757 .100 7.7666E+04  1.34 4.2064E+07   5.18 4.2064E+07GE-E
  397.630 .006  147.163 .100 2.9428E+05   .41 1.6289E+08   5.02 1.6289E+08GE-E
  420.456 .005  153.289 .100 1.3012E+06   .23 7.9119E+08   5.01 7.9119E+08GE-E
  444.658 .044  159.760 .101 3.5988E+04  1.86 2.4099E+07   5.33 2.4099E+07GE-E
  477.660 .326  168.583 .133 9.9919E+03  9.04 7.5855E+06  10.33 7.5855E+06GE-E
  489.782 .013  171.824 .100 2.8186E+05   .50 2.2370E+08   5.02 2.2370E+08GE-E
  499.288 .007  174.366 .100 7.0798E+05   .27 5.8149E+08   5.01 5.8149E+08GE-E
  508.976 .017  176.956 .100 1.8306E+05   .68 1.5562E+08   5.05 1.5562E+08GE-E
  578.397 .004  195.516 .100 3.5860E+04  1.17 3.8475E+07   5.14 3.8475E+07GE-E
  610.419 .012  204.078 .100 5.2553E+05   .52 6.2340E+08   5.03 6.2340E+08GE-E
  626.358 .001  208.339 .100 2.1629E+06   .22 2.7184E+09   5.00 2.7184E+09GE-E
  649.079 .007  214.405 .100 2.1921E+05   .47 2.9205E+08   5.02 2.9205E+08GE-E
  662.815 .008  218.072 .100 1.0998E+05   .77 1.5249E+08   5.06 1.5249E+08GE-E
  701.645 .002  228.439 .100 1.0679E+06   .25 1.6516E+09   5.01 1.6516E+09GE-E
  721.812 .019  233.821 .100 1.5291E+05   .80 2.4980E+08   5.06 2.4980E+08GE-E
  781.119 .003  249.650 .100 1.4283E+05   .31 2.7220E+08   5.01 2.7220E+08GE-E
  830.729 .407  262.865 .147 2.0937E+03 14.52 4.4997E+06  15.36 4.4997E+06GE-E
  835.321 .227  264.088 .117 3.8983E+03  7.59 8.4692E+06   9.09 8.4692E+06GE-E
  852.890 .013  268.768 .100 6.6145E+04   .53 1.4971E+08   5.03 1.4971E+08GE-E
  938.479 .093  291.567 .103 1.7418E+04  3.93 4.7657E+07   6.36 4.7657E+07GE-E
  942.369 .120  292.603 .105 1.3762E+04  4.78 3.7966E+07   6.92 3.7966E+07GE-E
  956.829 .014  296.455 .100 7.6335E+04   .54 2.1710E+08   5.03 2.1710E+08GE-E
  966.586 .028  299.054 .100 2.4452E+04  1.08 7.0973E+07   5.12 7.0973E+07GE-E
  990.855 .023  305.519 .100 2.5844E+04   .93 7.8838E+07   5.09 7.8838E+07GE-E
```

30D

TABLE III
-continued

966.586	.028	299.054	.100	2.4452E+04	1.08	[illegible]	[illegible]	[illegible]
990.855	.023	305.519	.100	2.5844E+04	.93	7.8838E+07	5.09	7.8838E+07GE-E
1021.740	.038	313.727	.101	1.6737E+04	1.42	5.4303E+07	5.20	5.4303E+07GE-E
1041.619	.012	319.011	.100	1.3274E+05	.40	4.4772E+08	5.02	4.4772E+08GE-E
1050.187	.049	321.288	.101	1.5077E+04	1.60	5.1701E+07	5.25	5.1701E+07GE-E
1074.161	.010	327.660	.100	2.2120E+05	.39	7.9396E+08	5.02	7.9396E+08GE-E
1109.346	.148	337.050	.108	9.7110E+02	4.90	3.7222E+06	7.00	3.7222E+06GE-E
1126.598	.013	341.654	.100	1.9176E+04	.49	7.5857E+07	5.02	7.5857E+07GE-E
1223.195	.002	367.433	.100	2.8656E+04	.63	1.3375E+08	5.04	1.3375E+08GE-E
1264.699	.012	378.510	.100	2.5488E+05	.46	1.2718E+09	5.02	1.2718E+09GE-E
1289.063	.051	385.051	.101	2.6770E+04	1.91	1.3883E+08	5.35	1.3883E+08GE-E
1395.533	.014	413.637	.100	1.2262E+05	.51	7.4988E+08	5.03	7.4988E+08GE-E
1413.489	.012	418.458	.100	1.4689E+05	.46	9.2324E+08	5.02	9.2324E+08GE-E
1442.663	.036	426.291	.100	3.0711E+03	1.86	2.0167E+07	5.33	2.0167E+07GE-E
1466.055	.467	432.571	.160	5.0178E+02	15.00	3.4109E+06	15.81	3.4109E+06GE-E
1470.844	.494	433.857	.166	4.8223E+02	15.48	3.3011E+06	16.27	3.3011E+06GE-E
1480.275	.309	436.389	.130	3.4543E+02	12.08	2.3974E+06	13.07	2.3974E+06GE-E
1494.453	.375	440.196	.142	3.5891E+02	11.68	2.5426E+06	12.71	2.5426E+06GE-E
1501.532	.482	442.096	.164	2.8852E+02	13.11	2.0648E+06	14.03	2.0648E+06GE-E

```
FITS       2.
    1  520  535        528
    2  883  922        902  910
RESULT     242.       2.         2.
ENFITIN    4.01972+01 100.       .1         1.         1.                  GE-E
ENFITIN    2.69527-01 200.       .1         2.                             GE-E
ENFITIN    -3.9305-07 300.       .1         3.                             GE-E
ENFITIN    -3.1317-09 400.       .1         4.                             GE-E
ENFITIN    1.72544-12 500.       .1         5.                             GE-E
EFFITIN    100.       2.8111 +02 5.         1.         1.                  GE-E
EFFITIN    200.       -2.386 +00 5.         2.                             GE-E
EFFITIN    300.       -1.253 -03 5.         3.                             GE-E
EFFITIN    500.       -6.230 -02 5.         4.                             GE-E
CALDATA               4.         4.
RESULT     242.       4.         4.
STOP
```

Berkeley SAMPO Library

At LRL Berkeley all SAMPO options are available in a special program library stored on a data cell that is directly accessible to the CDC-6600 computers. The SAMPO library contains binary and source decks of sections of the code; these sections correspond to different choices of input and output devices. The user needs to load only the sections that he is going to use and thus economize on field length requirements. By using the data cell library the program can be very conveniently loaded and executed without handling tapes or long source decks. Instructions for using SAMPO library are also on the data cell, and can be obtained by executing LIBCOPY (SAMPO, OUTPUT, INFORM). Table IV shows this information at present. Notice the date on the first line and be sure to have the latest information.

ACKNOWLEDGMENTS

I am greatly indebted to Stanley Prussin for his cooperation in the development of the analysis methods. The continuous cooperation and support of H. Wade Patterson, Alan Smith, and Roger Wallace is gratefully acknowledged. The use of the development versions of SAMPO program by Frederick Bernthal, Nickey Little, and Jerry Wilhelmy has provided valuable feedback and criticism towards improvement of the code.

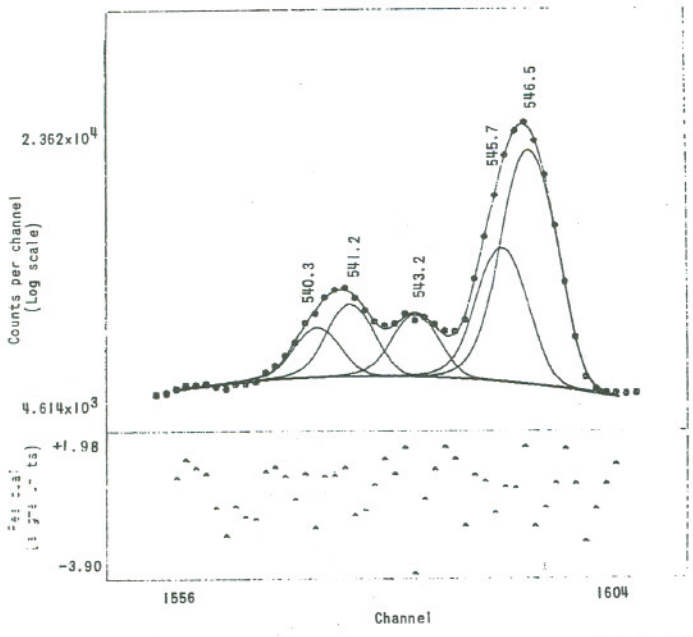


Fig. 10. A multiplet resolved in the spectrum of ^{176}Hf as shown on the CRT during an on-line run.

Table IV. Information on the SAMPO library which is stored on the data cell of CDC-6600 computers of LRL Berkeley. This gives the system control cards for loading and executing different program options. The user should obtain the latest version of this information from the data cell as instructed below.

```
INFORMATION OF SAMPO LIBRARY, LAST CHANGED ON DECEMBER 21, 1969.

SAMPO IS A FORTRAN PROGRAM WRITTEN TO PERFORM THE ANALYSIS DESCRIBED BY
J. T. ROUTTI AND S. G. PRUSSIN IN PHOTOPEAK METHOD FOR THE COMPUTER ANALYSIS
OF GAMMA-RAY SPECTRA FROM SEMICONDUCTOR DETECTORS, PUBLISHED IN NUCLEAR
INSTRUMENTS AND METHODS, VOL. 72, PP. 125-142, JULY 1969, AND ALSO IN
UCRL-17672, DECEMBER 1968. THE USER IS ADVISED TO CONSULT EITHER ONE OF
THESE REPORTS FOR THE EXPLANATION OF THE METHODS.

THE PROGRAM CAN BE USED FOR AUTOMATIC OFF-LINE DATA REDUCTION RUNS OR
FOR AN INTERACTIVE ON-LINE ANALYSIS WITH CRT VISTA AND TELETYPE INPUT
AND OUTPUT. THE WRITEUP WHICH EXPLAINS THESE OPTIONS AND THE DATA INPUT
CAN BE OBTAINED FROM THE AUTHOR, JORMA ROUTTI, LRL-BERKELEY, EXTENSION 5983.

SAMPO LIBRARY ON DATA CELL CONTAINS BINARY AND SOURCE DECKS OF SECTIONS
OF THE PROGRAM, AS WELL AS A SAMPLE INPUT AND OUTPUT. THE SUBSETS IN SAMPO
LIBRARY ARE LISTED BELOW, NAMES BEGINNING WITH B REFER TO RUNF COMPILED
PROGRAM SECTIONS WILE NAMES BEGINNING WITH S ARE THE CORRESPONDING SOURCE DECKS.

INFORM          =THIS INFORMATION OF SAMPO LIBRARY
INEX            =SAMPLE DATA INPUT DECK
OUTEX           =SAMPLE OUTPUT LISTING
BSAMPO,SSAMPO=MAIN PROGRAM FOR UP TO 1600 CHANNELS AND 100 PEAKS  FL=66000 OCTAL
BSAMPOL         =MAIN PROGRAM FOR UP TO 4100 CHANNELS AND 200 PEAKS  FL=74000 OCTAL
BCC,SCC         =CAL COMP OPTIONS FOR SPECTRA AND PEAK SEARCH        FL= 6000 OCTAL
BTV,STV         =CRT VISTA OPTIONS FOR RUNNING ON-LINE              FL=13000 OCTAL
BDT,SDT         =DATA TAPE READER FOR NICKEY LITTLE                 FL= 2500 OCTAL
BDT1,SDT1       =DATA TAPE READER FOR HOLLANDR GROUP                FL= 2500 OCTAL
BDT2,SDT2       =DATA TAPE READER FOR JERRY WILHELMY                FL= 2500 OCTAL
BDT3,SDT3       =DATA TAPE READER FOR DON LEBECK                    FL= 2500 OCTAL
BDT4,SDT4       =DATA TAPE READER FOR SOMEBODY ELSE, PLEASE SHOW UP FL= 2500 OCTAL
BDT5,SDT5       =DATA TAPE READER FOR SHASTA BCD TAPES              FL= 2500 OCTAL
BDT6,SDT6       =DATA TAPE READER FOR ESKOLA 1.13.1969              FL= 2500 OCTAL
BDT7,SDT7       =DATA TAPE READER FOR ASCON READER                  FL= 2500 OCTAL

THE SOURCE AND COMPILER LISTINGS CAN BE EASILY OBTAINED BY RUNNING THE JOB,

SAMPO,7,100,5000C.309302,JORMA ROUTTI
LIBCOPY(SAMPO,OUTPUT,INFORM)          TO GET UPDATED VERSION OF SAMPO LIBRARY
LIBCOPY(SAMPO,OUTPUT,SCC,SDT2)        TO GET SOURCE LISTINGS OF SCC AND SDT2
LIBCOPY(SAMPO,PUNCH,SCC,SDT2)         TO GET PUNCHED DECKS OF SCC AND SDT2
LIBCOPY(SAMPO,INP,SCC,SDT2)           TO GET COMPILED LISTINGS OF SCC AND SDT2
REWIND(INP)                           CORRESPONDING TO BCC AND BDT2 YOU NEED
RUNF(S,,,INP)                         THESE THREE CARDS.
LIBCOPY(SAMPO,OUTPUT,INEX,OUTEX)      FOR LISTING OF SAMPLE INPUT AND OUTPUT
 6/7/8/9
```

THE USE OF PRECOMPILED SUBSET ALLOWS THE USER TO EXECUTE A RUN WITHOUT HANDLING SOURCE DECKS OR LIBRARY TAPES. ONLY THE OPTIONS ACTUALLY USED NEED TO BE LOADED. SO FOR INSTANCE TO RUN A JOB WITH CARD INPUT AND CAL COMP OUTPUT OF SPECTRA USE THE FOLLOWING CONTROL CARDS.

```
SAMPO,10,200,74000.309302,JORMA ROUTTI
LIBCOPY(SAMPO,BIN,BSAMPO,BCC)
LODE(I=BIN,O=UNSATED)
XEQ.
EXIT.
DMP.
 7/8/9
SAMPO INPUT DATA
 6/7/8/9
```

COMPLETE LIST OF CONTROL CARDS FOR RUNNING SAMPO AT LRL-BERKELY IS GIVEN BELOW. USER HAS TO SELECT FROM THESE CARDS THE CARDS REQUIRED FOR HIS PARTICULAR RUN.

```
SAMPO,10,300,FIELD.309302,ROUTTI        REPLACE WITH YOUR JOB CARD,
                                        SET FIELD LENGTH DEPENDING ON SUBSETS
TTY(1000,JR)                            ONLY FOR ON-LINE RUNS WITH TELETYPE
LIBCOPY(SAMPO,BIN,BSAMPO)               FOR OF-LINE RUNS WITH CARD INPUT ONLY, OR
LIBCOPY(SAMPO,BIN,BSAMPO,BCC)           FOR RUNS WITH CAL COMP PLOTTING, OR
LIBCOPY(SAMPO,BIN,BSAMPO,BTV,BDT)       FOR CRT RUNS WITH MAGN.TAPE INPUT, OR
LIBCOPY(SAMPO,BIN,BSAMPO,               AND ANY OTHER OPTIONS DESIRED)
LIBCOPY(TLIBR,BIN,BTAPE)                IF YOU HAVE YOUR TAPE READER IN TLIBR
RUNF(S,,,,EROUT,BIN)                    IF YOU COMPILE YOUR OWN TAPE READER
REWIND(EROUT)                           IF LISTING OF COMPILATION OF TAPE
COPYBF(EROUT,OUTPUT)                    READER DESIRED
REQUEST TAPE5. INPUT TAPE GAMMA         ONLY IF SPECTRA ON MAGNETIC TAPE
DENSITY TAPE5,5.                        SPECIFIES DENSITY OF DATA TAPE
REWIND(TAPE5)                           ONLY IF NEEDED
REQUEST FILM. CRT VISTA 42              ONLY FOR ON-LINE RUNS WITH VISTA
LODE(I=BIN,O=UNSATED)                   LOADS SUBSETS COPIED AND COMPILED
XEQ.                                    EXECUTES THE PROGRAM
EXIT.                                   HOPEFULLY NORMALLY
DMP.                                    HOPEFULLY NOT
REWIND(INPUT)                           ONLY FOR ON-LINE          $     REPEAT
COPYBR(INPUT,NULL)                      RUNS WITH VISTA           $     UP
SEL(FIELD)                              FOR RECOVERING  FROM      $     TO
LOADE(I=BIN,O=UNSATED)                  ARITHMETIC AND            $     THREE
XEQ.                                    INPUT ERRORS              $
EXIT.                                                             $
DMP.                                                              $     TIMES
CXIT.                                   ONLY IF YOU COMPILE YOUR OWN TAPE READER
EREDIT.                                 EDITS THE FORTRAN ERRORS
FIN.                                    TERMINATION PROCEDURES
UNLOAD(TAPE5)                           ONLY IF TAPE5 WAS REQUESTED
RETURN(TAPE5)                           ONLY IF TAPE5 WAS REQUESTED
REWIND(TAPE14)                          ONLY IF PUNCH OUTPUT DESIRED
COPYCF(TAPE14,PUNCH)                    ONLY IF PUNCH OUTPUT DESIRED
REWIND(TAPE7)                           ONLY IF DUPLICATE RESULT TABLES DESIRED
COPYBF(TAPE7,OUTPUT)                    ONLY IF DUPLICATE RESULT TABLES DESIRED
 7/8/9                                  END OF RECORD
TAPE READING SUBROUTINE                 ONLY IF NEEDED FOR COMPILATION
CONSULT THE AUTHOR ABOUT GETTING ONE    ONLY IF YOU DO NOT HAVE ONE ALREADY
 7/8/9                                  ONLY IF TAPE READER IN THE DECK
DATA CARDS FOR SAMPO INPUT              CONSULT THE WRITEUP
 6/7/8/9                                END OF FILE
```

FOOTNOTES AND REFERENCES

*This name has been taken from Finnish mythology (Kalevala epos), in which a miracle well known as SAMPO fulfills all the wishes of its owner.

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6. William C. Davidon, Variable Metric

Method for Minimization, Argonne National Laboratory report ANL-5990, Nov. 1959;

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