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ANAIS - PROCEEDINGS

FIND - A COMPUTER PROGRAM FOR PEAK SEARCH IN GAMMA-RAY SPECTRA MESURED WITH Ge(Li) DETECTORS.

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RESUMO

O Programa FIND é um programa de computador escrito em FORTRAN IV, para ser usado na localização de picos em espectros gama medidos com detectores Ge(Li).O programa fornece a posição e estima energias e magnitudes relativas para todos os picos encontrados no espectro. A busca é feita por meio do cálculo da "negative smoothed second difference" do espectro experimental,como sugerido por Phillips e Marlow (1).

ABSTRACT

The program FIND is a FORTRAN IV computer code for peak search in spectra measured with Ge(Li) detectors. The program gives the position and estimates energy and relative significance for every peak found in the spectrum. The search in done by calculating a negative smoothed second difference of the experimental spectrum, as suggested by Phillips and Marlow (1).

The FIND program is a computer code written to be used a subroutine in the program ANALYSIS (2), in order to furnish the position in the spectrum to be analyzed. The ANALYSIS program is a FORTRAN IV computer code for spectral analysis, which calculates centroid, area and full width at half maximum of peaks in spectra measured with Ge(Li) detectors. These spectra can be very complex and for a good performance of the ANALYSIS program, all existing peaks in the regions being analyzed must be indicated. The program FIND attempts to make the peak search. The calculation of energy and relative significance are made in order to give the user additional information, but these are only estimates.

The method used for the peak search is that of Phillips and Marlow (1) which has been also used by McCullagh and Helmer (3) in the program GAUSS VII. Various types of other smooth functions have been proposed (4-5) and all of them can be classified as belonging to the general group of symmetric zero-area transforms. According to Phillips and Marlow (1), the simple square wave shape seems best to filter out the background continuum and the high frequency noise. Other transforms may be somewhat better in enhancing a true peak over a statistical fluctuation with a width of the order of a true peak.

THE PROGRAM FIND

The negative smoothed second difference, defined by Phillips and Marlow (1) so as to be positive at a peak, is calculated by a sliding transform as follows:

For an integer M, we define

$$SSD\ (5) = \sum_{H6=V5-M}^{V5+2M+1} H1 * IY1\ (H6)$$

where IY1 (H6) = number of data counts in the channel H6,

H1 = -1 for V5-M <= H6 <= V5-1

2 for V5 <= H6 <= V5

The H1 coefficients define a square wave function with zero convolution area which transforms IY1(H6) to the negative smoothed difference SSD(V5).

When M is approximately equal to the full width at half maximum of the peaks, the function SSD is large and positive at a peak centered between V5 and V5+M-1 and when the the background is smoothly varying, the expected value <SSD (V5)> is approximately zero because of the zero area transform of H1.

The statistical variance in the counts IY1(H6) is just IY1(H6) itself, therefore the variance in SSD(V5) is given by:

$$VAR\ (V5) = \sum_{H6=V5-M}^{V5+2M+1} H1 * H1 * IY1\ (H6)$$

Since the standard deviation is just the square root of the variance, the function defined as

$$SS(V5) = SSD(V5)/((VAR(V5))^{1/2})$$

is normally distributed around zero with unit standard deviation except in the vicinity of a peak or other sharply varying feature within a range of the width M.

The most proeminent feature in the background is usually the Compton edge but its full width at half maximum is quite large compared to that of a peak. So, when high resolution Ge(Li) detectors are used, the function SS (V5) is insensitive to Compton edges because the values of M being used correspond to those of peaks.

The quality of the search depends on the width M. Generally the performance of the search is good if just the mean width over the whole spectrum is used. For the case where the width is largelly varying, it can occur loss of peaks if just a mean value is used. In order to avoid this problem, the program uses a linear calibration for the local width. The calibration points, two channels with their respective widths,are given by the user.

The calculation of SS(V5) is carried out by varying V5 over the whole spectrum. The peak search starts from the low-energy end of the spectrum at a point chosen by the user through the input parameter INI.

The search is done over intervals of width 3M. If there is a peak at a channel H2, the funcion SS (V5) will be positive in the interval of width M centered at H2=V5-(M-1)/2 and negative in the two equal and adjacent intervals. At V5=H2, SS(V5) has its maximum. SS(H2) is not the total area of the peak centered at H2 but it increases with the amplitude and the width of the peak. In this sense, it is possible to compare two peaks and SS(H2) can be taken as an estimate of the peak's relative significance.

The function SS(V5) is also used to prevent statistical background fluctuations be taken as peaks. This is done through the input parameter SENS. The parameter SENS means the minimum value that SS (H2) can reach if a peak is considered to exist at H2. The value SENS=3.Ø has been found to give enough sensitivity to detect almost all valid peaks with little probability of including statistical background fluctuations.

Once a peak is found, tests are made to detect a possible multiplet by analyzing the increase and the decrease of SS (V5) in the interval. It is possible to indicate the peak's positions in a multiplet it the peaks are spaced by a distance greater than M.

The program has the option of estimating the peak energies. for this calculation, the user has to input the estimated energies of the same two channels given for the width calibration.

The program is listed in the appendix A.

DATA INPUT

This program uses the file number 15 for the experimental data counts and

the file Ø5 for other input data. The sequence and formats are as follows:

1. INI,FIM,SEMS (215,F8.2)
   INI is the channel where the search is to start,
   FIM is the last channel of the spectrum.
   SENS is the sensivity factor.
2. IY1 (I9,9I7)
   IY1 is experimental spectrum
3. CANAL1,LARG1, CANAL2, Larg2 (4F8.2)
   CANAL1 and CANAL2 are two channels used for calibrations.
   LARG1 and LARG2 are their respctive widths, given in channel units.
4. IOP1,E1,E2
   IOP1 = Ø for energy calibration,
   = 1 otherwise.
   E1 and E2 are the respective energies for the channels CANAL1 and CANAL2, given in KeV and needed for the option IOP1=1.

CONCLUDING REMARKS

The program was written to be used with spectra up to 4Ø96 channels, where the channel number zero stores the counting time. For spectra starting from channel number 1, the positions of the peaks will be shifted by-1 channel.

The program FIND showed a very good performance in very spectrum it has been tried for. Figure 1 shows part of a Melamine plus Ammonium Chloride thermal neutrons capture gamma-rays spectra measured with a pair spectrometer (6).

Table 1 shows the search results for the input parameter IOP1=Ø and SENS=3.Ø.

The peak search is an important step in the automatic spectral analysis. So, although the high quality of the peak search, it is necessary to keep in mind that, sometimes peaks are so weaks and personal sensivity has to be used to get the best result.

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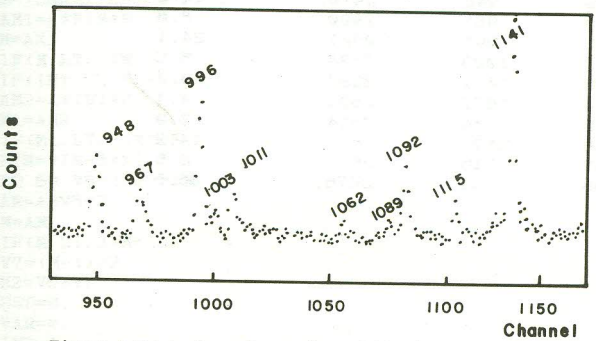

Figure I. Part of an Ammonium Chloride plus Melamine thermal neutrons capture gamma-rays spectrum, measured with a pair spectrometer.

TABLE I. Output for the region showed in fig.1.

PEAK NUMBER	PEAK POSITION	ESTIMATED ENERGY (KEV)	ESTIMATED REL. SIGNIF.
1	131	1600.	6.6
2	204	1678.	8.0
.			
.			
.			
29	948	2470.	14.2
30	967	2490.	8.6
31	996	2521.	24.1
32	1003	2528.	5.5
33	1011	2537.	9.3
34	1062	2591.	4.1
35	1084	2614.	3.9
36	1092	2623.	14.2
37	1115	2648.	8.5
38	1141	2676.	36.5

APPENDIX A. The FORTRAN IV list of the program FIND.

```
      DIMENSION IY1(4096),SS(4096),FAT(300)
      REAL LARG1,LARG2
      INTEGER H2,H4,H5,H6,V5,FIM,PICO(300),FIN,V6,V7
      READ(5,1)INI,FIM,SENS
    1 FORMAT(2I5,F8.2)
      READ(15,2)(IY1(I),I=1,FIM)
    2 FORMAT(I9,9I7)
      READ(5,3)CANAL1,LARG1,CANAL2,LARG2
    3 FORMAT(4F8.2)
      READ(5,4)IOP1,E1,E2
    4 FORMAT(I5,2F10.3)
      A=(LARG1-LARG2)/(CANAL1-CANAL2)
      B=A*(CANAL1+CANAL2)
      B=(LARG1+LARG2-B)/2
      AM1=A*FIM+B
      M=AM1
      IF(M.LT.3)M=3
      IF(INI.LE.M)INI=M+1
      AM2=A*INI+B
      M1=AM2
      IF(M1.LT.3)M1=3
      FIN=FIM-3*M1+1
  510 DO 50 V5=INI,FIN
      AM=A*V5+B
      M=AM
      IF(M.LT.3)M=3
      V7=(M-1)/2
      H2=V5+V7
      SSD=0.
      VAR=0.
      IND=1
   88 GO TO(55,66,77,110),IND
   55 H1=-1.
      H4=V5-M
      H5=V5-1
      GO TO 99
   66 H1=2.
      GO TO 98
   77 H1=-1.
   98 H4=H5+1
      H5=H5+M
   99 IND=IND+1
      DO 10 H6=H4,H5
      H3=IY1(H6)/100.
      SSD=SSD+H1*H3
      VAR=VAR+H1*H1*H3
   10 CONTINUE
      GO TO 88
  110 IF(VAR-.1)33,35,35
   33 SS(H2)=-100.00
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```
      GO TO 50
35    VAR=SQRT(VAR)
      SS(H2)=10*SSD/VAR
50    CONTINUE
      V7=(M1-1)/2
      V5=IN1+V7
      AFIN=AM1/2
      FIN=FIM-AFIN
      IND=0
      H2=V5
87    K1=0
      K3=0
      A1=SS(H2)
      IF(A1)60,60,61
61    IF(A1-SENS)60,62,62
62    AM=A*H2+B
      IF(AM.LT.3.0)AM=3.0
      H6=AM/2+1
      DO 64 H4=1,H6
      H5=H2-H4
      IF(H5.LE.V5)GO TO 60
      A2=SS(H5)
      A2=ABS(A2)
      IF(A1-A2)64,70,70
70    K3=K3+1
64    CONTINUE
      DO 67 H4=1,H6
      H5=H2+H4
      A2=SS(H5)
      A2=ABS(A2)
      IF(A1-A2)67,71,71
71    K1=K1+1
67    CONTINUE
      IF(K1.EQ.H6.AND.K3.GT.1)GO TO 75
      IF(K3.EQ.H6.AND.K1.GT.1)GO TO 75
60    IF(H2.EQ.FIN)GO TO 104
      H2=H2+1
      GO TO 87
75    IND=IND+1
      IF(IND.LE.300)GO TO 76
      IND=IND-1
      GO TO 105
76    PICO(IND)=H2-1
      FAT(IND)=SS(H2)
      H2=H2+H6+1
      GO TO 87
104   IF(IND.GT.0)GO TO 105
      WRITE(6,107)
107   FORMAT(1X,'NO PEAKS FOUND')
      GO TO 106
105   IF(IOP1.EQ.1) GO TO 220
      WRITE(6,44)
```

```
 44   FORMAT(////,' PEAK',4X,'PEAK',5X,'ESTIMATED',/,' NUMBER',
     *2X,'POSITION',2X,'REL. SIGNIF.',//)
      WRITE(6,201)(I,PICO(I),FAT(I),I=1,IND)
201   FORMAT(//,(I5,I11,F13.1)/(I5,I11,F13.1))
      GO TO 106
220   A1=(E1-E2)/(CANAL1-CANAL2)
      B1=A1*(CANAL1+CANAL2)
      B1=(E1+E2-B1)/2
      WRITE(6,224)
224   FORMAT(////,' PEAK',4X,'PEAK',6X,'ESTIMATED',5X,'ESTIMATED',/,
     *' NUMBER',2X,'POSITION',2X,'ENERGY (KEV)',2X,'REL. SIG.',//)
      DO 223 I=1,IND
      E=PICO(I)*A1+B1
      PRINT 225,I,PICO(I),E,FAT(I)
225   FORMAT(I5,I11,F13.0,F14.1)
223   CONTINUE
106   STOP
      END
```