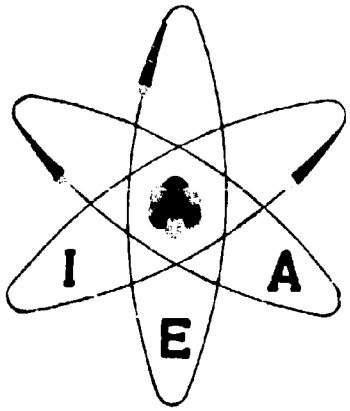

A PROGRAM IN "BASIC" LANGUAGE FOR ANALYSIS OF GAMMA SPECTRA, USING ON-LINE MINICOMPUTERS

F. W. LIMA and L. T. ATALLA

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INSTITUTO DE ENERGIA ATÔMICA
Caixa Postal 11049 (Pinheiros)
CIDADE UNIVERSITARIA "ARMANDO DE SALLES OLIVEIRA"
SAO PAULO — BRASIL

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F. W. Lima and L. T. Atalla

Coordenadoria de Radioquímica
Instituto de Energia Atômica
São Paulo - Brasil

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SUMMARY

A program in "INSTRUMENT BASIC" language is proposed for analysis of gamma-ray spectra obtained with Ge (Li) detectors and accumulated in multichannel analysers on-line with minicomputers. The program locates the peaks, evaluates the corresponding energy values, the net peak areas and the standard deviation of the areas

INTRODUCTION

Many advantages arise from the use of minicomputer, on-line with the analyser, for the interpretation of gamma spectra. In case of preparation of programs for ultimate use in activation analysis problems, the interference of the programmer with the equipment is often necessary up to the point where all the parameters for the program have been chosen. On-line computers are extremely useful for this phase of the work. If the program language is a conversational one, such as "BASIC", the advantages of the on-line computer can be exploited at their highest capacities. "BASIC" language is also a good starting point for beginners in programing and it is powerful enough for an experienced programmer to make use of it for advanced work.

In this paper a program is presented in "INSTRUMENT BASIC"[1] language, which is a "BASIC" language adapted for use with the 5402A Hewlett-Packard System, composed of a multichannel analyser (4096 channels, Model 5401B), a 2100A computer (8K memory, expandable to 32K) and a teleprinter, Model HP 2752A. Tape perforation and tape reading can be done through the teleprinter, although perforation and reading will be much quicker if fast tape punch and fast tape reader are used. In our case we used a HP Model 2895A tape punch and a HP Model 2748A tape reader.

The program, which is written for gamma-ray spectra obtained with Ge-Li detectors, can cover the whole memory of the analyser or smaller parts of it, such as one half, leaving the other half for accumulation of spectra for comparison or for subtraction of background. The listing of the program contains about 1900 characters for spectra stored in 2048 or 4096 channels and it is compatible with a 8K computer memory. The number of characters involved is smaller than the one proposed by Kemper and van Kempen[2], which is also written in "BASIC", for spectra accumulated in 400 channels, but involving about 4800 characters and containing the requirement that data are read into the computer memory in a separate file in order to avoid exceeding the maximum number of characters permitted by the computer time sharing system. The execution time for the program by Kemper and van Kempen is very fast, about 28.8 seconds for a 400 channels capacity. The execution and typing time for the program presented in this paper is equal to about 7 minutes for a spectrum accumulated in 2048 or 4096 channels, corresponding to a sample composed of ^{241}Am, ^{170}Tm, ^{137}Cs, $^{152\text{-}154}Eu$, ^{22}Na,

^{57}Co, ^{60}Co. Data-reading is included in the program itself.

Indexed variables are avoided and used only parsimoniously during the calibration step, in order not to put restrictions on the memory size of the computer by having to use a DIMENSION statement that occupies an appreciable part of the computer memory. The program is conceived in such a way that after calculations are carried out in connection with a peak, the corresponding data are printed and removed from the computer memory, leaving it available for the following set of calculations concerning the next peak.

THEORY

The complete program is made up of two parts: the first one is calibration of the adress or channels scale of the analyser in terms of energy units. The second part of the program analyses the spectra by locating the peaks, determining the centroid values for the peaks, calculating their corresponding energies in keV, the area for each peak and the associated standard deviation. A loop is introduced in the program to re-start the calculations for another sample, without having to go through the calibration steps for each new sample to be counted. However, the calibration step can be repeated as many times as one wishes by typing "STOP" after the analysis of a spectrum has been completed.

The areas of the peaks are calculated by summation of the number of counts in each channel of the peak and without assuming a Gaussian peak shape. If such an assumption is made, allowance should be made for assimetry of the peaks. Kemper and van Kempen[2] used the same procedure for the same reason.

Calibration

For calibration a linear relation between energy and channel-numbers is assumed and calibration of the channels scale is made with only two points since gain and zero stability of the equipment is very good, even if a peak stabilizer is not used. The assumption of linear relation between energy and channel-numbers is more close to truth the smaller the number of channels involved.

The choice of the lower and upper channel for a peak is made in such a way that the left and right boundaries for a peak do not lay in the "valley" immediately before and after a peak. Instead, Covell method[3] is used and the channels are chosen at the beginning of the steepest and practically linear part of the peak, on both sides of the peak. Choosing a smaller number of channels on both sides of the centroid, rather than including all channels from the centroid to valleys, has the advantage of avoiding interferences from other peaks that might exist immediately before and after the peak for which calculation is being carried out by the computer.

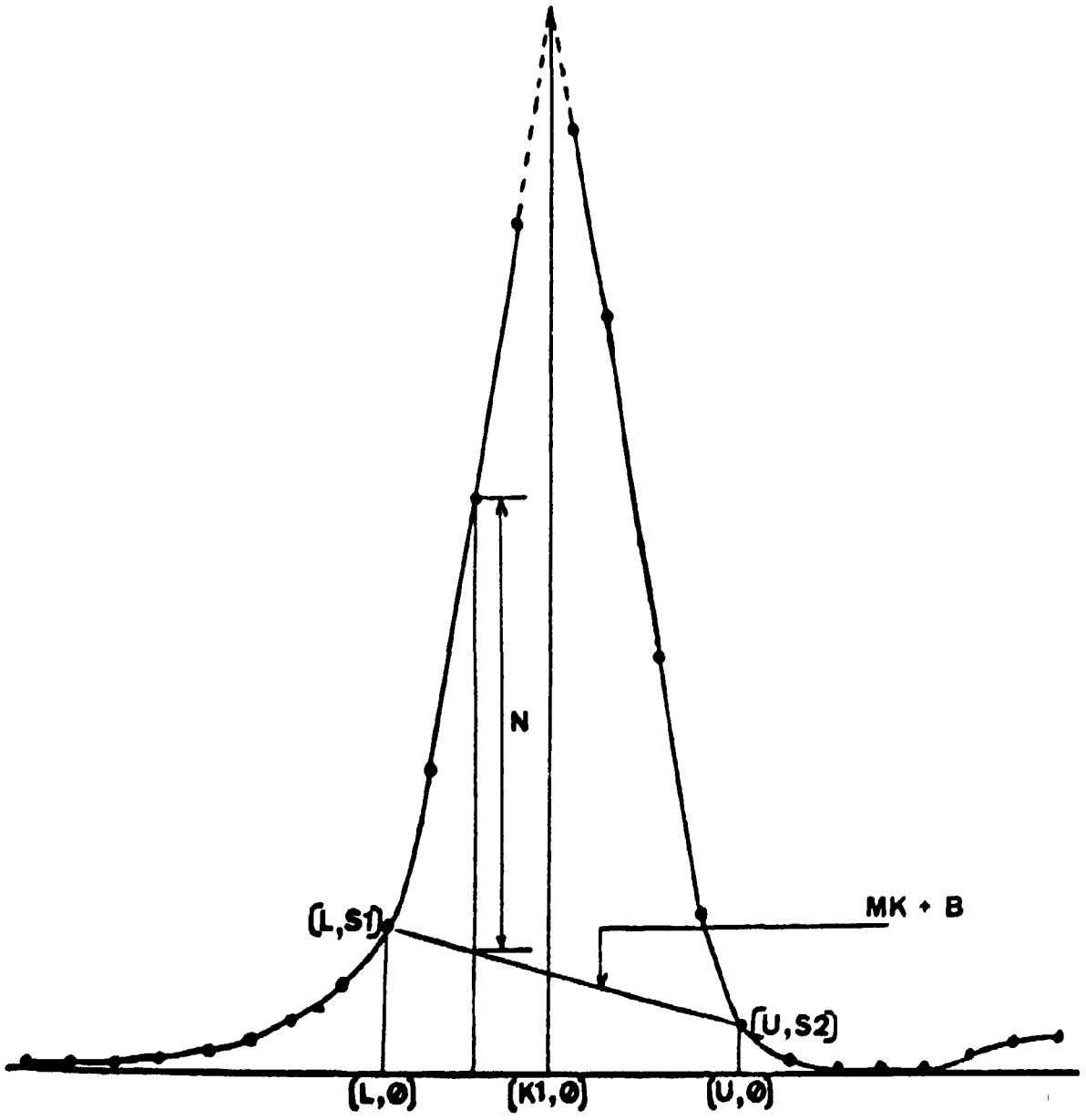
The number of channels L1 to be considered in each side of a peak, by the program, during the analysis of a spectrum, is a function of the slope R of the calibration line "energy versus channel-numbers", that is

$$L1 = INT(3*1/R + 0.5) \qquad (1)$$

In this way the number of channels in a peak is recalculated if the amplifier gain is altered by the user. "INT" stands for "integer in". *means multiplication

If too high values are taken for boundaries on both sides of the peak, meaning a very small number of channels in a peak, the value for the relative standard deviation V/B3, will also be too high (V is the standard deviation for the net area value, as given by equation (7), and B3 the net area of the peak). The choice of the boundaries at the beginning of the almost linear part of the peak, on both sides of the peak, has shown, in practice, to be a good compromise, giving a peak with sufficient number of channels for area calculations and avoiding interferences from other peaks that are too near the one being analysed. As it will be seen, provision is made in the program in such a way that overlapping and unresolvable peaks are duly indicated. Practice has shown that the number of channels in half a peak, as defined by expression (1), is adequate.

FIGURE 1
SCHEMATIC INDICATION OF SYMBOLS FOR CALCULATING
NET AREA AND PEAK CENTROID
(see text)



After the operator chooses the lower channel (L) of a calibration peak, Figure 1, the upper channel (U), the counts S1 and S2 in these channels are registered by the program. The program calculates next the slope and the intercept for the straight line, MK + B, passing through the points (L,S1) and (U,S2). The trapezoidal area defined by the points (L,Ø), (L,S1), (U,S2) and (U,Ø) is subtracted, channel by channel, from the total area of the peak. This subtraction step will give the net values N for the number of counts per channel.

The summation of the N values will give the net area for the peak. The centroid K1 of a peak is calculated by the ratio of the sum of the first moment (product of channel content N and corresponding channel number K) by the net area of the peak, for K varying from L to U:

$$K1 = \sum_{K=L}^{U} NK \Big/ \sum_{K=L}^{U} N \qquad (2)$$

The ratio of the difference between the energy values H2 and H1 for the calibration peaks and the corresponding centroid differences, gives the value R in keV per channel:

$$R = (H2-H1) / (K2-K1) \qquad (3)$$

In general the calibration line does not pass through the origin of the graph "energy versus channels", and the point XØ were this line intercepts the abcissa, is calculated by

$$X\emptyset = K2-H2/R = K1-H1/R \qquad (4)$$

For the calibration step, the program requests (statement 40) the number of channels that shoud be considered in the calibrating peaks. This can be answered by the operator by a previous visual inspection of the oscilloscope image of the two calibrating peaks. The next question regards the lower channel and the energy value for each of the calibrating peaks (statement 80, Table 1). With these entries the program will print the values of R, XØ and the time T, in minutes, during which the calibration spectrum was accumulated.

Spectrum Analysis

After registration of a spectrum on the multichannel analyser it is advisable to smooth the original spectrum (statement 360). The smoothing can improve statiscally poor information by performing a weighted average on the data represented by the spectrum and in this way the registration of too many overlapping peaks is avoided. In order to do this the counting in each channel is substituted by the sum of twice the contents in a channel, plus one time the contents of the channels immediately before and after that especific channel and dividing this sum by 4. This procedure is repeated for all channels in the chosen interval of the spectrum.

If the user decides to smooth the spectrum he should type "1" when the computer asks "do you want to smooth? " or "Ø" if such is not the case.

One should be aware that smoothing the data may distort the statistics and give rise to the appearance of small peak-like maxima that cannot be distinguished from true photopeaks of comparable magnitude[4]. Practice with the use of the program will help the operator in distinguish these ghost peaks from actual ones and when it is advisable to smooth or not.

By using a pulser during the accumulation of the spectrum it is possible to correct for losses in count rate due to pulse pile-up at high dead-times[5]. In order to do that the pulser accumulation data are first registered on the analyser in the absence of the radioactive source whose spectrum is to be analysed. The pulse height of the pulser should be set at a value such that the pulser peak will lie at the farther right end of the spectrum. The fractional loss of peak area, when counting at low and high dead-times, for the pulser and for the photopeak area representing gamma-rays, should be the same. In this way a correction is made by means of statements 380 and 880 in the program, in which the correction factor Q2 is obtained and used in statement 960 for area and standard deviation correction, when high dead-times occur due to very active samples. The data requested by the program in statement 380 are the ones obtained by counting only the pulser in the absence of actual radioactive sources.

After the pulser data have been provided by the operator the next step is the choice of the interval or zone of the spectrum to be analysed, defined by channels Z1 and Z2 (statement 400). The program registers the counting values C in each channel K of the interval Z1 to Z2. A comparison is made of the counts C in channel K with the counts in channels lower and higher by two units with respect to channel K, i.e., (K-2, C1) and (K+2,C2). The condition for a peak to "exist" in channel K is, Guzzi et al.[6]:

$$C > C1 + P^{*}SQR(C1) \quad (5)$$

$$C > C2 + P^{*}SQR(C2) \quad (6)$$

with SQR standing for "square root of".

P, in the above expressions, is a "Sensitivity Factor" used to avoid interpretation, by the program, of statistical counting fluctuations as peaks and has an empirical value between 1 and 2. In this way, only counting values C exceeding C1 and C2 by once or twice the standard deviation in these two channels, are retained by the program in order to calculated the centroid for the peak and to proceed with subsequent calculations. The value of P is requested by the program in statement 290.

Once a peak has been identified by its centroid value, the net area of that peak is calculated for the 2L1 + 1 channels in the peak. If B4 is the total uncorrected area for a peak, the standard deviation V of the net area is calculated by

$$V = SQR(B4+((2^{*}L1+1)/2)\uparrow 2^{*}(S2+S1)) \quad (7)\ (a)$$

A peak is retained as a true peak if the net area B3 of the peak is larger or at least equal to 2 times the standard deviation, that is,

$$B3> = 2^{*}V \quad (8)$$

This condition, plus the ones expressed by (5) and (6), are required for the analysis of a spectrum in the interval from the energy corresponding to channel Z1 up to channel Z2. After the highest energy peak is analysed by the program, the statistical fluctuations of the counts superimposed over the compton continuum, caused by higher energy gammas rays existing above the chosen energy range, will be of the same order of magnitude as the counting rate in

(a) The symbol ↑2 indicates "to the 2nd power"; the asterisk indicates multiplication

each channel laying above the compton continuum. To avoid printing of data corresponding to this part of the spectrum, in which true peaks may not exist, a further empirical condition is imposed, stating that the net counting rate in a peak area must be at least equal to 15 counts per minute. This would correspond to about one to two counts per minute for each channel above the compton continuum or background.

In order not to waist time with calculations which are not useful, such as the calculations corresponding to channels or energy values above the highest energy peak of interest, present in the spectrum, the *Z2* value can be put equal to the channel number where the last peak of interest is located, plus 20 channels, for instance. The last peak of interest present in the spectrum can be visually located by inspection of the spectrum on the display of the oscilloscope.

After calculation of the net area B3 and standard deviation V for a peak, these values are divided by the counting or live time during which the spectrum was accumulated, giving the final results in counts per minute. Both values are printed out together with the channel number K3 for the centroid and its value in energy units, (K3-X0)*R.

In case of overlapping peaks, the calculation of the centroid by formula (1) will displace the value of K3 to the right, since the products NK will be affected by the high N values of the second peak. After the first overlapping peak has been surpassed and the program starts to analyse the peak that overlaps the first one, the contrary will happen, that is, the value of the new K3 will be displaced to the left. This will cause an inversion on the listing of the channels with a peak being registered at channel, for instance, 1738.22 and then another one at 1736.08.

To prevent this, other conditions than the ones expressed by (5) and (6), for the searching of a peak, are required, that is, the counting C3 and C4 at channels K-1 and K+1 should be smaller than the counts C at the channel K corresponding to the channel of maximum content of a peak:

$$C3 < C \tag{9}$$

$$C4 < C \tag{10}$$

The difference between the channel K of maximum content in a peak, registered by the analyser, and the centroid K3 calculated by formula (1), should not be larger than ± 0.5, if the peak is symmetric. In case of overlapping peaks, it has been observed that this difference should not be larger than 2 otherwise the inversion, on registering the channels, will happen, with registration of ghost peaks. For this reason the following condition should also be imposed (statement 950):

$$ABS(K3-K) < 2 \tag{11}$$

in which K is the channel of maximum content of a peak, and K3 is the centroid calculated by formula (1). ABS stands for "absolute value of". If condition (11) is not fulfilled the program will not calculate the area for the peak corresponding to the centroid K3. Instead, the program will folow to the next K value (statement 950 and 990).

The indication of "overlapping peaks" is obtained by comparing the content values of the

channels that lie at the right side of the channel of maximum content K, i.e., from channels K+1 to K+L1 (statements 680, 690, 700, 720). If there is an inversion in the contents of the peaks in this interval (statement 720) the program will print "overlapping peaks" (statement 980)

Other information given by the program are the number of channels "L1" in half a peak that were used for calculations (statement 670 and 1000) and the time "T" during which the spectrum was accumulated (statement 25 and 26; 270; 330 and 331; 1000).

This program is not intended for precise determination of energies since the calibration of the channel axis is made on the assumption of a linear correlation between channel-number and energy, which is rigourously valid only for small channel interval. The approximation, however, is sufficiently good for activation analysis work, where other information is available for the identification of the radioactive species, such as some previous chemical group separation, decay curves, irradiation times, etc.. The approximation for the energies that one may obtain with this program can be evaluated by comparing the values shown in Table 2 with a catalog of gamma-ray energies values, such as the one prepared by Pagden et al.[7].

APPLICATION

To run the program, whose list is presented in Table 1, the operator will first count the calibrating source, for instance, cobalt 60 and cesium 137. It is not necessary to register the time during which the counts were accumulated, since this time will be registered by the analyser through statements 25 and 26. Counting can be interrupted at any moment before the end of the preset time, at the operator convenience, and the registration of the elapsed live-time will be made the same way.

After the calibrating spectrum has been registered by the analyser the operator will comand RUN by the teleprinter. The program will then ask which radioisotopes were used for calibration (statement 10). Next question will be the number of channels that should be considered for calculations in each peak. This number can be chosen by the operator after a visual inspection of the calibration spectrum on the oscilloscope of the analyser. Next the program asks the lower channel and the energy value for each of the two calibrating peaks. After these data have been provided by the operator the computer will calculate and print the slope R in keV per channel, the point X0 where the calibrating straight line intercepts the abcissa or channel axis and the time T, in minutes, during which the calibrating spectrum was accumulated. A PAUSE statement will be printed by the program during which time the operator will comand the analyser to accumulate pulses coming from the pulser and with no radioactive source on the detector. When the accumulation time has elapsed the operator will type the letter C and the teleprinter will then write CONTINUE followed by the question SENSITIVITY FACTOR, to which the operator will answer with a number that practice has indicated convenient (usually in between 1 and 2).

The next instruction or question put up by the computer is "CHECK EXTERNAL OF ANALYSER". It is quite common that the operator, after visual examination of the spectrum, forgets to connect the External key of the analyser. A number typed by the user after that question, and after checking if the analyser is actually connected to the computer, will be followed by a REMARKS statement, when the user will type the pertinent data and

informations in connection with the spectrum that has been registered by the analyser. At this point the spectrum is made up only of the pulser peak.

The following question is "DO YOU WANT TO SMOOTH", to which the operator will answer Ø, meaning "No". It is preferable to have the original data for the pulser, which are quite reproducible.

To the following question CHANNEL AND CPM FOR THE PULSER the answer should be Ø,Ø because no data have yet been obtained for the pulser. The spectrum interval in which the operator is interested is supplied by him after the question "SPECTRUM INTERVAL Z1, Z2".

After these questions have been answered by the user, the data for the pulser, with no radioactive source on the detector, will be calculated by the computer and printed by the teleprinter. The channel number (nearest integer in the printed centroid value) and the CPM for the pulser will be latter used for correction of pulse pile-up, which occurs during counting of actual samples, due to high dead- times.

When the printer types PAUSE again the actual sample is counted and the above procedure is repeated. In this case, when the teleprinter asks for CHANNEL AND CPM OF THE PULSER, the data obtained by counting the pulser alone, with no radioactive source, should be typed by the operator, meaning, the channel number of maximum content and the CPM previously registered. The value for Z2 should exclude the pulser peak, otherwise the pulser data would also be smoothed, what is not convenient, as said before.

For the spectrum corresponding to an actual sample it is advisable to smooth the spectrum (answer 1 to the question DO YOU WANT TO SMOOTH) or too many overlapping peaks will be printed during the scanning of the spectrum. The whole operation of computing, smoothing and printing the spectrum takes about 7 minutes for 4096 channels. The operator can follow and check the zone of the spectrum that is being smoothed or computed by observing the displacement of the luminous point on the oscilloscope of the analyser.

In Table 2 an example is presented of the application to the spectrum of a sample composed of the following radioisotopes: ^{241}Am, ^{57}Co, ^{22}Na, ^{137}Cs, ^{54}Mn, ^{60}Co. The 661.635 keV peak for ^{137}Cs and the 1332.49 keV peak for ^{60}Co were used for calibration. In Table 2 the Sensitivity Factor P was set equal to 2.

TABLE 1

LISTING OF THE PROGRAM

```
LIST
1  REM "SPECTRUM ANALYSIS"
10  PRINT "RADIOISOTOPES FOR CALIBRATION";
20  INPUT O
25  CALL READ(0,T)
26  LET T=T/100
30  DIM H[2]
40  PRINT "NUMBER OF CHANNELS IN CALIBRATION PEAKS";
50  INPUT L3
60  FOR I=1 TO 2
70  LET A=E=0
80  PRINT "LOWER CHANNEL AND ENERGY FOR PEAK";I;
90  INPUT L,H[I]
100  LET U=L+L3-1
110  CALL READ(L,S1)
120  CALL READ(U,S2)
130  LET M=(S2-S1)/(U-L)
140  LET B=S1-M*L
150  FOR K=L TO U
160  CALL READ(K,D3)
170  LET N=D3-(M*K+B)
180  LET A=A+N
190  LET E=E+N*K
200  NEXT K
210  IF I=2 THEN 240
220  LET K1=E/A
230  NEXT I
240  LET K2=E/A
250  LET R=(H[2]-H[1])/(K2-K1)
260  LET X0=K2-H[2]/R
270  PRINT "R=";R,"X0=";X0,"T=";T
280  PAUSE
290  PRINT "SENSITIVITY FACTOR";
291  INPUT P
310  PRINT "CHECK EXT.ANALYSER";
311  INPUT W
320  PRINT "REMARKS"
321  INPUT O1
330  CALL READ(0,T)
331  LET T=T/100
```

```
340  LET Q2=1
350  LET S5=0
360  PRINT "DO YOU WANT TO SMOOTH";
370  INPUT S5
380  PRINT "CHANNEL AND CPM FOR PULSER";
390  INPUT K1,Q3
400  PRINT "SPECTRUM INTERVAL Z1,Z2";
410  INPUT Z1,Z2
420  IF S5=0 THEN 530
430  LET K2=Z1+2
440  CALL READ(K2-1,D4)
450  CALL READ(K2,D2)
460  CALL READ(K2+1,D3)
470  LET S=(D4+2*D2+D3)/4
480  CALL WRITE(K2,S)
490  LET D4=D2
500  LET D2=D3
510  LET K2=K2+1
520  IF K2<Z2 THEN 440
530  LET K=K1
540  IF K=0 THEN 560
550  GOTO 740
560  PRINT " CANAL          KEV          CPM          SD"
570  FOR K=Z1+2 TO Z2
580  CALL READ(K,C)
590  CALL READ(K-2,C1)
600  CALL REA)(K+2,C2)
610  CALL READ(K-1,C3)
620  CALL READ(K+1,C4)
630  IF C<C1+P*SQR(C1) THEN 990
640  IF C<C2+P*SQR(C2) THEN 990
650  IF C<C3 THEN 990
660  IF C <= C4 THEN 990
670  LET L1=INT(3*(1/R)+.5)
680  FOR F=K+1 TO K+L1
690  CALL READ(F,C)
700  CALL READ(F+1,C5)
710  IF C/T<2 THEN 730
720  IF C5>C+2*SQR(C) THEN 980
730  NEXT F
740  LET B4=B3=E=0
750  LET L1=INT(3*(1/R)+.5)
760  CALL READ(K-L1,S1)
770  CALL READ(K+L1,S2)
780  LET M=(S2-S1)/(2*L1+1)
790  LET B=S1-M*(K-L1)
800  FOR X=K-L1 TO K+L1
```

```
810  CALL READ(X,Y)
820  LET B4=B4+Y
830  LET N=Y-(M*X+B)
840  LET B3=B3+N
850  LET E=E+N*X
860  NEXT X
870  IF K1=0 THEN 910
880  LET Q2=ABS(Q3*T/B3)
890  LET K1=0
900  GOTO 560
910  LET V=SQR(B4+((2*L1+1)/2)↑2*(S2+S1))
920  IF B3 <= 2*V THEN 990
930  LET K3=E/B3
940  IF B3/T<15 THEN 990
950  IF ABS(K3-K)>2 THEN 990
960  PRINT K3;(K3-X0)*R;(B3/T)*Q2;(V/T)*Q2
970  GOTO 990
980  PRINT K;TAB(15),(K-X0)*R;TAB(30)"OVERLAPPING PEAKS"
990  NEXT K
1000  PRINT "L1=";L1,"T=";T
1010  PRINT
1020  PAUSE
1030  GOTO 310
9999  END

READY
```

TABLE 2

DATA OUTPUT FOR A SAMPLE COMPOSED OF AM241, CO57, NA22, CS137, MN54, CO60.

```
RUN
RADIOISOTOPES FOR CALIBRATION?CS137,CO60 PEAK 2.
NUMBER OF CHANNELS IN CALIBRATION PEAKS?11
LOWER CHANNEL AND ENERGY FOR PEAK 1     ?1181,661.635
LOWER CHANNEL AND ENERGY FOR PEAK 2     ?2369,1332.49
R= .564517      X0= 13.627      T= 10
PAUSE
CONTINUE
SENSITIVITY FACTOR?2
CHECK EXT.ANALYSER?1
REMARKS
?PULSER DATA.
DO YOU WANT TO SMOOTH?0
CHANNEL AND CPM FOR PULSER?0,0
SPECTRUM INTERVAL Z1,Z2?4010,4040
 CANAL          KEV          CPM          DP
 4025.46      2264.75      3347         18.6384
L1= 5           T= 10

PAUSE
CONTINUE
CHECK EXT.ANALYSER?1
REMARKS
?AM241, CO57, NA22, CS137, CO60, MN54.
DO YOU WANT TO SMOOTH?1
CHANNEL AND CPM FOR PULSER?4025,3347
SPECTRUM INTERVAL Z1,Z2?50,2500
 CANAL          KEV          CPM          DP
 118.303      59.0915      7913.06      77.8447
 229.606      121.924      762.351      40.9376
 255.36       136.463      124.543      38.3494
 645.091      356.472      60.3609      29.8477
 919.045      511.124      4033.11      41.7884
 1186.08      661.867      5400.25      33.9866
 1492.95      835.101      2378.87      25.2547
 2092.61      1173.62      2103.61      21.9372
 2272.06      1274.93      1066.8       14.6274
 2374.78      1332.91      1851         19.5428
L1= 5           T= 10

PAUSE
```

(Note: It is not necessary to count the pulser alone before a new spectrum, The same CPM value 3347 can be used. Channel number of maximum content for pulser should be checked in oscilloscope for each new spectrum.)

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SUMÁRIO

Apresenta-se um programa em linguagem "Instrument Basic" para análise de espectros de raios gama obtidos por intermédio de detectores de Ge-Li e registrados em analisadores multicanais acoplados a minicomputadores. O programa localiza os picos correspondentes às energias dos raios gama detecta determina o valor dessas energias, as áreas dos picos correspondentes, já excluindo a área do trapézio devido à contagem de fundo, e determina ainda, os valores dos desvios padrões de tais áreas.

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