



IT9700078

1T4700078

ENEA

ENTE PER LE NUOVE TECNOLOGIE,
L'ENERGIA E L'AMBIENTE

Dipartimento Energia

DESCRIPTION OF THE COMPUTER CODE PRINS, PROGRAM FOR INTERPRETING GAMMA SPECTRA, DEVELOPED AT ENEA

ROBERTO BORSARI

Centro Ricerche "Ezio Clementel", Bologna

RT/ERG/95/15

**NEXT PAGE(S)
left BLANK**

R
VOL 28 No 0

RIASSUNTO

Il codice di calcolo PRINS, PRogramma per l'INterpretazione automatica degli Spettri gamma, è stato sviluppato dallo scrivente in collaborazione con il servizio SECC (Service Etude Comportement du Combustible) del centro CEA di Grenoble.

In seguito è stato aggiornato e migliorato all'ENEA in modo indipendente.

Prerogative del codice PRINS sono:

- 1) Un potente algoritmo di individuazione dei picchi;
- 2) Una accurata valutazione degli errori;
- 3) Possibilità di una calibrazione automatica canali-energia.

ABSTRACT

The computer code PRINS, PRogram for INterpreting gamma Spectra, has been developed in collaboration with CENG/SECC (Centre Etude Nucleaire Grenoble / Service Etude Comportement du Combustible).

Later it has been updated and improved at ENEA.

Properties of the PRINS code are:

- 1) A powerful algorithm to locate the peaks;
- 2) An accurate evaluation of the errors;
- 3) Possibility of an automatic channels-energy calibration.

**NEXT PAGE(S)
left BLANK**

CONTENTS

1. Introduction
2. Review of the general concepts of gammametry
 - 2.1 Photo - electric effect
 - 2.2 Compton effect
 - 2.3 Pair production effect
 - 2.4 Constitution of a spectrum
 - 2.4.1 Conversion of the analogical signals
 - 2.4.2 Analogical - digital conversion
 - 2.4.3 Multichannel analyser
3. Interpretation of a spectrum
 - 3.1 Procedure for interpreting a spectrum
4. The basic equation
 - 4.1 Correction due to the radio-decay during counting time
5. Peak searching algorithm
6. Best-fit algorithm
 - 6.1 Error due to the best-fit algorithm
7. Student's test
8. Minimum detectable
9. Channels - energy calibration function
 - 9.1 Automatic calibration
 - 9.2 Interactive calibration
10. Programming / system features
11. Acknowledgements
12. References

**NEXT PAGE(S)
left BLANK**

1. Introduction

A radio nuclide gamma emitter is an unstable nuclide that emits one, or more, gamma rays when it decays to the ground state.

These gamma rays can be recorded in a gamma spectrum, which is the distribution of the gamma ray intensity versus their energy.

To interpret a gamma spectrum means to evaluate which and how many radio nuclides were present in the source at a given instant, starting from the shape of the spectrum and the parameters of the recording.

2. Review of the General Concepts of Gammametry

A spectrum of gamma rays is characterised by a curve representing the distribution of the gamma rays intensity versus the energy.

The detection of these gamma rays is performed by means of diodes, Germanium or Silicon compensated with Lithium, or H.P. Germanium (high purity), that work at low temperature and in a vacuum environment.

The interaction of the gamma photons with the detectors is ruled by different phenomena:

- 1) Photo-electric effect;
- 2) Compton effect;
- 3) Pair production effect.

2.1 Photo - Electric Effect

The photons interact with the external electronic layers of the detector atoms (external photo-electric effect), or with those of the internal layers (internal photo-electric effect).

In both cases the incident photon vanishes and the collided electron is ejected with energy:

$$E_e = h \cdot \nu - E_b$$

with:

E_e = electron energy

h = Planck's constant

ν = photon frequency

E_b = binding energy of the electron (negligible compared with the photon energy)

The ejected electron produces an ionisation in the detector crystal proportional to its energy.

In the case of the internal photo-electric effect, the change of position of the electron involves some transitions of the external electrons with emission of fluorescence X rays.

The fluorescence photons may produce, in their turn, photo-electric effect on the external electrons; the electrons ejected with this mechanism are called Auger electrons.

The photo-electric effect is predominant at low energy, its probability decreases rapidly when the energy increases and, versus the atomic number Z of the detector, it is about proportional to Z^5 .

When the incident photon energy increases, the internal photo-electric effect gives place progressively to the Compton effect, and later to the pair production effect.

2.2 Compton Effect

The incident photon, with energy $h \cdot \nu_0$, interacts with an electron of the internal layers; the electron is ejected with a certain speed and the incident photon is scattered with a reduced energy $h \cdot \nu_1$.

In the process, the energy and the momentum are conserved (the momentum of the ejected electron is compensated by a nucleus recoil).

If the scattered gamma, of $h \cdot \nu_1$ energy, is absorbed in the crystal, the detection will give only one peak, the sum of all secondary ionisation.

Then we have the same result as the photo-electric effect, because the phenomenon is very rapid and the electronic devices cannot react so rapidly.

If the scattered photon leaves the detector, the absorbed energy is equal to the difference $h \cdot \nu_0 - h \cdot \nu_1$, and the resulting peak will be statistically smaller than the previous one.

The probability of Compton interaction decreases when the photon energy increases (but not so rapidly as in the photo-electric effect), and it is about proportional to Z/A (Z atomic number, A mass number); therefore the Compton effect is predominant in absorbers with an intermediate atomic number.

2.3 Pair Production Effect

The interaction consists in the disappearance of the incident photon and the production of the pair electron-positron.

A photon energy ($h \cdot \nu_0$) greater than 1022 keV is needed; 511 keV being the rest energy of both the electron and the positron.

The energy exceeding 1022 keV is transferred, as kinetic energy, in part to the pair electron-positron, in part to the nucleus, in such a way as to conserve the momentum (the interaction always takes place close to a nucleus).

The electron and the positron lose their kinetic energy by ionisation in the detector, and later the positron reacts with an electron of the crystal, with a process named annihilation: both particles vanish and their mass is transformed into two photons, with energy of 511 keV, emitted in opposite directions.

These two photons, in their turn, may interact with the crystal by photo-electric or Compton effect.

Because of all that, the presence, in a spectrum with peaks of high energy, of a 511 keV peak due to the absorption of one photon, and a smaller 1022 keV peak due to the simultaneous absorption of both photons (less probable).

When one of the two annihilation photons leaves the detector, we obtain an energy peak of $h \cdot \nu_0 - 511$ keV (simple escape peak), if both photons leave the detector, we obtain an energy peak of $h \cdot \nu_0 - 1022$ keV (double escape peak).

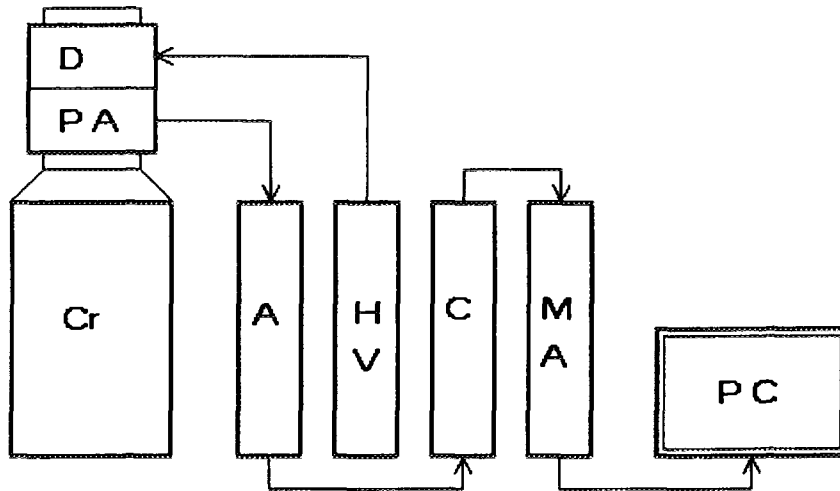
If the energy of the incident gamma ($h \cdot \nu_0$) is high enough, these two latter peaks are more important than the total absorption peak.

The probability of pair production interaction increases rapidly, from the threshold of 1022 keV, with the energy of the incident gamma (in opposition to the Compton and photo-electric effects), versus the atomic number Z it is proportional to Z^2 .

In practice the reply of a gamma ray detector are electric impulses proportional to the energy of the incident photon (photo-electric peak), and impulses representative of a fraction of the incident photon energy (Compton plateau).

2.4 Constitution of a Spectrum

Fig. 2.1 shows a scheme of a gamma spectrometry chain.



D = diode
Cr= cryostat
HV = high voltage
MA = Multichannel analyser
PA = pre-amplifier
A = shape amplifier
C = analogical-digital converter
PC = personal computer

Fig. 2.1

2.4.1 Conversion of the Analogical Signals

a) In the detector.

The initial signal is constituted by the gamma photons that enter the detector.

Of these photons we want to measure the energy and the quantity per unit of time.

At present for this purpose the detector is usually a cylinder of high purity Germanium (hp GE), with electric contacts that enable us to apply a high voltage between two surfaces, in general, one surface close to the axis, and the lateral surface (coaxial detector).

This voltage, close to 5000 volts, produces a radial electric field to obtain a desert zone of charges (reverse polarisation).

To obtain a reverse current, weak enough (some ηA), the detector is cooled down to the liquid nitrogen temperature (about $-196\text{ }^{\circ}C$) by means of a cryostat.

We have seen (§ 2.1, 2.2, 2.3) that the gamma photons produce electric charges in the detector, by interaction with the electron layers of the atoms.

These charges are collected by the conductor contacts.

When the gamma photons are completely absorbed, the total sum of charges produced and collected is proportional to the energy of the incident photons; this makes the line spectrometry of the gamma photons possible, and so the identification of the emitter nuclides.

b) In the pre-amplifier.

The pre-amplifier uses a field effect transistor as a first component because of the high input impedance.

To reduce the background noise, this pre-amplifier is cooled down to the liquid nitrogen temperature as well as the crystal detector.

The reduction of the background noise improves the peaks resolution (reduction of the peak width).

The pre-amplifier function is to transform the variations of the collected number of charges into voltage variations of duration equal to the charges collection time in the detector (about 100 ns).

c) In the shape amplifier.

The rapid variations of voltage are shaped to optimise the ratio signal/background and to obtain the best resolution.

Moreover they are amplified to provide a level signal suitable for the analogical - digital converter (about 10 volts max.).

2.4.2 Analogical - Digital Conversion.

This consists in converting the maximum amplitude of an impulse in a numeric value that will be identified as an address in the storage memory.

Two methods can be used.

The more ancient (Wilkinson method) consists in charging a condenser at the voltage to be measured, and then in discharging it with known quantities of electricity; the number of these quantities constitutes the numeric value of the conversion.

In practice, the condenser is disconnected and discharged by means of a constant current source; the duration of the discharge is measured with a high frequency clock.

The conversion is stopped when the charge reaches zero.

Then the condenser is reconnected to analyse the next impulse.

The disadvantage of this method is having a conversion time proportional to the impulse amplitude.

In the second method the conversion is performed by successive comparisons between the impulse amplitude and a voltage produced by a digital-analogical converter.

This technique is named weighted codification.

The conversion time is independent of the impulse amplitude.

In both methods the conversion module provides the busy signals that permit measuring the active counting time, that is, they allow correcting the loss of counts during the conversions.

2.4.3 Multichannels Analyser.

The analyser permits stocking the information from the converter and, when the counting is closed, their transmission to a computer.

Stocking consists in adding "+1" to the content of the memory-block at the address fixed by the converter (at the end of the conversion).

The numeric value of the address is proportional to the impulse amplitude.

If a module to correct the loss of counting (Westphal, Harms) is used, the correction consists in adding "+n" instead of "+1".

The whole of the memory-block contents versus their addresses constitutes a spectrum of number of counts versus the analyser channels.

Usually the maximum number of channels in a spectrum is 4096 or 8192 (even 16384) , the maximum content of a channel may reach about four thousand million ($2^{32} = 4.29 \cdot 10^9$).

The analyser also constitutes a header that contains the information about the spectrum.

The header is usually stocked in the first channels of the spectrum.

3. Interpretation of a Spectrum

The general shape of a spectrum is made up of two parts.

One corresponds to a continuous background, the other to the peaks of total absorption of the photons energies; these peaks are situated above the background.

These peaks constitute the interesting part of the information.

It is, in particular, the surface of these peaks that will have to be determined to evaluate the source activity.

Fig. 3.1 shows a spectrum recorded with a coaxial diode.

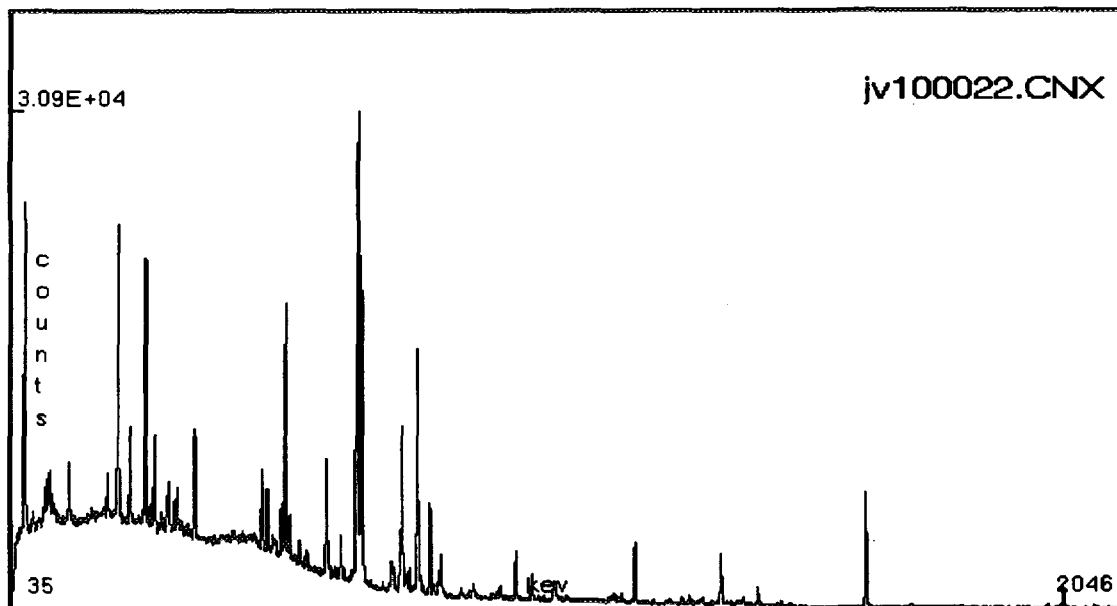


Fig. 3.1 Spectrum of 4096 channels recorded with a coaxial diode (*)

3.1 Procedure for Interpreting a Spectrum

To interpret a spectrum we have to go back from its general shape to the number of atoms of every emitter present in the radioactive source at a given instant "T".

The procedure adopted in the PRINS code is the following.

(*) *The spectra used for the figures in this report belong to CEA/CENG/SECC (Commissariat Energie Atomique / Centre Etude Nucleaire Grenoble / Service Etude Comportement du Combustible) and to CEA/CEC/SEA (Commissariat Energie Atomique / Centre Etude Cadarache / Service d'Experimentation des Accidents) .*

1) Recognition of the peaks of total absorption (of the photon energy) above the continuous background.

In particular we need to find the peak position in the spectrum (the central channel of the peak), its height above the background, its width at half-maximum (number of channels between the two inflexion points), and its boundaries.

2) Tests on the peak quality: Student's test and test on the WHM (Width at Half-Maximum); possible rejection of the peak.

3) Determining the background level beneath every peak.

4) Best-fit of every peak with a gaussian curve; if two or more peaks are close enough, the number of gaussian curves to best-fit, at the same time, is equal to the number of the interfering peaks (multiplet).

5) Determining the gaussian curve surfaces best-fitted on the peaks; if the best-fit algorithm leads to a singular system, the surfaces are determined by histogram.

6) Calibration channels - energy by means of a calibration function (usually a 2nd degree polynomial), determined from the positions of certain peaks whose reference energy is known.

7) Estimation, for every peak, of the related source term, from the detected fraction, by means of a global efficiency curve which it takes into account:

a) the collimator, that determines the solid angle under which the source is seen by the detector;

b) the self-absorption of the radioactive source;

c) the absorption of the structures that surround the source;

d) the diode efficiency versus the incident ray energy.

This efficiency curve is established with an additional procedure (outside the PRINS code) by means of a spectrum recorded with a radioactive source, whose activities and self-absorption are known; or with a method named "self determination of the efficiency curve", that consists in determining, first, the shape of the efficiency curve, by means of the multi-lines nuclides present in the same source to be measured, and later in fixing the ordinate by means of a spectrum recorded with a source (usually CO^{60} or CS^{137} , or both) whose apparent activity is known.

This procedure evaluates also the uncertainty (function of the energy) of the efficiency curve.

8) Correction due to the absorption of a S.S. (Stainless Steel) shield, if used between the diode and the source, in order to limit the counting.

It is suitable to keep this correction out of the efficiency function, because this shield may be added at the last moment, and with different thickness from case to case.

9) Comparison of the energy of the detected peaks with the reference energy of the lines in a gamma-library; attribution, sometimes multiple, of the peaks to certain lines of the library.

The gamma library is set up with an additional procedure (outside the PRINS code); the library contains all the nuclear data including the uncertainty on the branch factors of the lines (gamma %).

Moreover the procedure determines the interferences among the lines, i.e. lines whose energies are in a range of the same order as the detector resolution.

10) Calculation of the number of atoms from the surface of every peak (application of the basic equation), correction due to the radioactive decay during counting time, correction of the interferences among the lines attributed to the same peak.

Weighed average among the results related to the lines of the same nuclide.

Some steps of the procedure to interpret a gamma ray spectrum are described in detail in the following paragraphs.

4. The Basic Equation

From the gamma-ray source to the result (number of atoms of a given nuclide, at a given instant, in a given volume), calculated by means of a peak of the spectrum, the information undergoes a series of subsequent degradations.

a) For the gamma beam:

- Self-absorption of the source and absorption by its container;
- Reduction due to the collimator (solid angle);
- Absorption due to the S. S. (stainless steel) shield, if one is present;
- Answer of the diode (efficiency at the gamma energy).

b) For the electric signal:

- Transmission of the electronic chain (dead time).

c) In the calculation:

- Evaluation of the peak surface.

The hypothesis, made in the interpretation of a gamma spectrum, according to the gaussian statistics, is the existence of a surface related to every peak, named "gaussian surface", proportional to the number of photons emitted by the radio nuclide at that energy.

This hypothesis is translated into the following equation, which is the basis of the spectrum interpretation.

$$(4.1) \quad SG_i = \lambda \cdot N \cdot \gamma_i \cdot T_e \cdot \rho(E_i) \cdot \varepsilon(E_i)$$

with:

SG_i = gaussian surface of the peak related to the "i" line of energy E_i ;

λ = radioactive constant of the emitting nuclide;

N = number of atoms of the emitting nuclide present in the source;

γ_i = absolute intensity (or branch factor) of the "i" line;

T_e = equivalent counting time, usually equal to the active time (real time - dead time);

$\rho(E_i)$ = proportional factor, function of the energy, that takes into account all factors related to the energy, except the absorption loss due to the S.S. shield, and a factor related to the collimator system, i.e.:

- proportional factor due to the self-absorption of the source and the absorption by its container;
- proportional factor due to the collimator system (solid angle from which the source is seen by the diode, and the interactions of the gamma beam with the inner side of the collimating channel);
- proportional factor due to the efficiency of the diode at the given energy (intrinsic efficiency).

The function $\rho(E_i)$ is named absolute efficiency, it is established experimentally, as stated in § 3.1.

The best representation of the efficiency curve has been obtained by means of the formula:

$$(4.2) \quad \log[\rho(E)] = a + b \cdot \log(E) + c \cdot [\log(E)]^2 + d \cdot [\log(E)]^3$$

a, b, c and d being the results of a best-fit with a polynomial of degree 3.

Usually an efficiency curve is defined by two determinations of this type: one valid for the energies smaller than a joint value, the other for the energies beyond it.

$\varepsilon(E_i)$ = proportional factor, function of the energy, due to the loss through absorption of the S.S. shield.

ε represents the transmitted fraction of the gamma beam by the S. S. shield. It is:

$$\varepsilon(E_i) = e^{-\mu(E_i) \cdot X}$$

with:

$\mu(E_i)$ = linear absorption coefficient of the S. S. at the energy E_i (in mm^{-1});

X = shield thickness (in mm).

The best representation of the function $\mu(E)$ has been obtained with the formula:

$$(4.3) \quad \log[\mu(E)] = a + b \cdot \{\log[\log(E)]\} + c \cdot \{\log[\log(E)]\}^2 + d \cdot \{\log[\log(E)]\}^3$$

a, b, c and d being the results of a best-fit with a polynomial of degree 3.

From the basic equation (4.1) we obtain:

$$(4.4) \quad N = \frac{SG_i}{\lambda \cdot \gamma_i \cdot T_e \cdot \rho(E_i) \cdot \varepsilon(E_i)}$$

4.1 Correction Due to Radio-Decay During Counting Time

The equation (4.4) (basic equation) does not take into account the variation of the atoms number $N(t)$, of the emitting nuclide, during counting time, due to the radio-decay.

If we take as a reference instant the time at the beginning of the counting ($t=0$), N is equal to:

$$(4.1.1) \quad N = \frac{1}{T_r} \cdot \int_0^{T_r} N_0 \cdot e^{-\lambda t} \cdot dt$$

with:

T_r = counting time;

N_0 = number of atoms of the emitting nuclide at $t=0$;

then:

$$(4.1.2) \quad N = \frac{N_0 \cdot (1 - e^{-\lambda T_r})}{\lambda \cdot T_r}$$

Therefore, if N is the value that we would obtain without correction (it represents the average value of the number of atoms during the counting):

$$(4.1.3) \quad N_0 = N \cdot \frac{\lambda \cdot T_r}{1 - e^{-\lambda T_r}}$$

The correction is important for nuclides with half-life of the same order as the counting time.

5. Peak Searching Algorithm

The peaks of total absorption are, at first, located with the analysis of the first derivative of the counting curve.

As a first derivative of the counting in the "I" channel, we take the derivative in the same channel at the parabola of the least squares fitted on the counts of the five channels I-2, I-1, I, I+1, I+2 (smoothness on 5 channels), or of the seven channels I-3, I-2, I-1, I, I+1, I+2, I+3 (smoothness on 7 channels).

The option can be chosen by an index in the input file of general data.

The algorithm searches (fig. 5.1) the number of the channel of the left boundary IG, the one of the right boundary ID, the number of the channel where the derivative has its maximum positive value ID1 (first inflexion point), the one where the derivative has its minimum negative value ID2 (second inflexion point).

Then the algorithm checks the second derivative (second derivative also calculated on channel I at the least squares parabola).

If the second derivative is positive in the channels between IG and ID1, negative between ID1 and ID2, positive again between ID2 and ID (fig. 5.1), the algorithm goes on to search the next peak.

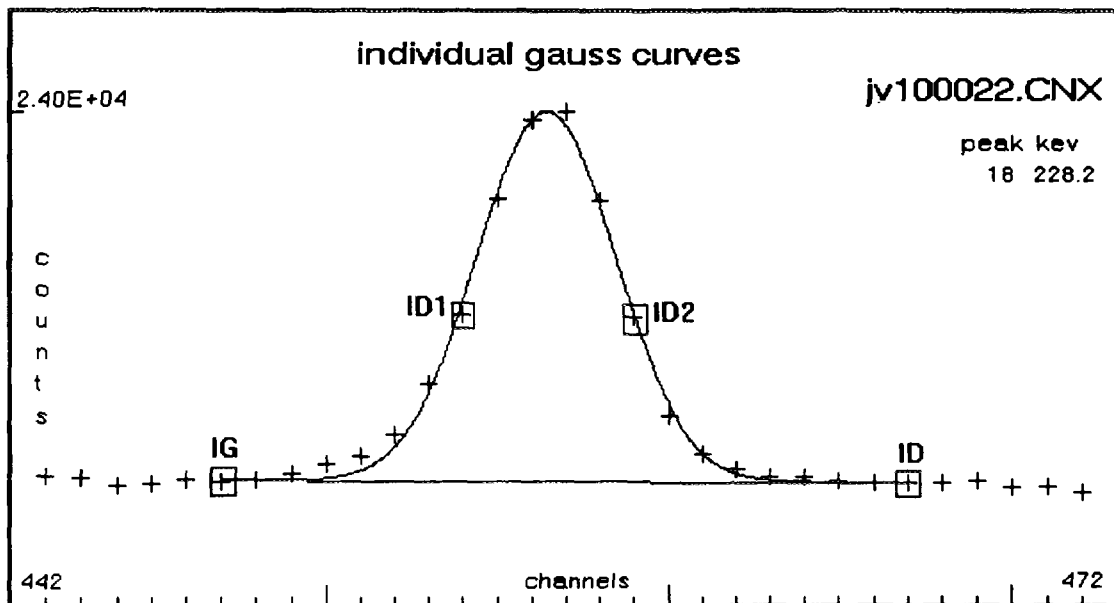


Fig. 5.1 Peak defined with the first derivative analysis

In case the behaviour of the second derivative is not as expected, the algorithm defines additional peaks, between the channels IG and ID, in the following manner.

1) Case in which the second derivative is negative, in one or more channels, between the left boundary IG and the first inflexion ID1, or between the second inflexion ID2 and the right boundary ID:

In both cases the algorithm defines an additional peak on the side of the peak already defined by means of the first derivative analysis.

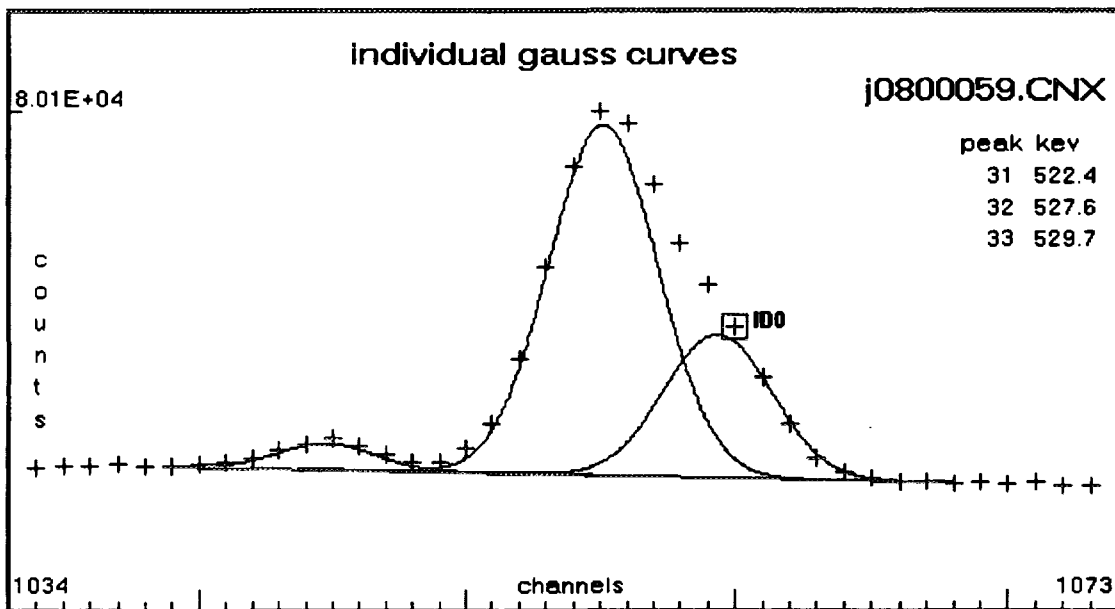


Fig. 5.2.a Peak number 33 has been defined with the second derivative analysis on the side of a peak defined with the first derivative analysis

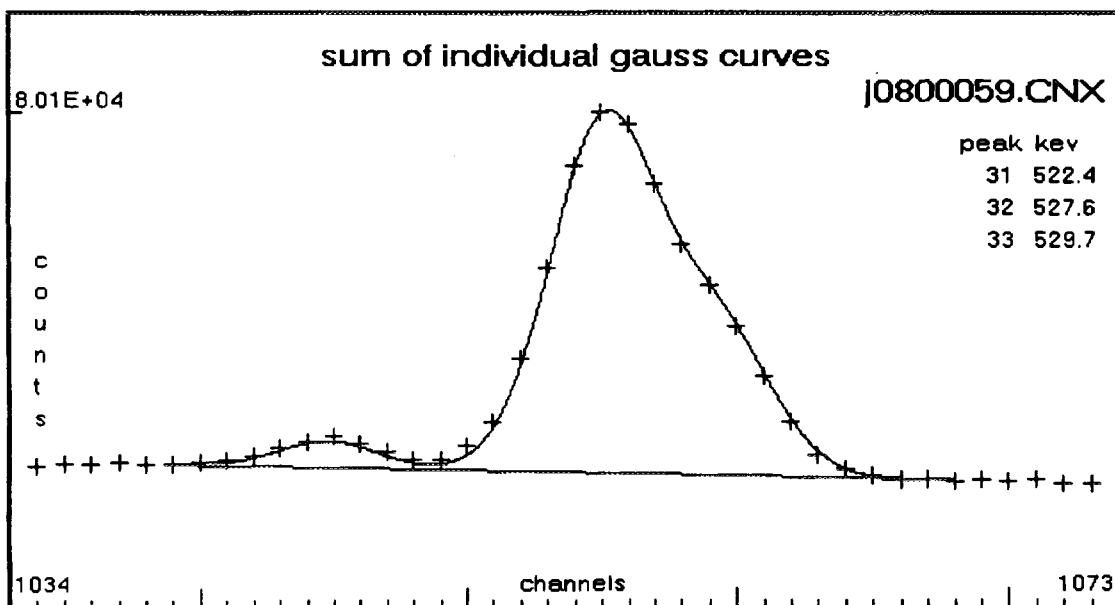


Fig. 5.2.b Sum of the individual Gauss curves of fig.5.2.a

The new peak is centred on the channel in which the second derivative has the minimum negative value (maximum concavity downwards) ID0, the counting in the same channel is taken as its height, and the expected resolution of the diode for the given channel (or energy) is taken as its WHM (Width at Half-Maximum).

These will be the initial parameters of the new peak for the best-fit.

Fig. 5.2.a shows one peak and Fig. 5.3.a shows two peaks defined in this way.

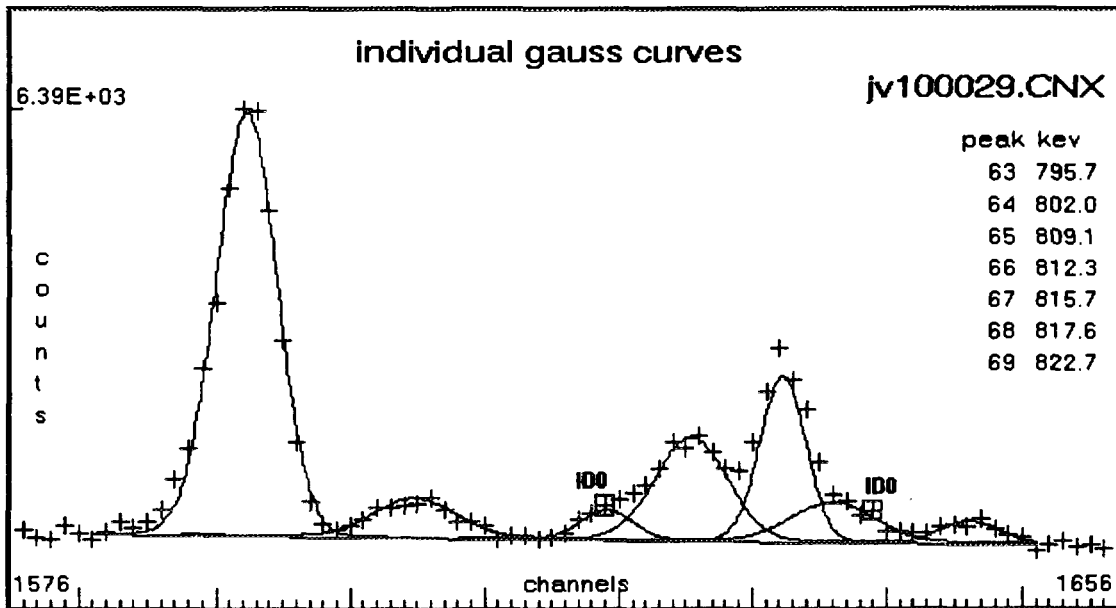


Fig. 5.3.a Peaks number 65 and 68 have been defined with the second derivative analysis on the side of a peak defined with the first derivative analysis

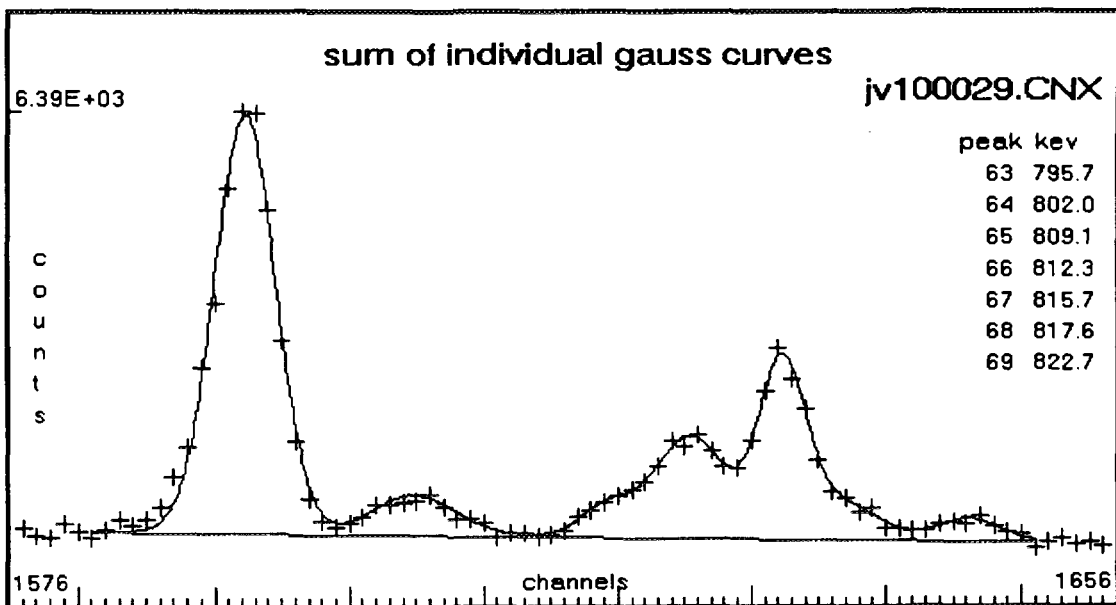


Fig. 5.3.b Sum of the individual Gauss curves of fig.5.3.a

2) Case in which the second derivative is positive, in one or more channels, between the first inflexion point ID1 and the second ID2:

In that case (fig. 5.4.a/c), first, is located the channel between ID1 and ID2 in which the second derivative has the maximum positive value ID0 (maximum concavity upwards).

Then the algorithm searches between ID1 and ID0, and between ID0 and ID2 the channels in which the second derivative has the minimum negative value, ID10 and ID02.

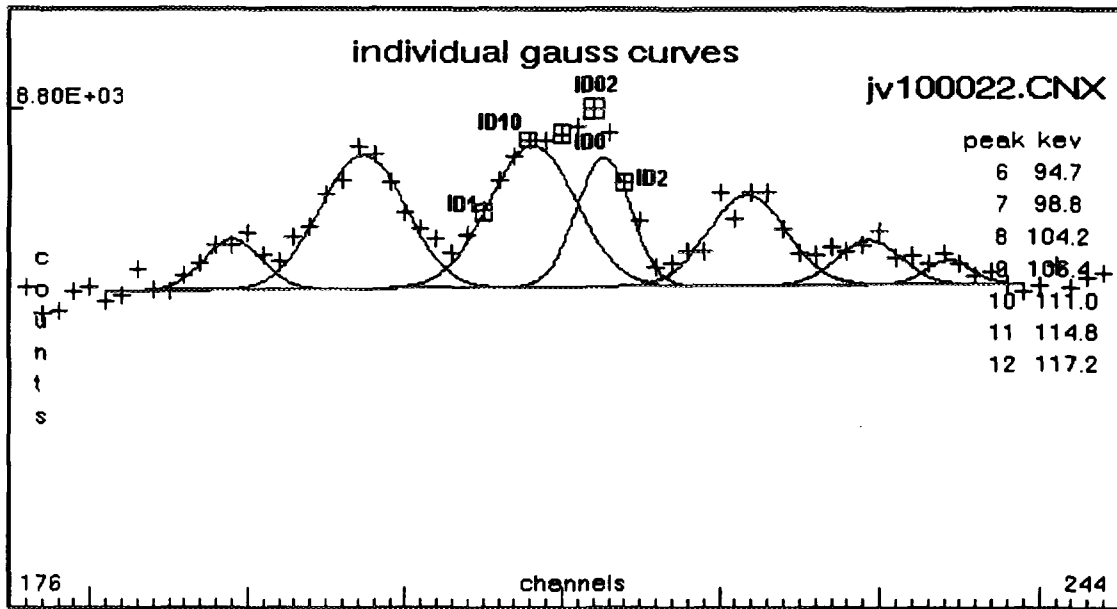


Fig. 5.4.a Peaks number 8 and 9 have been defined with the second derivative analysis between the inflexion points of a peak defined with the first derivative analysis

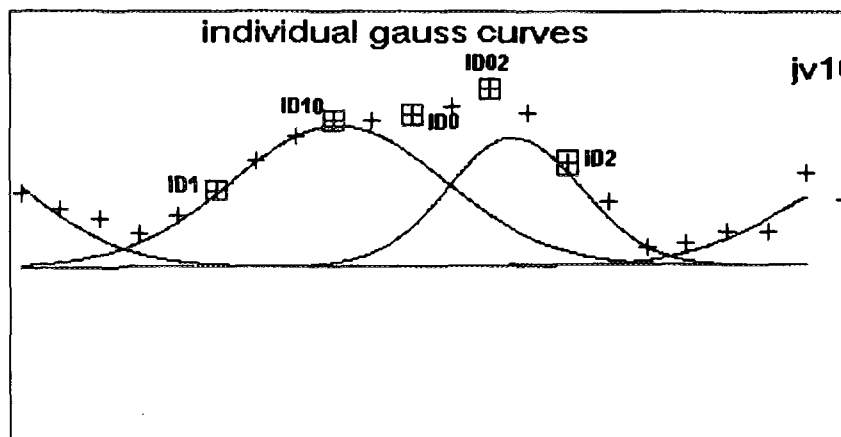


Fig.5.4.c Zoom from fig. 5.4.a

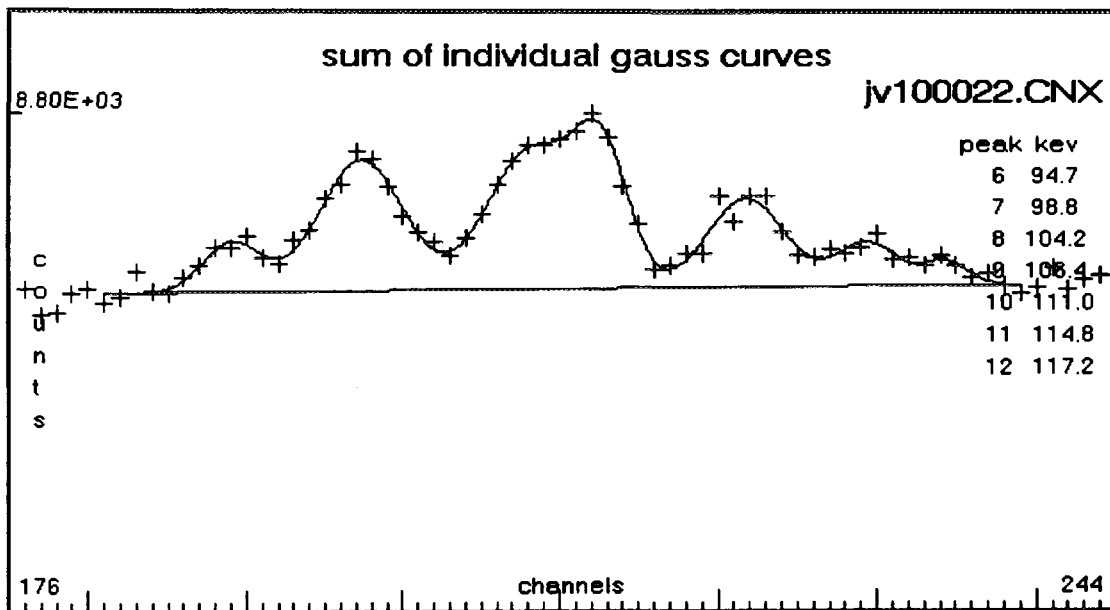


Fig. 5.4.b Sum of the individual Gauss curves of fig.5.4.a

At this stage the peak, already defined with the first derivative, is substituted by two peaks. These two peaks are centred at the channels ID10 and ID02, their heights are equal to the counting in the same channels, and each WHM is equal to half distance between the inflexion points of the original peak.

These will be the initial parameters of the new peaks for the best-fit.

With the above-described procedure, with the second derivative analysis, we may add up to three peaks to a peak defined only with the first derivative analysis: one on the left side, one on the right side (leaving the parameters of the original peak unchanged), and one between the inflexion points (in this case the parameters of the original peak are redefined).

Below we shall call quasi-peaks the peaks defined with the second derivative analysis.

The addition of the quasi-peaks generally makes the convergence for the algorithm of best-fit (least squares by iteration /4/) more problematic.

It is obvious that for a group of peaks (close peaks submitted to best-fit at the same time) as those of fig. 5.3.a or those of fig. 5.4.a, the non-convergence and consequently, the evaluation of the peak surfaces by histogram, would mean a complete loss of information.

In fact there is not a satisfactory method to distinguish between the surfaces of two or more peaks in close interaction by histogram.

The search for more information implies the risk of loss of all available information.

For this reason, the peak searching algorithm keeps separate, by means of an index, the peaks defined with the first derivative analysis from those defined with the second derivative analysis (quasi-peaks), and **takes a step backwards** every time the algorithm of best-fit does not converge.

The logic applied is the following:

- 1) If in the group of peaks submitted to best-fit there is only one quasi-peak and the

convergence is not reached, this peak is suppressed and the best-fit is tried again. In case the peak were defined between the inflexion points of a peak defined with the first derivative, this one takes the original parameters again. (Later the algorithm of the correction of the interactions among lines of the gamma library, will attempt to separate the different contributions to a peak attributed to more than one line).

2) If in the group of peaks submitted to best-fit there are more than one quasi-peak and the convergence is not reached, these quasi-peaks are suppressed, one at a time; the peak that degenerates first, during the best-fit process, is suppressed.

(In case the peak that degenerates is one defined with the first derivative, anyway a quasi-peak is suppressed).

The best-fit is tried again after every suppression; the procedure is stopped as soon as the convergence is reached or if all quasi-peaks have been suppressed.

When only peaks defined with the first derivative are left, the non-convergence is very unlikely.

The groups of peaks shown in fig. 5.2.a, fig. 5.3.a and fig. 5.4.a, all converge without suppression; fig. 5.2.b, fig. 5.3.b and fig. 5.4.b show the sum curves of the best-fit gauss curves.

In all cases the sum curve is very close to the experimental counts.

6. Best-Fit Algorithm

We consider an isolated peak above the Compton background (fig.6.1).

The experimental measurements give us a number of recorded counts for each channel:

$YE(I)$ = experimental content of the channel I.

We assume number I itself as abscissa $X(I)$ of channel I.

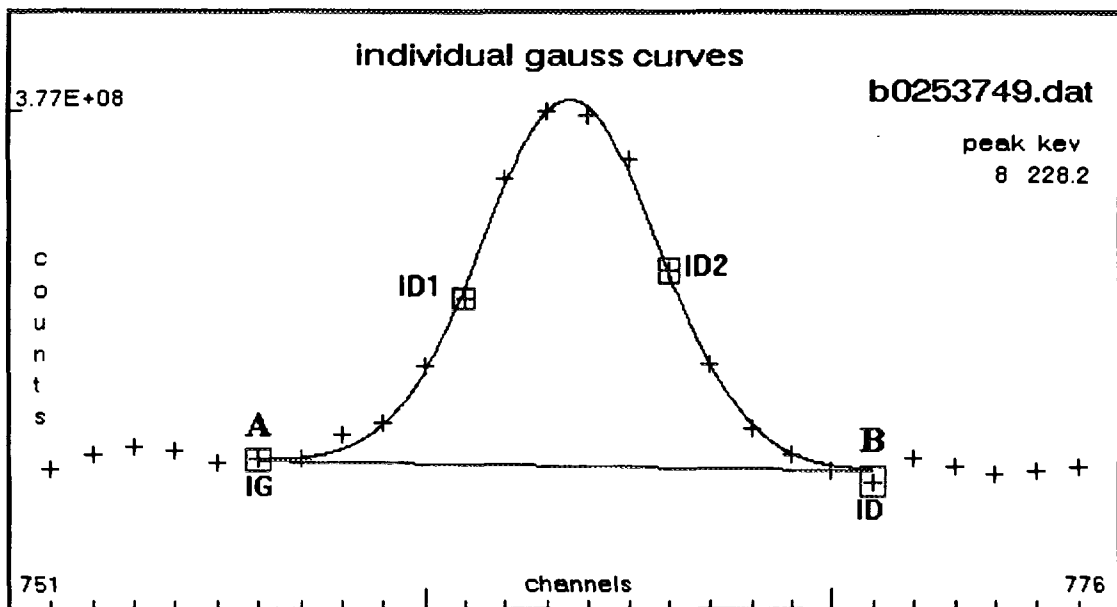


Fig. 6.1 Isolated peak of the spectrum "b0253749.dat" with 8192 channels

The peak search algorithm has individuated for the peak (fig.6.1):

- 1) IG = number of the left boundary channel;
- 2) ID = " of the right boundary channel;
- 3) ID1 = " of the first inflexion point channel;
- 4) ID2 = " of the second inflexion point channel.

The background beneath the peak is determined by the AB line (fig.6.1), of equation:

$$(6.1) \quad y = m \cdot x + q$$

$$\text{with: } m = \frac{YE(ID) - YE(IG)}{X(ID) - X(IG)} \quad q = YE(IG) - m \cdot X(IG)$$

We have to best-fit a Gauss curve on the experimental counts above the AB line.
The most usual parametrisation of a Gauss curve is:

$$(6.2) \quad f(x) = y \cdot e^{-\left[\frac{c1 \cdot (x-z)}{w}\right]^2}$$

with: $c1 = 2 \cdot \sqrt{\log(2)}$
 x = current abscissa
 z = abscissa of the middle
 $y = f(z)$ = ordinate in the middle
 w = width at half-maximum

In order to evaluate correctly the error on the Gauss surface, due to the best-fit algorithm, it is convenient to express the Gauss equation as a function of the surface A, rather than its height in the middle y .

Since:

$$(6.3) \quad A = y \cdot w \cdot c2$$

$$\text{with: } c2 = \sqrt{\frac{\pi}{4 \cdot \log(2)}}$$

the Gauss equation becomes:

$$(6.4) \quad f(x) = \frac{A}{w \cdot c2} \cdot e^{-\left[\frac{c1 \cdot (x-z)}{w}\right]^2}$$

The three parameters A, z, w determine the Gauss curve.

The ordinates calculated on the Gauss curve, channel by channel, $YC(I)$, are function of the channel abscissa $X(I)$, of the three parameters A, z, w, and of the background:

$$(6.5) \quad YC[X(I), A, z, w, m, q] = \frac{A}{w \cdot c2} \cdot e^{-\left[\frac{c1 \cdot (X(I)-z)}{w}\right]^2} + m \cdot X(I) + q$$

The problem comes down to finding out the five parameters A, z, w, m, q that determine the Gauss curve closer, in the sense of the least squares, to the experimental curve; i.e. the parameters that minimise the sum:

$$(6.6) \quad S = \sum_I P(I) \cdot [YE(I) - YC(X(I), A, z, w, m, q)]^2 \quad IG \leq I \leq ID$$

P(I) are weight factors to be used because the experimental counts have different precisions (equal to the square root of the counts themselves); it is easily proved that the weight factors which reduce the precisions to the same scale are:

$$(6.7) \quad P(I) = \frac{1}{YE(I)}$$

The problem is solved with the system:

$$(6.8) \quad \begin{cases} \partial S / \partial A = 0 \\ \partial S / \partial z = 0 \\ \partial S / \partial w = 0 \\ \partial S / \partial m = 0 \\ \partial S / \partial p = 0 \end{cases}$$

If we leave the function YC in the form (6.5), the system (6.8) becomes non linear versus some of the unknown parameters.

It is possible to linearize the problem with the Gauss-Newton method.

We fix the starting values for the parameters A, z, w, m, q, and name them A0, z0, w0, m0, q0; these values are chosen as follows (fig.6.1):

$$(6.9) \quad \begin{aligned} z_0 &= \frac{[X(ID1) + X(ID2)]}{2} \\ w_0 &= X(ID2) - X(ID1) \\ m_0 &= \frac{YE(ID) - YE(IG)}{X(ID) - X(IG)} \\ q_0 &= YE(IG) - m_0 \cdot X(IG) \\ A_0 &= [YE(Z_0) - m_0 \cdot z_0 - q_0] \cdot w_0 \cdot c^2 \end{aligned}$$

We put:

$$(6.10) \quad \begin{aligned} A &= A_0 + \delta A \\ z &= z_0 + \delta z \\ w &= w_0 + \delta w \\ m &= m_0 + \delta m \\ q &= q_0 + \delta q \end{aligned}$$

We replace the function (6.5) with its development in Taylor series, in the neighbourhood of

the point $P0(X(I), A0, z0, w0, m0, q0)$, up to the first derivative terms:

$$(6.11) \quad \begin{aligned} YC[X(I), A, z, w, m, q] \cong YC(P0) + \\ + (\partial YC / \partial A)_{P0} \cdot \delta A + (\partial YC / \partial z)_{P0} \cdot \delta z + (\partial YC / \partial w)_{P0} \cdot \delta w + \\ + (\partial YC / \partial m)_{P0} \cdot \delta m + (\partial YC / \partial q)_{P0} \cdot \delta q \end{aligned}$$

Therefore, instead of the (6.6) we have:

$$(6.12) \quad \begin{aligned} S' = \Sigma, P(I) \cdot [YE(I) - YC(P0) + \\ - (\partial YC / \partial A)_{P0} \cdot \delta A - (\partial YC / \partial z)_{P0} \cdot \delta z - (\partial YC / \partial w)_{P0} \cdot \delta w + \\ - (\partial YC / \partial m)_{P0} \cdot \delta m - (\partial YC / \partial q)_{P0} \cdot \delta q]^2 \end{aligned}$$

$$IG \leq I \leq ID$$

In this equation the unknown quantities are the increments of the parameters: δA , δz , δw , δm , δq .

The system that we obtain by setting the stationary conditions (6.13) is linear versus the unknown quantities themselves.

$$(6.13) \quad \begin{cases} \partial S' / \partial \delta A = 0 \\ \partial S' / \partial \delta z = 0 \\ \partial S' / \partial \delta w = 0 \\ \partial S' / \partial \delta m = 0 \\ \partial S' / \partial \delta q = 0 \end{cases}$$

By solving the system (6.13) we obtain the values: δA , δz , δw , δm , δq , with which we correct the starting parameters in the following way:

$$(6.14) \quad \begin{aligned} A0 &= A0 + \delta A \\ z0 &= z0 + \delta z \\ w0 &= w0 + \delta w \\ m0 &= m0 + \delta m \\ q0 &= q0 + \delta q \end{aligned}$$

We can repeat the procedure taking the new values $A0$, $z0$, $w0$, $m0$, $q0$, as starting parameters and we will obtain new corrections.

We can iterate until a given criterion of convergence is satisfied, or a reasonable number of iterations is reached.

The procedure is easily extended to whatever number of peaks in interference; the order of the system to be solved, at every iteration, is three times the number of peaks plus two for the background; the background line is defined by the left boundary of the first peak and the right one of the last peak.

As an alternative option we can keep the coefficients "m" and "q" of the background equal to their starting values, and best-fit only on the parameters of the Gauss curves.

With this option the order of the system is just three times the number of peaks and the best-fit algorithm is numerically more stable.

The option can be chosen by an index in the input file of general data.

6.1 Error Due to the Best-Fit Algorithm

The variance (square of the standard error) on the estimated parameters is calculated in the following way (/4/), (with reference to a single peak and with the equations in the same order as in the system (6.13)):

$$(6.15) \quad \begin{aligned} \text{Var}(A) &= \frac{S^2}{N-K} \cdot A^{-1}(1,1) \\ \text{Var}(z) &= \frac{S^2}{N-K} \cdot A^{-1}(2,2) \\ \text{Var}(w) &= \frac{S^2}{N-K} \cdot A^{-1}(3,3) \end{aligned}$$

where:

$$S^2 = \sum_I [YE(I) - YC(I)]^2 \quad IG \leq I \leq ID \quad \text{sum of the squares of the residues}$$

$$N = ID - IG + 1 \quad \text{number of channels belonging to the peak}$$

$$K \quad \text{number of parameters (order of the matrix)}$$

$A^{-1}(I,I)$ main diagonal terms of the inverse matrix of the coefficients matrix of the linear system solved in the last iteration.

Then the error due to the best-fit on the surface "A", ERBF, is:

$$(6.16) \quad ERBF = \frac{\sqrt{\text{Var}(A)}}{A} \quad \text{in "relative standard error" units.}$$

For peaks in close interaction this source of error becomes predominant compared with the statistical error, and in the calculation of the atoms number, compared with the error related to the efficiency curve and with the error on the branch factor of the gamma lines.

For peaks such as peaks number 65, 67, 68 of fig. 5.3.a, the amount of the relative standard error due to the best-fit exceeds 50%, for peak number 9 in fig. 5.4.a it is about 40%.

7. Student's Test

The Student's test value (STV) for a peak is defined as follows:

$$(7.1) \quad STV = \frac{YD(ID1) - YD(ID2)}{\sigma[YD(ID1) - YD(ID2)]}$$

with:

YD(ID1) = value of the first derivative in the 1° inflexion point

YD(ID2) = " " 2° " "

σ [YD(ID1)-YD(ID2)] = absolute standard error on YD(ID1)-YD(ID2)

This value increases with the size of the peak, compared with its background level, and with its sharpness.

Only the peaks with STV greater than a given threshold STT (Student's test threshold) are conserved and dealt with.

The absolute error σ depends on the counting of the channels on which every derivative is calculated.

Since every counting is affected by a standard error that, according to Poisson's law, is equal to the square root of the counting itself, applying the propagation error law, we can express σ as a function of the countings.

(The mathematical details are omitted).

8. Minimum Detectable

A peak detected is conserved only if its STV (Student's test value) is greater than a given threshold STT (Student's test threshold).

We can wonder which is the minimum surface of a peak, in a given spectrum, at a given energy, to be conserved and dealt with.

To answer we need to know the resolution of the detector at the given energy and the background level at that energy.

The resolution of a detector is the width at half-maximum (WHM) of the detected peaks, it is a physical datum of the detector and depends on the energy and on the experimental conditions.

The background level at the given energy can be evaluated by interpolation among the backgrounds of the detected peaks of the same spectrum or, in a range without peaks, considered equal to the counting level.

We name:

RE = resolution of the detector at the given energy (in channels)

BG = background level at the given energy (in counts)

STT = Student's test threshold (undimensioned number).

From the formula of Student's test value it is possible to deduce the height of the Gauss curve Y_0 corresponding to the threshold value:

$$Y_0 = f(\text{RE}, \text{BG}, \text{STT})$$

(The mathematical details are omitted).

The minimum detectable surface (MDS) at the given energy, with the given background level, will be that of a Gauss curve with maximum height Y_0 and RE as width at half-maximum.

$$(8.1) \quad MSD = Y_0 \cdot RE \cdot \sqrt{\frac{\pi}{4 \cdot \log(2)}}$$

From this MSD it is possible to go back to the number of atoms, at the reference instant, for a nuclide emitting at the same energy, with the same procedure adopted to exploit the spectrum peaks.

9. Channels - Energy Calibration Function

A gamma spectrum is the whole of the counts, recorded during the acquisition time and stocked in the channels of a multichannel analyser.

The number of the channel, where an impulse is recorded, is correlated with the range of the impulse itself, therefore with the quantity of ionisation induced by the gamma ray in the diode.

If the gamma ray has been completely absorbed (photo-electric effect) the quantity of ionisation is correlated with its energy.

The channels-energy calibration function is a function associating an energy value to each channel.

It is usually a second degree polynomial (parabola):

$$e = f(k) = a + b \cdot k + c \cdot k^2$$

with:

e = energy (kev)

k = channel number

a, b, c = coefficients

Otherwise it is a line: $e = f(k) = a + b \cdot k$

When the spectrum is interpreted, in particular to attribute the peaks of the spectrum to the lines of the gamma library, the calibration function is essential.

Because of the unavoidable derive of the electronic chain, the calibration function must be verified and adjusted for each spectrum.

We can do this ajustement in an automatic or in an interactive way.

9.1 Automatic Calibration

The automatic calibration can be done by means of:

- a) auto-calibration on calibration sources;
- b) auto-calibration on the identified lines.

The auto-calibration on calibration sources consists in putting, directly close to the diode, a gamma source at low energy (e1) (e.g.: Am²⁴¹ to exploit its emission at 59.54 kev) and one at high energy (e2) (e.g.: Zn⁶⁵ to exploit its emission at 1115.52 kev).

Starting from an initial calibration function, the peaks related to the calibration sources can be identified by the code on the basis of their energies (or positions) and their likely surfaces.

The research is done in spaces of spectrum wide enough, and the likely surfaces are given with an appropriate tolerance.

(The data related to the calibration sources are read in the input file of general data).

If the research is successful the code re-defines the calibration function as the line individuated by the two points (can1,e1), (can2,e2); where can1 and can2 are the numbers of the central channels of the two peaks.

The auto-calibration on the identified lines consists in comparing the energies of the peaks of the spectrum to the lines of the gamma library, first using an initial calibration function, and

then re-defining as a calibration function the least squares parabola fitted on the positions of the peaks considered as correctly attributed by the code.

The code considers a peak as correctly attributed if it has been attributed to a line belonging to a nuclide which has in the gamma library a number of lines greater than or equal to a minimum number NRMIN, and whose other lines are, at the same time, associated to peaks; otherwise the corresponding peak would have a surface less than the minimum detectable surface (MSD), plus the standard error on this surface ($\sigma(\text{MDS})$).

(NRMIN is also read in the input file of general data).

With the new calibration function the peaks will be definitively attributed to the lines of the gamma library.

9.2 Interactive Calibration

After preparing the list of the peaks and attributing them an energy by means of an initial calibration function, the code enables the user to associate certain peaks to lines of the gamma library in an interactive way.

Then the code re-defines as a calibration function the least squares parabola fitted on the positions of the associated peaks.

If the associated peaks are only two the function will be a line.

The energies of the peaks are re-calculated with the new calibration function before comparing them with the lines of the library.

Figures from 9.2.1 to 9.2.4 show the screens of the interactive program.

The interactive program can be called in execution during the execution of PRINS (by means of an index in the input file of general data) with a "call system", then the control returns to PRINS.

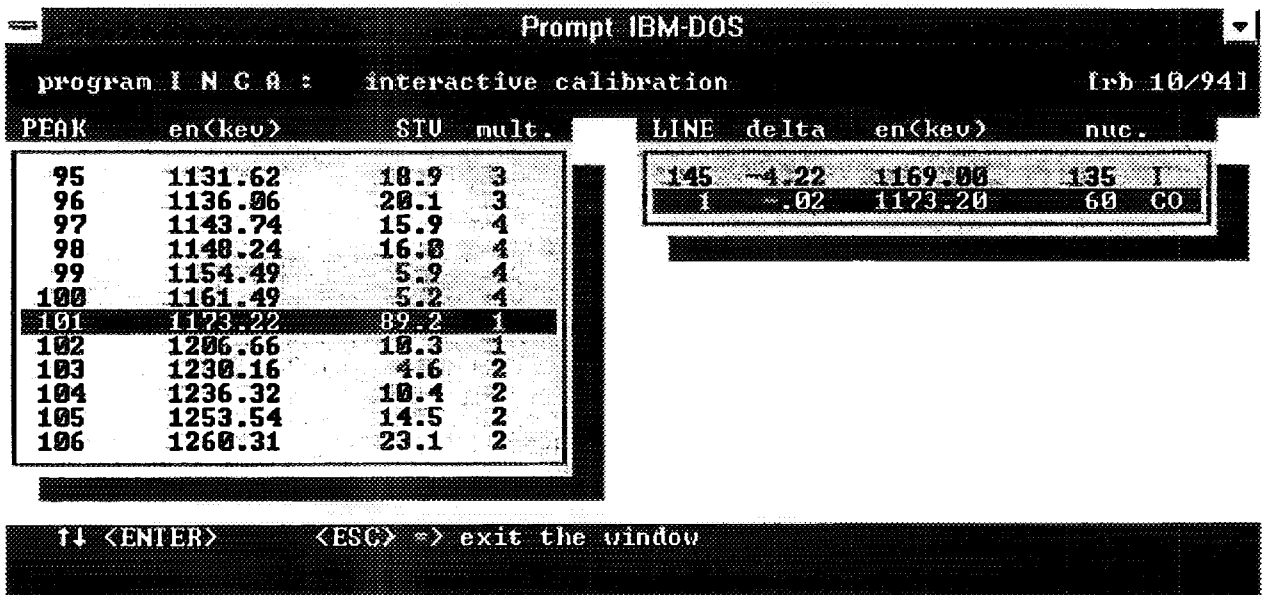


Fig. 9.2.1 The code suggests associating the closer line, the 1173.20 keV line of the 60 CO, to peak n. 101 of energy 1173.22 keV, chosen by the user in the left window. The user can choose this association or another from among those appearing in the right window.

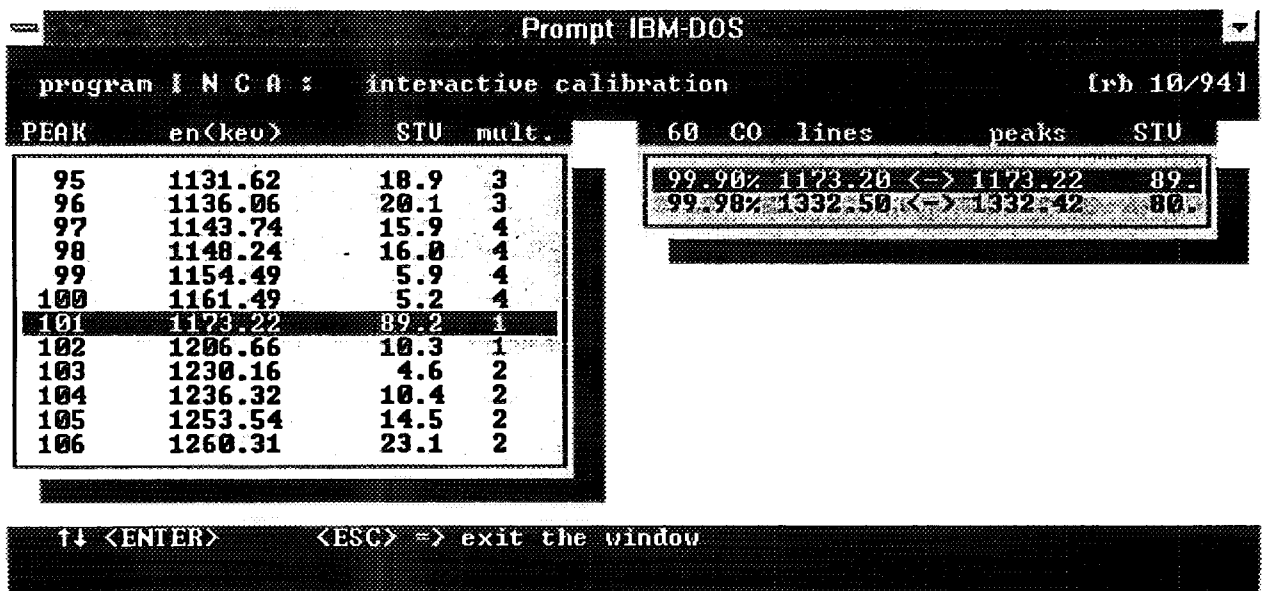


Fig.9.2.2 The right window shows the peaks closer to each line of the nuclide associated in the previous screen. This allows the user to verify the likelihood of his association.

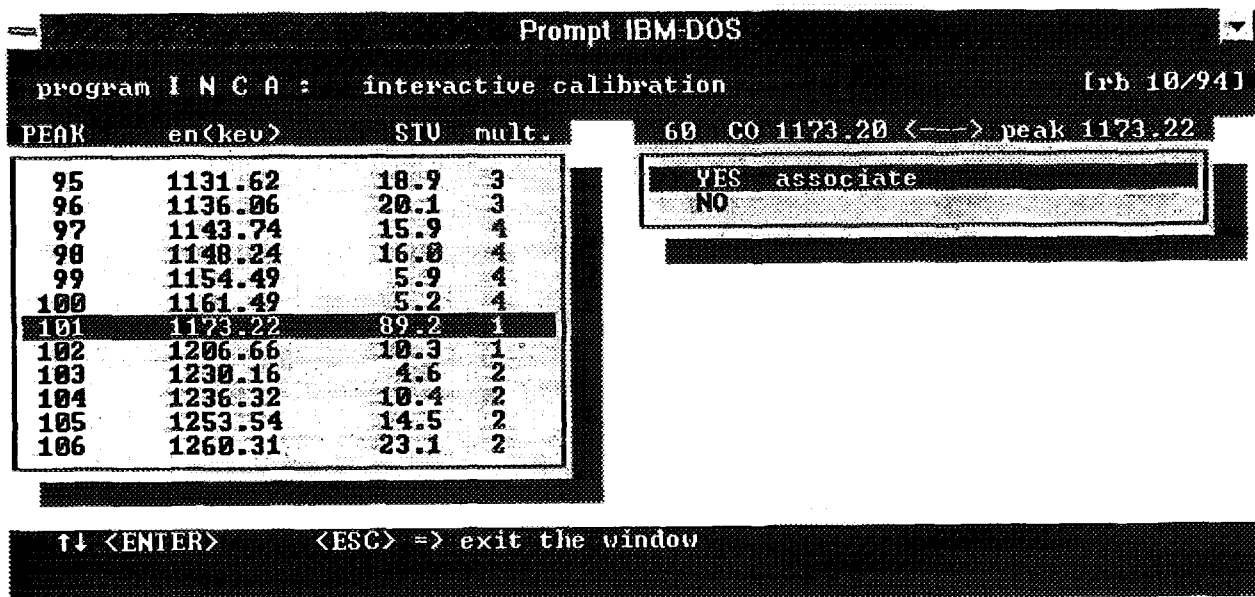


Fig.9.2.3 In this screen a confirmation for the association is asked.

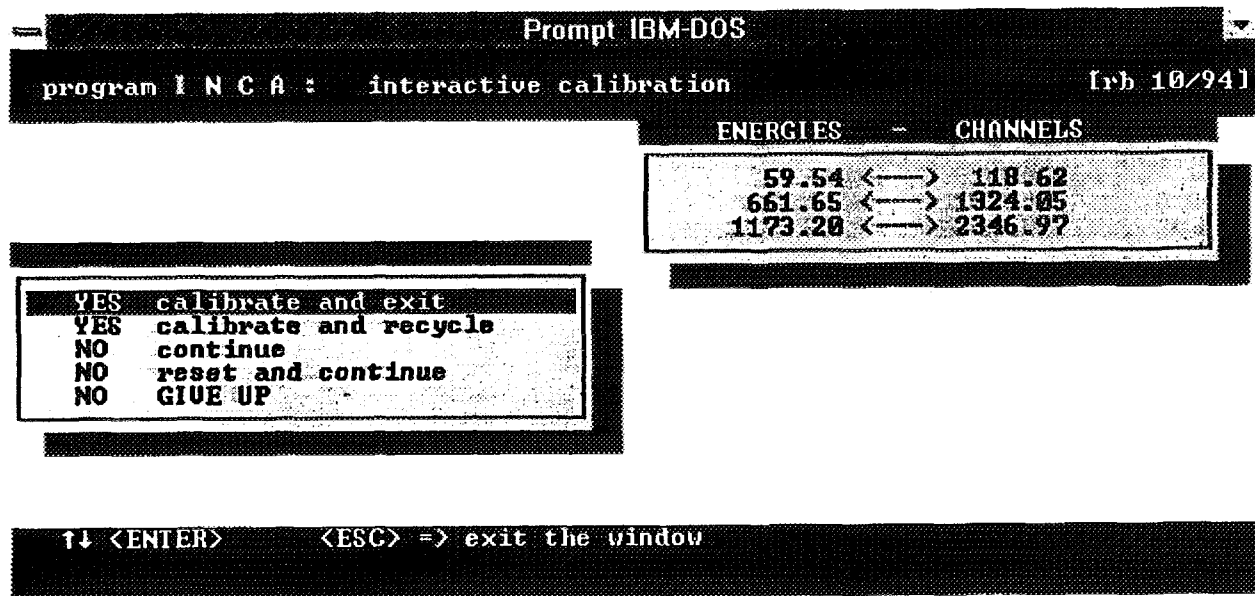


Fig. 9.2.4 After ending the associations (with the <ESC> key), the user can choose to:

- 1) calibrate, leave the calibration program, and return to PRINS;
- 2) calibrate and repeat the calibration starting from the new calibration;
- 3) add other associations;
- 4) reset and restart with the associations;
- 5) abandon the interactive calibration, and return to PRINS.

10. Programming / System Features

The PRINS code is equipped with four additional procedures.

- 1) SETLIB : outputs the gamma library in a format suitable for PRINS;
- 2) EFFCURVE : establishes the efficiency function;
- 3) INCA : allows the user to calibrate interactively;
- 4) PRINS_GR : graphics utility: enables the user to see how the peak searching algorithm and the best-fit algorithm have worked. (All the spectrum figures in this report have been drawn with this utility).

The PRINS code and all its additional procedures are written in standard FORTRAN 77.

PRINS and SETLIB can be compiled for and can be run on every operating system.

EFFCURVE, INCA and PRINS_GR, because of their graphic outputs, require to be compiled with Microsoft FORTRAN ver. 5.1 or with Microsoft FORTRAN Power Station ver. 1.0 (for DOS), and to be run on PC DOS.

In the present version of PRINS the dimensions of the matrixes are as follows:

- 1) matrixes related to the number of channels in the spectrum: 8192;
- 2) " lines in the gamma library: 600;
- 3) " detected peaks: 550.

With the previous dimensions and compiled with the Lahey F77-EM/32 FORTRAN compiler, ver. 5.01, for PC DOS (in real mode), the size of the executable module of PRINS is about 440 Kbytes.

The execution time on a PC DOS IBM 486 DX2 (66 MHz) is about 10 seconds for a spectrum with 8192 channels and about 120 - 150 peaks.

11. Acknowledgements

Special thanks to the colleague Mrs Liliana FERRI for her indispensable help.

12. References

/1/ François MICHEL - *Contribution à l'étude et à la réalisation d'une méthode d'examen par scrutation gamma en réacteur nucléaire de recherche de dispositifs d'irradiation* - Rapport CEA-R-4963

/2/ Roberto BORSARI - *Aggiornamento del codice di calcolo PRINS (PRogramma per l'INterpretazione automatica degli Spettri gamma)* - Rapporto ENEA CT-FCD-00001

/3/ Roberto BORSARI - *Codice di calcolo LINA: calcolo dell'errore associato al risultato, in numero di atomi, dei radionuclidi presenti nella sorgente* - Rapporto ENEA QT-WCH-00001

/4/ Anestis ANTONIADIS - *Least squares in linear and non linear models* - Lecture course in Institute Laue Langevin (Grenoble) 1987

/5/ Yardley BEERS - *Introduction to the theory of errors* - Addison Wesley

/6/ SNEDECOR and COCHRAN - *Statistical Methods* - Ames Iowa

/7/ Giuseppe CICCHITELLI - *Probabilità e statistica* - Maggioli 1984

/8/ W. T. EADIE, D. DRIJARD, F. E. JAMES, M. ROOS, B. SADOULET - *Statistical methods in experimental physics* - North Holland / American Elsevier (1971)

/9/ C. R. RAO - *Linear statistical inference and its applications* - J. Wiley & Sons (New York 1973)

/10/ B. EFRON - *Maximum likelihood and decision theory* - Annuals of Statistics (1982)

/11/ R. KINSEY - *ENDF 102, Data Formats and Procedures for the Evaluated Nuclear Data Files* - Brookhaven National Laboratory Upton, New York 1979

Edito dall'Enea
Funzione Centrale Relazioni Esterne
V. le Regina Margherita, 125 - 00198 Roma
Finito di stampare nel mese di dicembre 1995
presso il Tecnografico