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# THEORY OF AND COMPUTER AIDED NEUTRON ACTIVATION ANALYSIS

by

SEMİHA SAĞLAM

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## A B S T R A C T

Neutron activation analysis, NAA, has become a widely used and important analytical technique, not only in trace analysis but also in determining alloy elements and minor constituents. The micro qualitative and quantitative analysis can usually be performed by NAA in various fields, such as biology, criminology, geochemistry, cosmochemistry, industry etc. Thus, the field of application of the method is very wide.

In this study, first the basic concepts and principles of NAA is introduced. The detection methods and various types of detectors are discussed. The use of computers in NAA problems are also given. Then, a predeveloped computer code, Gretel, which is set up for routine batchwise processing of spectrometric data obtained by GE(Li) detectors is introduced. This code, programmed originally for the IBM 370/165 computer, is adopted to the UNIVAC 1106 computer in BU for further studies. The UNIVAC version of the program, the input and the output data are finally recorded onto a magnetic tape.

Also, another computer code prepared for NAA, Corgam, which was studied previously is introduced briefly. The comparison of these two codes are given at the end of this study.

## Ö Z E T

Günümüzde Nötron Aktivasyon Analizi, NAA, yöntemi ile çeşitli malzemelerde, bu malzemeleri teşkil eden elementlerin cins ve miktarlarının tayini büyük önem kazanmıştır. Diğer analitik yöntemlere kıyasla daha hassas sonuçlar veren bu yöntem, bugün bioloji, kriminoloji, jeokimya ve kosmokimya gibi birçok alanlarda kullanılmaktadır.

Bu çalışmada, NAA'nın temel kavram ve prensipleri, analizde kullanılan spektrometre sistemleri incelenmiş ve değişik detektör tipleri tanıtılmıştır. Nötron aktivasyon analizi sonuçlarının değerlendirilmesinde karşılaşılan güçlüklerden biri, uzun zaman alan hesaplamalardır. Bilgisayarların hızlı hesaplama yetenekleriyle bunların giderilmesinden ayrıca söz edilmiştir. Bu amaçla, daha önce hazırlanmış ve Ge(Li) tipi spektrumları inceleyen bir bilgisayar programı, Gretel, tanıtılmış ve programda gereklili takım düzeltmeler, çizim altprogramlarının program mantığını bozmadan çıkartılması gibi, yapılarak yalnız tasarlandığı üzere IBM 370/165 tipi bilgisayarlarla değil, UNIVAC-1106 tipi bilgisayarlarla da kullanılabilmesi sağlanmıştır. Program bu yeni şekliyle bir manyetik teybe kaydedilmiş ve gelecek kullanıcılar için saklanmıştır.

Ayrıca, NAA problemleri için hazırlanmış bir diğer bilgisayar programı olan Corgam kısaca tanıtılmış ve bu iki programın kıyaslaması da çalışmanın sonunda sunulmuştur.

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## I. INTRODUCTION

### 1.1. GENERAL

The nuclei of atoms are stable only when they contain a certain number of neutrons and protons. In other words, the number of excess neutrons in the nucleus of an atom determines whether that atom is radioactive or not. However, all elements found in nature with atomic number greater than 83 (bismuth) are radioactive. They belong to chains of successive decays, and all the species in one such chain constitute a radioactive family or series. Besides the naturally occurring radioactivity which was first discovered by H. Becquerel, [Fr-62, Ra-69], there are also some radioactive nuclei artificially produced.

The name of radioactivity implies that radiation is emitted. As will be seen in the next chapter, radiation may be in the form of  $\alpha$ ,  $\beta$  and  $\gamma$  rays. Since these radiations penetrate and cause ionisation and damage in the body, they may be used for various types of testing, such as tracer techniques. Activation analysis is the most sensitive tool for analysis of trace elements in many materials.

The activation analysis may be defined as a method of measuring concentrations of constituents in a given sample by measuring the characteristic radiations emitted by the radioactive nuclei resulting from nuclear transmutations. First, originally Hevesy and Levi used thermal neutron activation to determine the concentration of dysprosium in impure

yttrium, in 1936 [He-36]. Then, increasing application of radionuclides to analytical problems led to a rapid growth of activation analysis. The activation product provides a specific method for its identification and measurement. For example, for a given problem, a specific method can be selected based on the properties of the sensitivity required in the analysis, the presence of interfering reactions, the location of a suitable irradiation facility and cost.

The activation method is now used frequently in combination with gamma-ray spectrometry in order to simplify or even to eliminate chemical separations. The digital computers are also used for the analysis of gamma-ray spectra and many computer programs are prepared not only to resolve the gamma-ray spectra, but also to calculate the weight of the activated elements from their induced radioactivities. These programs are prepared especially for three types of systems [Li-65, Be-73]. These systems may be:

1. A large centralised computer facility which can analyse batchwise punched tape on which gamma spectrometric data have been collected.
2. A time-shared teleprocessing system linking various spectrometric installations to a centralised computer.
3. A minicomputer used at the laboratory site for both data acquisition and analysis.

The programs prepared for these systems, deal with especially NaI(Tl) type or Ge(Li) type spectra.

Through its nuclear character, the neutron activation technique is a powerful analytical tool not only in trace

analysis but also in determining alloy elements and minor constituents. Therefore, the field of application of the method is very wide. It can be used to determine traces in ultrapure elements, in biological materials and minerals, in industrial product identification by trace characterization, in geochemistry and cosmochemistry, etc [Ko-69, Ch-60, Fa-73].

In this thesis, all these subjects mentioned above will be discussed briefly in the separate subchapters. In addition, a computer code for Ge(Li) type spectra, Gretel, will be examined in a detailed form and compared with another one prepared for NaI(Tl) type spectra.

## 1.2. OUTLINE OF THE THESIS

The main purpose of the thesis is to investigate the theory and application of the neutron activation analysis, NAA, and make a detailed study of Gretel which is a computer code used to analyze the gamma spectra obtained by Ge(Li) detectors.

The thesis is composed of five chapters and a number of appendices. These can be summarized as follows:

The first chapter is the general introduction of the thesis, covering its purpose and results, and the method of neutron activation analysis.

The second chapter is mainly based on the theory of NAA; the basic principles of activation analysis and gamma-ray spectrometry are examined in detail. First, in the subchapter 2.1 natural radioactivity, radioactive decay and radioactive equilibrium are discussed briefly. In the subchapter 2.2 interaction of neutrons is studied. In the 2.3 interaction of gamma rays with matter and the main effects of this interaction, such as photoelectric effect, Compton scattering and pair-production, are introduced briefly. Then, the detection of gamma rays by means of different types of counters, especially scintillation and semiconductor counters are explained in detail.

The subchapters 2.5 and 2.6 introduce the gamma-ray spectrometry and the basic principles of NAA. Since the use of computers in NAA is an important tool, the last subchapter examines this subject in a summary form.

In chapter 3, Gretel is introduced and investigated in detail; theory of the code, analysis of gamma spectra obtained by Ge(Li) detectors with computer, the smoothing procedure to minimize the influence of the statistical counting fluctuations and the principles for searching of the peaks and the computation of the peak areas found by two different methods are discussed in the following subchapters. In the last subchapter 3.3, the modification of the code which was recorded originally by the use of IBM 370/165 to UNIVAC-1106 is given in detail.

In the following chapter 4, introduction of another code, CORGAM, that has been studied in a previous thesis is given and comparison of these two codes in a tabular form is made. Then, in the chapter 5, discussion and conclusion of the thesis and some suggestions for the use of Gretel are given in a short form.

Finally, some mathematical methods used in Gretel and the listing of Univac version of the code, the listing of input and output data are given as appendices A to K.

### 1.3. NEUTRON ACTIVATION ANALYSIS

Activation analysis is based on the principle that when a material is irradiated by the nuclear particles produced in a nuclear reactor, particle accelerator or other suitable source, some of the atoms present in the material will interact with the bombarding particles and be converted into different isotopes of the same element or isotopes of different elements, depending on the nature of the bombarding particles. In many cases, the isotopes produced are radioactive. The subsequent emission of beta or gamma radiations from these nuclei is characteristic of the particular isotope. If each different induced radioactivity can be distinguished or separated from all other radioactivities produced, then the amount of each radioactivity is a measure of the quantity of the parent isotope present in the material [Wa-63].

The sensitivity of the neutron activation analysis method can be considered to be about parts per billion, ppb, for reactor irradiations and parts per million, ppm, level for irradiations with neutron generators. In fact, the sensitivity and the accuracy of the analysis are frequently based on the ability to distinguish the radiation of the radioisotopes of interest from the other activated constituents of a sample. Besides NAA, analysis with photons and charged particles can be considered [Ho-71].

Besides the high sensitivity of thermal activation analysis, this technique offers a number of other advantages such as the simplicity of the nuclear reaction, transparency of most materials to thermal neutrons and non-destruction of the sample. In principle, in most cases only neutron capture reactions have to be considered and there is no change in the chemical nature of the irradiated samples.

Unfortunately, thermal neutron activation can not solve a number of important trace analysis problems, for instance those of the light elements, such as carbon, nitrogen and oxygen. These problems can sometimes be solved by applying photons or charged particles such as protons, deuterons, etc. If neutrons and protons essentially analyze the whole mass of the sample, this is not true for charged particle analysis, as these have a very short range. While all analytical techniques require some chemical treatment before the analysis; the NAA may require the chemical treatment only after irradiation and often after removal of surface contamination. One further advantage of neutron activation analysis, NAA, is in many cases, the selectivity or even specificity of its nature. First, the activation is a reaction of the nucleus and thus independent of the chemical state of the considered element. Further, the relatively simple nature of the nuclear reaction allows one to establish with great certainty the isotope or isotopes which gave rise to the measured species. Besides chemical criteria, nuclear ones can increase the certainty of identification of elements, as, for instance, half-life measurements, type of Disintegration and energy measurements of the emitted radiation.

Gamma-ray spectrometry appears to be a powerful tool in this respect. By applying gamma scintillation spectrometry to activation analysis, it becomes possible to analyze simultaneously a number of different elements. With the use of germanium lithium drifted detectors, gamma spectrometry has developed in a spectacular way. These detectors have a very high resolving power [So-72, Ho-71].

The procedure is often summarized as follows: Irradiate a sample and a standard under the same conditions; count

both under the same conditions; the ratio of these rates will be equal to the ratio of the masses of the elements of interest. If one takes activation in a thermal reactor as an example, it should be remembered that among many other parameters the neutron energy varies from a thermal energy of 0.025 eV up to about 20 MeV. Consequently activation not only occurs with thermal neutrons, but also with epithermal and fast neutrons. Besides, the activation can vary from place to place in the reactor. The flux gradient may not be the same in standard or sample or even over the entire sample itself. Many other complexities may be met during activation, such as unsuspected reactions, production of the isotope of interest by second order reactions or radioactive growth of a daughter isotope, absorption of radiations, instability of the instrumentation, non-linearity in detector response, etc.

From this short list of possible sources of error it is concluded that activation analysis is a complex analytical technique and that experience is required to obtain satisfactory results. But all these complexities have not prevented it from developing rapidly. At the beginning, it was mainly used in the field of trace determination in high purity materials; applications are now increasingly used in different fields such as biological sciences, geochemistry, criminology, environmental sciences, etc. Since 1969, cosmochemistry is also added to these fields. For instance, the analysis of Apollo Lunar material is widely performed by activation analysis [Ho-71]. More and widespread applications are to be expected in the future.

## 2. THEORY

### 2.1. RADIOACTIVITY

Some nuclei undergo spontaneous decay or disintegration. This process is known as radioactivity. The discovery of radioactivity goes back two historical events: 1) The discovery of x rays by W.C.Roentgen in 1895, 2) In 1896, H.Becquerel reported his experimental results; after exposure to bright sunlight crystals of the uranyl double sulfate emitted a radiation which blackened a photographic plate after penetrating black paper, glass and other substances. Then, Pierre and Marie Curie concluded that the uranium rays were an atomic phenomenon characteristic of the element and not related to its chemical or physical state. They, then introduced the name "radioactivity" for the phenomenon [Fr-62, Ha-65].

There are three kinds of radiations emitted by the radioactive substances. These rays can be distinguished from each other in two ways: First, by the difference in the ease with which the rays can pass through matter. Second, by the direction in which their path is bent by the application of a magnetic field. The most easily absorbed rays are  $\alpha$  particles which are deflected by both electric and magnetic fields. This deflection shows that its charge is positive. It is also concluded that it is composed of a doubly ionized He atom,  $\text{He}^{++}$ . The second type of radiation requires roughly 1000 times as much matter to bring it to rest. These particles, named  $\beta$ , are reflected much more readily by magnetic fields than  $\alpha$ .

particles but in the opposite direction. They, therefore, carry a negative electrical charge. The properties of these particles are similar to those of fast moving electrons. The third type of radiation, called  $\gamma$  ray is even more penetrating than  $\beta^-$  particles. The gamma-rays can only be stopped by several centimeters of lead. These rays are not deflected by magnetic or electric fields. They are electromagnetic radiations of the same kind as X rays, light and radio waves, but of very short wavelength.

The emission of  $\alpha$  and  $\beta$  particles cause a change in atomic number or mass number of the nucleus. If a nucleus emits an  $\alpha$  particle, whose charge is 2 and whose mass is 4 on the atomic weight scale, then obviously the nucleus that remains after the event will carry two units less of positive charge and four units less of mass. Since a  $\beta^-$  particle is negatively charged, its emission will cause an increase of one unit in the nuclear positive charge. On the other hand, the emission of a  $\gamma$ -ray produces no change in atomic number of the nucleus; but only a decrease in its energy content. In most cases, the emission of gamma-rays is a secondary consequence of either an  $\alpha$  or a  $\beta$  decay. Following the initial decay, the residual nucleus is frequently left with excess energy which may emit one or more  $\gamma$ -rays.

Besides the naturally occurring radioactivity, some radioactive nuclei are artificially produced. First in 1934 I.Curie and F.Joliot discovered that boron, aluminum and magnesium could be made radioactive by bombardment with the  $\alpha$  rays [Fr-62]. At that time, many laboratories put into operation devices for the acceleration of hydrogen ions and helium ions to energies at which nuclear transmutations were produced. Then, many artificially produced radioelements have found important applications in some fields, such as che-

mistry, physics, biology, medicine and engineering.

### 2.1.1. Radioactive Decay

Radioactive decay is a statistical process. The probability of one nucleus in a group of nuclei decaying in a finite time interval is independent of the time. In other words, the probability of decay at two different times  $t_1$  and  $t_2$  will be the same.

The probability  $P$  of decay of one nucleus in a time interval  $\Delta t$  can be written as,

$$P = \lambda \Delta t \quad (2.1)$$

where  $\lambda$  is decay constant of the isotope. The number of nuclei decaying from a group of  $N$  nuclei will be,

$$-\Delta N = NP = N\lambda \Delta t \quad (2.2)$$

If the time interval is very small, e.g. (2.2) can be written as,

$$-dN/dt = \lambda N \quad (2.3)$$

integrating this equation and taking  $N_0$  as the number of nuclei present at time  $t=0$ , one obtains,

$$N = N_0 e^{-\lambda t} \quad (2.4)$$

This equation shows that the number of radioactive nuclei decreases exponentially with time.

According to eg. (2.3), the number of nuclei decaying per unit time is equal to  $(\lambda N)$ . This is called the activity of the sample [Ou-75, Ha-65]. Multiplying both sides of eg. (2.4) by  $\lambda$ ;

$$\lambda N = \lambda N_0 e^{-\lambda t}$$

or,

$$A = A_0 e^{-\lambda t} \quad (2.5)$$

where  $A$  is the activity at time  $t$  and  $A_0$  is the initial activity at time  $t = 0$ . Equation (2.5) shows that the activity also changes with time exponentially.

### 2.1.2. Radioactive Equilibrium

Among the radioactive nuclei there are many examples of chains of decays in which a radioactive parent decays to a daughter which is also radioactive, and so on. In such a case, it is especially important to know how much of that is produced.

In the case of a radioactive parent decaying to form a radioactive daughter, the daughter product is produced at the rate of the parent's decay. However, the daughter itself decays, and this decay is proportional to the amount of daughter that is present.

Considering  $N_1$ , the number of parent atoms and  $N_2$ , the number of daughter atoms as functions of decay constants and time, it is possible to write the decay rate of the parent, according to eg. (2.3), as,

$$dN_1/dt = -\lambda_1 N_1$$

or taking  $N_1 = N_{1,0} e^{-\lambda_1 t}$

$$dN_1/dt = -\lambda_1 N_{1,0} e^{-\lambda_1 t} \quad (2.6)$$

The analogous equation for the daughter is,

$$dN_2/dt = R_F - \lambda_2 N_2 = \lambda_1 N_{1,0} e^{-\lambda_1 t} - \lambda_2 N_2 \quad (2.7)$$

where  $R_F$  represents the rate of formation of the daughter and it is equal to  $(\lambda_1 N_{1,0} e^{-\lambda_1 t})$ ; the second term  $(-\lambda_2 N_2)$  represents the decay term.

Rearranging the equation (2.7) which is a 1<sup>st</sup> order linear differential equation, for the solution of which(\*), one obtains,

$$N_2 = \frac{\lambda_1}{\lambda_2 - \lambda_1} N_{1,0} (e^{-\lambda_1 t} - e^{-\lambda_2 t}) \quad (2.8)$$

Just what happens depends largely on the ratio of the half lives:

a) In the case of the parent having a much longer half-life than the daughter, ( $\lambda_2 \gg \lambda_1$ ),  $\lambda_1$  is very small and can be allowed to approach zero in eq. (2.8). The resulting equation which gives the amount of the product nuclide as a function of time, takes the form,

$$N_2 = \frac{\lambda_1}{\lambda_2 - \lambda_1} N_{1,0} (1 - e^{-\lambda_2 t}) \quad (2.9)$$

---

(\*) Solution of this equation is given in the appendix B in more detail.

or,

$$N_2 = K(1 - e^{-\lambda_2 t}) \quad (2.10)$$

The significance of  $K$  becomes apparent if  $t$  approaches to infinity. Then  $N_2 = K$  and  $K$  is the equilibrium value that  $N_2$  approaches as time goes on.

The form of the build-up or saturation factor  $(1 - e^{-\lambda t})$  is shown in the figure (2.1)

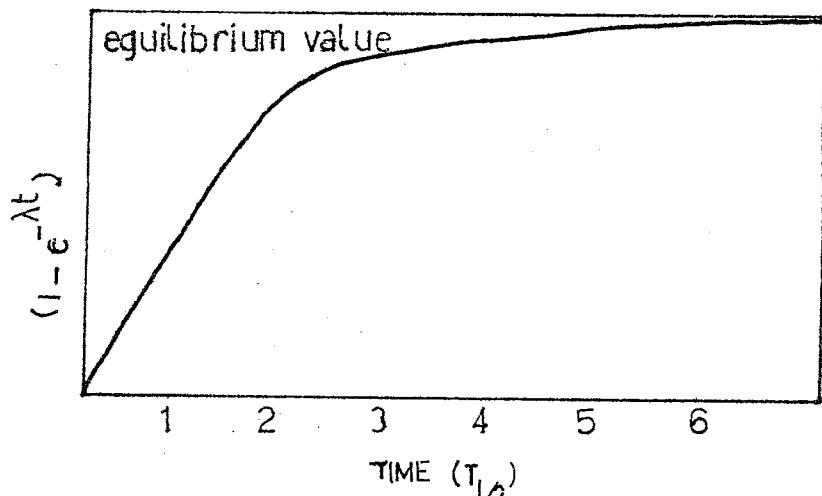


Fig. 2.1. Build up of a radioactive nuclide created at a constant rate [EL-59].

b) If  $\lambda_2 > \lambda_1$ , but not great enough for one to ignore the decay of the parent during the growth of the daughter, then the situation is called transient equilibrium. Fig.(2.2) shows the growth and decay of a parent and its daughter.

As shown in fig.(2.2), the amount of daughter at first increases, then reaches a maximum, and finally decreases at the same rate as the parent with which it is in transient equilibrium(\*) .

(\*) Detailed explanations for that subject can be supplied from many text books, such as [EL-59, Ha-69, Wi-66, Se-67, Ou-75].

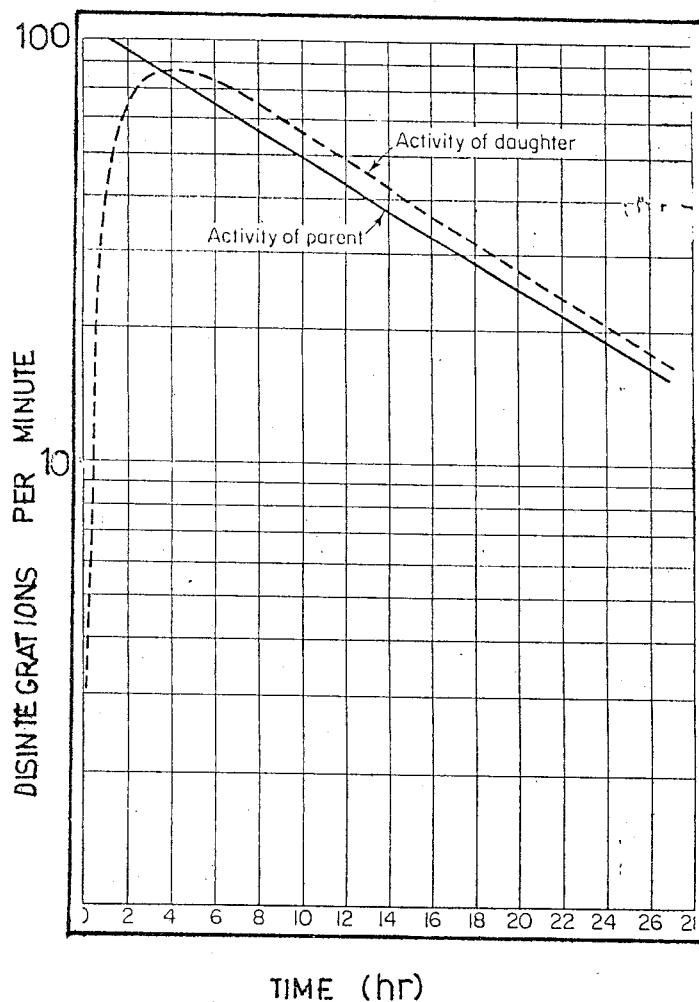


Fig. 2.2. Growth and decay of daughter in transient equilibrium with parent.

## 2.2. INTERACTION OF NEUTRONS WITH MATTER

Since neutrons are not charged and are much heavier than electrons, they do not interact significantly with electrons. They are also not repelled by electric fields; even very low energy (thermal) neutrons readily penetrate and react with nuclei. Therefore, neutrons are not easily detected by most counting instruments because they do not ionize. They must be detected by their secondary effects. In other words, for the detection of neutrons, a nuclear reaction must have reasonably high probability and must result in the production

of some other form of easily detectable radiation, such as charged particles or gamma-ray. Suitable reactions(\*) fall into four general categories as follows:

Activation reactions: These reactions result in the production of excited nuclei with reasonable long life times. Samples of suitable materials, usually thin foils, are exposed to neutron irradiation. They are then removed from the neutron flux and their radioactivity is measured usually by  $\beta$  or  $\gamma$  counting. The most important of those reactions is the  $(n,\gamma)$  reaction. This process is also known as radiative capture, since one of the products of the reaction is instantaneous gamma-rays.

Activation reactions are very useful for the detection of neutrons. That subject will be studied in detail in the later subsections.

Transmutation reactions: Neutrons may be captured by nuclei and cause the prompt emission of charged particles such as protons, deuterons or alpha particles. In that case, the incident neutron must supply sufficient energy to overcome the force binding the charged particle to the compound nucleus for the reaction to take place. Besides those, sometimes two or more neutrons are emitted when a nucleus is struck by a high energy neutron. These processes here are of the  $(n,2n)$  or  $(n,3n)$  types. A closely related process is the  $(n,pn)$  reaction which also occurs with highly energetic incident neutrons.

Fission: When a neutron collides with a heavy nucleus, the nucleus splits into two large fragments with the release of considerable energy. This process is known as fission. The fission process provides a technique for detecting neutrons

(\*)These explanations and more detailed form of them can be obtained from many text books, such as [Ch-61, La-72, Wa-62, Wi-66].

in the presence of very intense gamma radiation.

Scattering: When a moving particle collides with another particle, the kinetic energy is exchanged between them according to the laws of conservation of energy and momentum. There are two types of collisions: First, if the potential energy of the system remains unchanged, kinetic energy being conserved during the collision, the phenomenon is called elastic scattering. Second is the inelastic scattering in which one of the particles is left in an excited state after collision. Here momentum and total energy of the particles before and after collision are conserved. However, kinetic energy is not.

In each scattering event, part of the kinetic energy of the neutron is transferred to initially stationary and heavier nucleus; as a result of that they are slowed down. Then the slowed down neutrons become more effective in causing nuclear reactions.

The emission of gamma radiation, as a result of the reactions described above is due to the release of excess energy of the excited nucleus. The energy of that gamma-ray is equal to the difference between the energy levels of the excited and stable states of the nucleus. In some cases two or more gamma-rays of discrete energies are emitted in cascade. Those gammas are usually emitted within  $10^{-13}$  sec. Then  $\beta$  particle,  $\alpha$  particle and electron capture decays occur. Sometimes that excited state has a characteristic half-life of its own. Whenever that half-life is of the order of  $10^{-7}$  to  $10^{-6}$  sec, or longer; the excited state is called an isomer of the product. The subsequent decay of that isomer by the emission of a gamma ray is called an isomeric transition. A typical example is given for  $\text{Co}^{60}$  in the figure(2.3).

The  $^{60}\text{Ni}$  nucleus formed by the  $\beta^-$  decay of  $^{60}\text{Co}$  is rapidly converted by the emission of 2.50 MeV gamma-ray. This conversion takes place by the emission of a photon of 1.17 MeV and immediately thereafter a photon with 1.33 MeV.

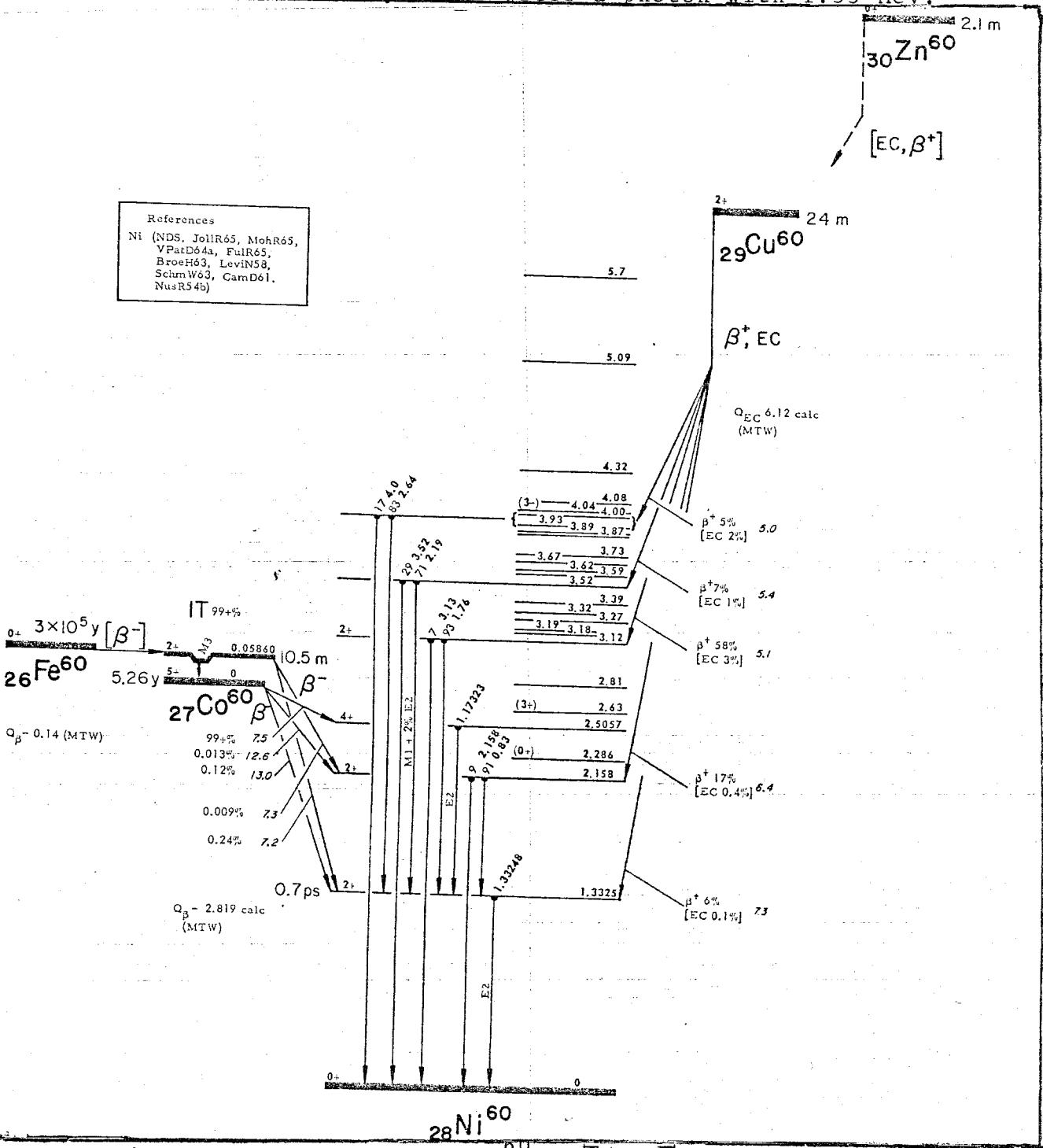


Fig. 2.3. Decay scheme of  $^{60}\text{Co}$  [Le-68].

A more complicated one is  $^{152}\text{Eu}$ . It has an average level spacing of about 5 keV above 100 keV. It decays to the spherical nucleus  $^{152}\text{Gd}$  and to the deformed nucleus  $^{152}\text{Sm}$ . Deformed and spherical states are expected close to the ground state. It is very difficult to determine the configurations of these levels in  $^{152}\text{Eu}$  [Eg-74]. The decay scheme of  $^{152}\text{Eu}$  can be seen in figure(2.4).

The detection of those gamma rays by suitable detectors and the analysis of that spectrum may be used to identify the radiating nuclide, its amount, etc. In the following subchapters, detection of gamma-rays, analysis of spectra obtained from unknown nuclei and, qualitative and quantitative analysis techniques will be examined in detail.

### 2.3. INTERACTION OF GAMMA RAYS WITH MATTER

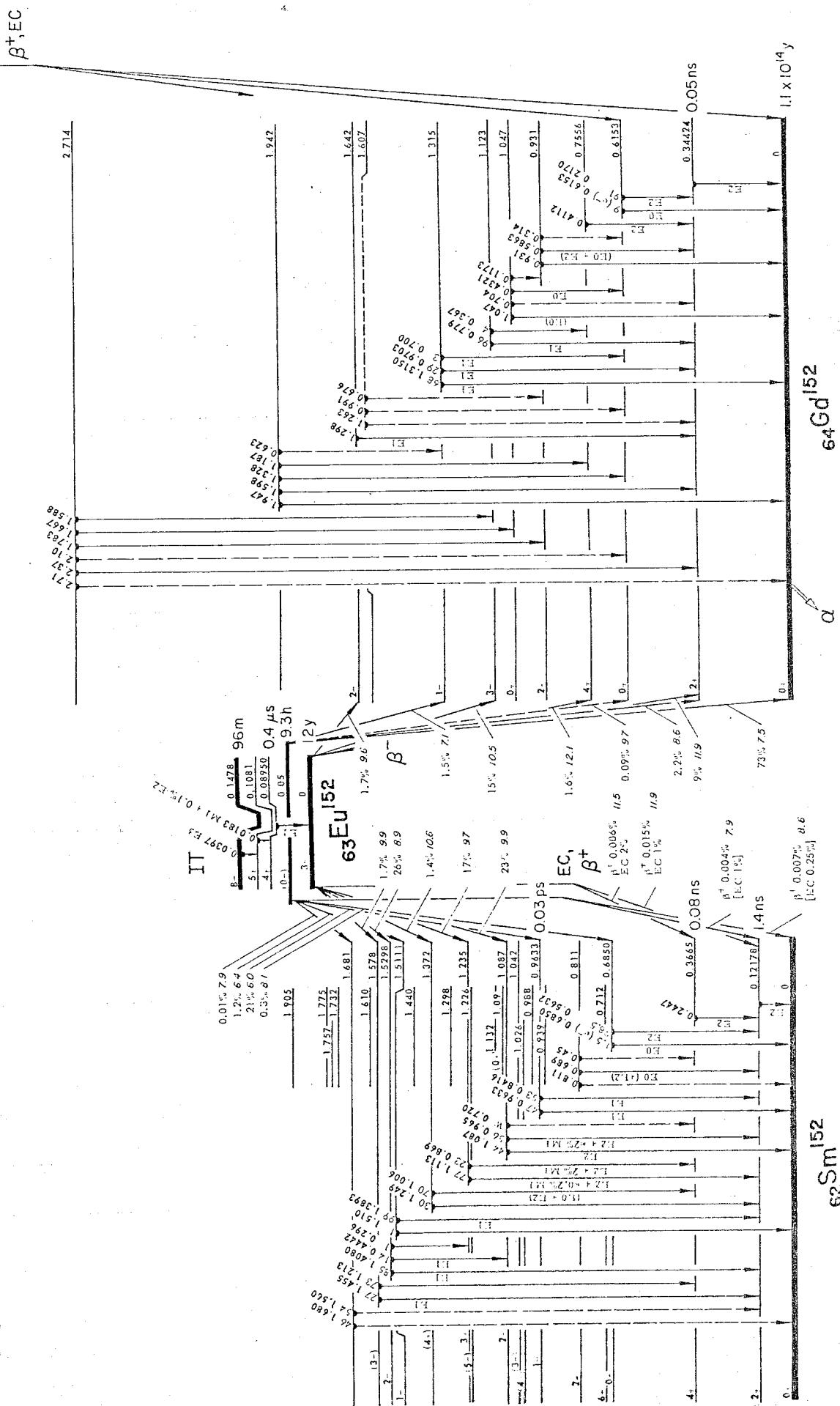
Electromagnetic radiation of high photon energy usually originates from excited atomic nuclei and is called  $\gamma$  ray or X ray. These rays are usually classified according to their mode of origin, not their energy.

There are a number of processes which can cause gamma-rays to be scattered or absorbed. A catalogue of the possible processes by which the electromagnetic field of the  $\gamma$ -ray may interact with matter has been put in the following systematic form by Fano [Fa-53];

Kinds of interaction:

- 1- Interaction with atomic electrons
- 2- Interaction with nucleons
- 3- Interaction with the electric field surrounding nuclei or electrons

Fig. 2.4 Velocity profile of  $[\text{Le}-68]$



4- Interaction with the meson field surrounding the nucleons.

Effects of interaction:

- a) Complete absorption
- b) Elastic scattering (coherent)
- c) Inelastic scattering (incoherent)

There are 12 ways of combining these interactions and effects, thus in theory there are 12 different processes by which gamma-rays can be absorbed or scattered. Many of these processes are infrequent. Three of them, photoelectric effect, compton scattering and pair production, are the most important effects. Figure(2.5) illustrates the relative importance of the three main interactions.

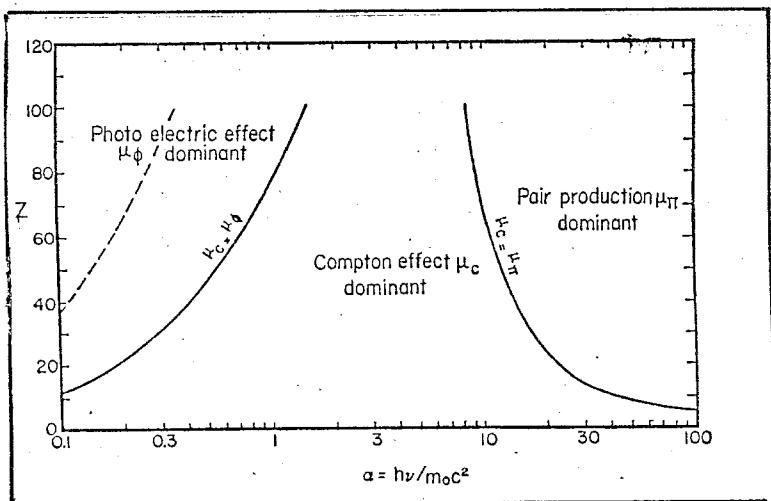


Fig. 2.5. Relative importance of the three main  $\gamma$ -ray interactions as a function of the absorber atomic number  $Z$  and the photon energy in the units of  $M_0C^2$  are given (the dotted curve indicates the Rayleigh scattering) [Aj-60].

These effects will be examined in the following sub-chapters.

The minor effects which are of interest in special cases are as follows [Ev-55];

Rayleigh Scattering (1b): Gamma rays scattered by small angles resulting in only a small recoil, especially when their energy is low. The recoil is then often absorbed by a whole atom or molecule. This scattering is more likely for high Z than for low Z materials.

Thomson Scattering (2b): Thomson scattering can combine coherently with Rayleigh scattering. Because of the large mass of the nucleus, the effects are small but appear to have been detected.

Delbruck Scattering (3b): Delbruck scattering is due to virtual electron pair formation in the field of the nucleus. The effect is extremely small.

Nuclear Resonance Scattering (2c): This type of scattering involves the excitation of a nuclear level by an incident photon, with subsequent reemission of the excitation energy.

Photodisintegration of nuclei (2a): It is possible whenever the photon energy exceeds the separation energy of a neutron or proton. Except for  $^9\text{Be}(\gamma, n)$  and  $^2\text{H}(\gamma, n)$ , these effects are generally confined to the high energy region above approximately 8 MeV.

Meson Production (4a): Meson production requires photon energies above 150 MeV.

### 2.3.1. Photoelectric Effect

Below energies of about 0.1 MeV the predominant mode of  $\gamma$ -ray interaction in all medium and high Z absorbers is the photoelectric process. In this process the photon energy is used to remove one of the electrons from an inner shell of an atom of the absorber element. Clearly this process can occur only if the incoming gamma-ray has an energy higher than the binding energy of the electron to be removed. Thus, the energy of incident photon can be determined from the kinetic energy T of the ejected electron and the binding energy E of the atomic level from which it was ejected by the use of the expression,

$$h\nu = T + E \quad (2.11)$$

where,  $h\nu$  represents the energy of incident photon,  $\nu$  being frequency and  $h$  being Planck's constant.

When the experimental mass attenuation coefficient  $\mu/\rho$  for the photoelectric effect is plotted as a function of  $\lambda$  of the incident photon, a series of jumps corresponding to the binding energy of the different orbits can be observed (e.g. Fig. 2.6).

These energies are given by Moseley's law, [Se-64],

$$E = Rhc \frac{(Z-\sigma)^2}{n^2} \quad (2.12)$$

where,

$$Rhc = 13.605 \text{ eV}$$

Z is the atomic number

$n$  is the quantum number of different electronic orbits (in the K series  $n = 1$ , in the L series  $n = 2$ , etc.).

$\sigma$  is the screening constant which has the approximate value 3 for the K shell, 5 for the L shell etc. Figure(2.6) shows these jumps for platinum.

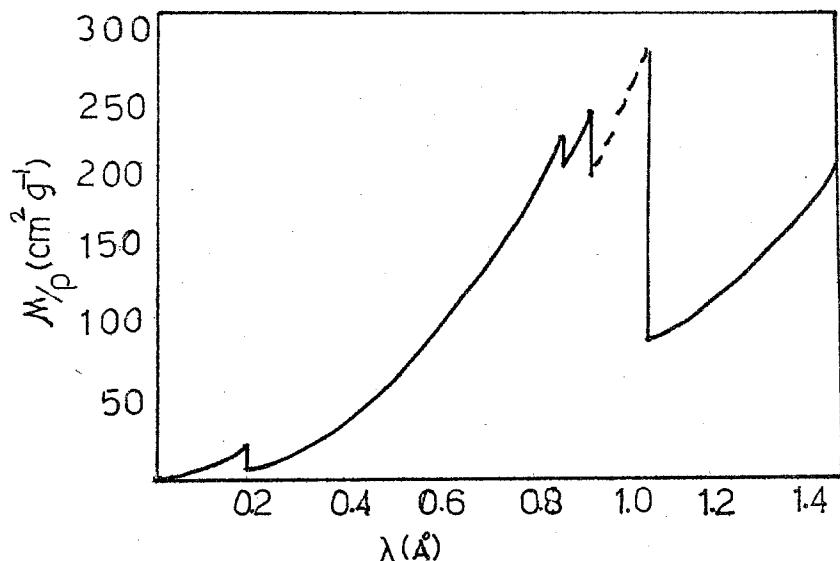


Fig. 2.6. Mass absorption coefficient of platinum as a function of the wavelength of the incident ray [Se-64].

The vacancy created by the ejection of an electron from the inner shell is filled by an outer electron falling into it, and this process may be accompanied by the emission of fluorescent radiation. Alternatively it is possible that no fluorescent radiation is emitted but that an electron from an outer shell is ejected. For instance, a vacancy in a K shell may be filled by an L electron and another L electron emitted with energy  $E_k - 2E_L$ . Similarly, if the K vacancy is filled by an L elektron and an M elektron is emitted, the ejected electron will have the kinetic energy  $E_k - E_L - E_m$ . These and similar processes are called AUGER processes.

### 2.3.2. Compton Scattering

Compton scattering is inelastic (incoherent) scattering of photons with the atomic electrons. In this type of effect, the photon energy is considered to be large enough compared to the atomic binding energy  $E$ , so that the atomic electrons may be considered as free electrons. The incident photon momentum  $h\nu_0/c$  is conserved between the scattered photon and the struck electron. Except for the trivial case of zero scattering angle, the direction of the scattered photon is not parallel to the direction of the incident photon. The scattered photon must therefore have a smaller momentum and a smaller quantum energy than the incident photon. The remaining momentum and energy are imparted to the struck electron.

Assuming that the struck electron is at rest and unbound, the schematic representation of the Compton scattering is given in figure (2.7). Where,  $h\nu$  represents the energy of the incident photon,  $h\nu'$  is the energy of the scattered photon,  $\theta$  is the angle through which the photon scatters,  $\psi$  is the angle at which the electron recoils.

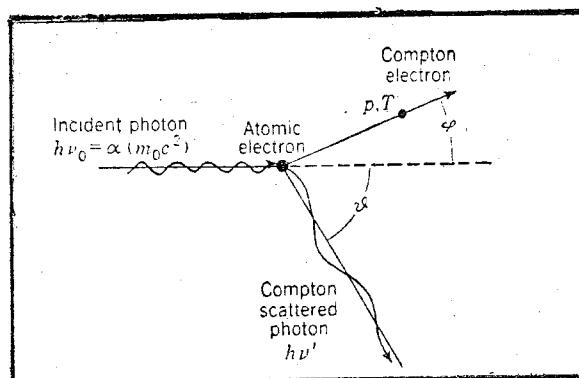


Fig. 2.7. The schematic representation of Compton scattering.

From the conservation of energy,

$$hv = hv' + T \quad (2.13)$$

where  $T$  represents the kinetic energy of scattered electron.

The energy of the scattered photon,  $hv'$ , in terms of  $hv$ ,  $\theta$  and  $\alpha$  which is a dimensionless parameter and equal to  $hv/M_0 C^2$ , by using the energy and momentum conservation of the system can be written as,  $[A_j - 60]$ .

$$hv' = \frac{hv}{1+\alpha(1-\cos\theta)} \quad (2.14)$$

It will be seen that  $hv' = hv$  for  $\theta = 0^\circ$  for any  $\alpha$  and that

$$hv' = \frac{1}{2} M_0 C^2 \quad \text{at} \quad \theta = 180^\circ \quad \text{with} \quad \alpha \gg 1 \quad (2.15)$$

$$hv' = M_0 C^2 \quad \text{at} \quad \theta = 90^\circ \quad \text{with} \quad \alpha \gg 1 \quad (2.16)$$

Then the kinetic energy of the recoil electron in terms of  $\phi$  and  $\theta$  is

$$T = hv - hv' = hv \frac{\alpha(1-\cos\theta)}{1+\alpha(1-\cos\theta)} \quad (2.17)$$

### 2.3.3. Pair Production

At photon energies above  $2 M_0 C^2 = 1.02$  MeV pair production is a possible effect. It is the transformation of a gamma ray into an electron-positron pair, also called materialization. When a recoil is absorbed by an electron, the threshold energy required by the conservation of energy and

momentum is  $4 MC^2$ , and there are two electrons and a positron acquiring appreciable momentum. In a cloud or bubble chamber they form a triplet; [Se-64]. Pairs can also be produced by heavy particle collision, by electron-electron collisions, in mesonic decay and by internal conversion in some gamma transitions.

The angular distribution of the electron-positron pairs is difficult to predict theoretically. If  $T_-$  and  $T_+$  are used to denote the kinetic energies of these pairs, they can be given as

$$T_+ + T_- = h\nu - 2 M_0 C^2 \quad (2.18)$$

where  $2 M_0 C^2$  is the threshold energy required to create these pairs. [Detailed information about these processes can be obtained in many books, such as Aj-60, Ev-55, Se-64]

#### 2.4. DETECTION OF GAMMA RAYS

Gamma rays are quantized electromagnetic waves emitted as a result of spontaneous changes between energy states of excited nuclei. Gamma rays are usually observed by detecting secondary charged particles, such as photoelectrons ejected from atoms, Compton electrons resulting from interactions with unbound electrons, positron-electron pairs created in the vicinity of a nucleus which lies in the path of the gamma-ray, or photons emitted when the gamma ray interacts with a nucleus.

In many cases one may say that a gamma-ray transition has been observed even though a gamma ray does not leave the nucleus. The most predominant process alternative to gamma -

ray emission is the internal conversion emission of a bound electron. For a gamma-ray transition involving an energy greater than 1.02 MeV a positron-electron pair may be emitted from the nucleus instead of a gamma ray or a conversion electron. This process, called internal pair creation, has the same relationship to external pair production as internal conversion has to photoelectron emission. In special cases when the emission of gamma rays is completely forbidden the transition may take place either by internal conversion, or if this energy is greater than 1.02 MeV, by pair production.

Finally, it may be said that the gamma-ray transitions may be detected by the observation of charged particles external to the atom following interaction with the  $\gamma$  rays. It may also be detected by measuring the internal conversion electron lines emitted from the atom itself. Most of the devices and techniques used for the measurement of gamma rays, actually analyze the secondary electrons. The only exception is the diffraction crystal spectrometer which analyzes the gamma rays directly by Bragg reflection. The ideal device for the detection and measurement of gamma rays would have high efficiency, good resolution and corresponding to each  $\gamma$  ray present, would yield a single peak or line. Since there are many interactions of gamma rays with matter, continuous distributions as well as discrete lines are frequently produced. There are only a few special types of spectrometers which will eliminate continuous distribution and yield only one line for each gamma ray present [A<sub>j</sub>-60]. They do so generally with a considerably smaller efficiency than for the ordinary electrons. The most common devices for  $\gamma$ -ray detection are the ionization chamber, proportional counter and Geiger-Müller counter. [Pr-64, En-66, Ou-75]. But the NaI (TL) scintillation counter is the most widely used device which will be examined in the following subchapter. In recent years, with

the development of semiconductor counters which have considerably good resolution, these counters have found wide use. So the second subchapter of this chapter deals with the semiconductor detectors in detail and Li drifted type is especially examined as the computer code studied in this thesis, Gretel, makes use of this type of semiconductor detector.

#### 2.4.1. Scintillation Detectors

One of the oldest methods of nuclear radiation detection is to make use of light scintillations. Although the basic principles remain the same, the techniques used have changed greatly. These techniques are particularly useful in the measurement of the energies of  $\beta$  and gamma rays. Besides these, the solid or liquid phosphors which are used with the scintillation detectors can absorb the  $\beta$  particles or the secondary electrons produced by gammas. Consequently, measurements of the energies of these particles are possible.

Figure( 2.8) is a schematic diagram of a scintillator and the electronic arrangement(\*) used in a counting system.

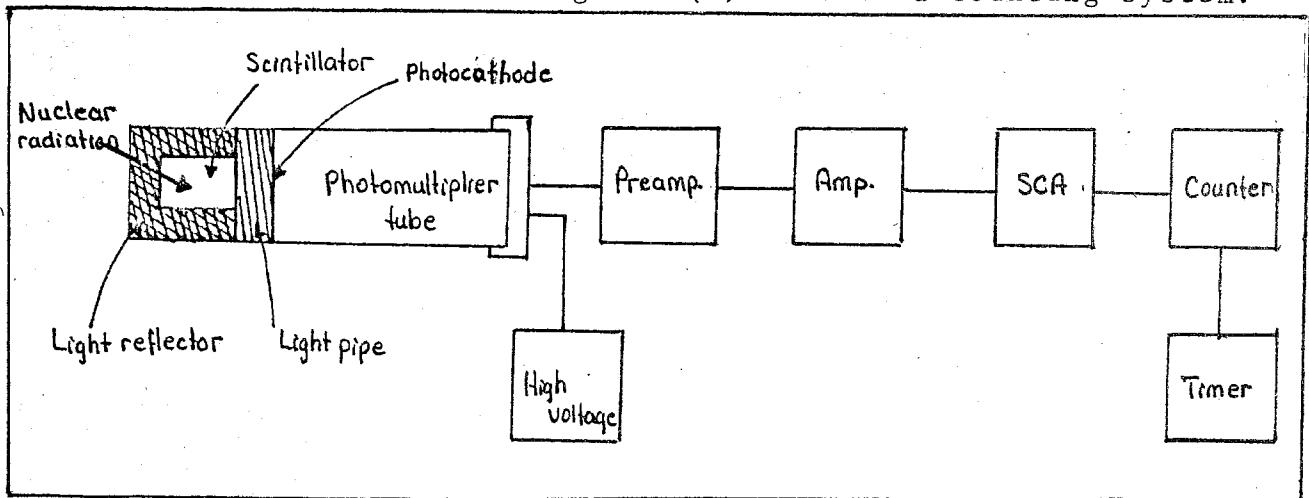


Fig. 2.8. Schematic diagram of a basic scintillation detection system [Bo-82].

(\*) This electronic arrangement is taken from NE laboratory notes prepared by F.Borak.

A wide variety of scintillators is in use today. Table 2.1 gives them and some of their characteristics.

TABLE 2.1. Properties of several scintillators [Pr-64]

Materials	Dens- ity, g/cm <sup>3</sup>	Wavelength of maximum emission, Å	Relative beta-ray pulse height	Alpha- beta ratio, %	Decay time, sec
1. Anthracene crystal.....	1.25	4,400	100	9	$3 \times 10^{-8}$
2. Trans-stilbene crystal.....	1.15	4,100	60	9	$4-8 \times 10^{-9} (\beta)$
3. Liquid phosphors	0.86	3,500-4,500	40-60	9	$2-8 \times 10^{-9}$
4. Plastic phosphors	1.06	3,500-4,500	28-48		$3-5 \times 10^{-9}$
5. NaI(Tl).....	3.67	4,200	210	44	$3 \times 10^{-7}$
6. LiI(Eu).....	4.06	4,700	70	95	$1.2 \times 10^{-6}$
7. CsI(Tl).....	4.51	4,200-5,700	55-95		$1.1 \times 10^{-6} (\beta)$ $0.43 \times 10^{-4} (\alpha)$
8. ZnS(Ag) (powder)	4.10	4,500	200	100	$4-10 \times 10^{-8}$ (fast component) $4-10 \times 10^{-8}$ (slow component)

As can be seen in table 2.2, one of the most widely used scintillators is the NaI(Tl). When approximately 0.5 % of thallium is added to sodium iodide, a crystal grown from the mixture has the property of emitting light in the visible range of wavelength upon the passage of an ionizing particle. The crystals are generally made cylindrical in shape and the container is provided with a glass window adjacent to one of the flat ends. In order to get the maximum yield of light out of the window, a layer of reflecting material is packed between the surfaces of the crystal and the container walls. To convert the light scintillation to an electronic pulse the packed crystal mounted on a photomultiplier tube by using heavy grease for optical contact with the face of the tube. Typical photomultiplier tubes have a photosensitive layer on the inside of the flat end of the tube. When photons from the scintillation event eject photoelectrons from this layer, the

electrons are attracted to a dynode assembly where multiplication takes place. A voltage divider is arranged so that each successive dynode is at a voltage of 70 to 200 volts. For each photoelectron emitted from the photosensitive surface a burst containing  $10^6$  or more electrons depending on the voltage, is collected at the anode. The amplitude of the final pulse depends on the initial number of photoelectrons which in turn depends on the number of photons produced by an ionizing event in the crystal [Aj-60].

#### 2.4.2. Semiconductor Counters

The operation of a semiconductor detector is analogous to the operation of an ionization chamber. In an ionization chamber the incident radiation produces positive ions and electrons, and an electrical signal is obtained by collecting these ions. In a semiconductor counter the incident radiation produces electrons and holes; then information about the radiation is obtained by collecting them. One major difference is that only 3.5 eV has to be expended to produce an electron - hole pair in a semiconductor, while the value is approximately 30 eV in an ionization chamber [Ou-75].

To understand the operation of the semiconductor counter, it can be considered as a bar of a uniform crystal with electrodes attached at the both ends as seen in figure (2.9),

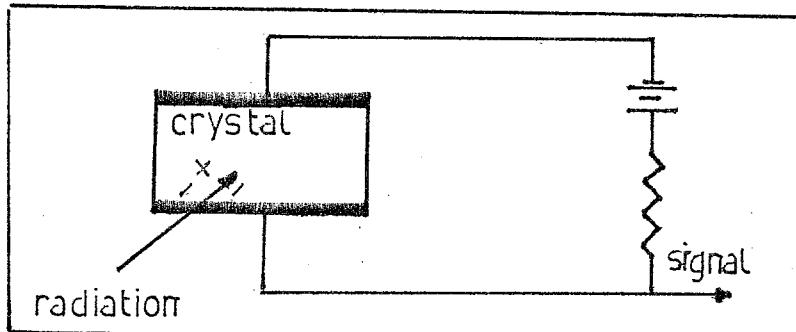


Fig. 2.9. Single crystal semiconductor counter [Ou-75]

When radiation falls on the crystal, electron-hole pairs are produced and when they are collected by the electrodes, a signal is obtained across the resistance, the height of which is proportional to the energy expended by the radiation in the material.

Energy resolution is usually an important factor in selecting a detector material. Energy resolution depends on the number of electron-hole pairs produced by the radiation. The energy required to produce an electron-hole pair is lower in a semiconductor than in an insulator. Hence the resolution of semiconductor detectors will be much better than that of detectors made of insulators.

The electron-hole pairs produced should be free to move in the detector and should be able to reach the electrodes. If the detector contains traps produced by impurities and defects, the electrons may be captured before reaching the electrode. Therefore only single crystals with the least number of traps are used for detectors. Trapping centers enhance recombination of holes and electrons, which will also reduce the pulse height.

#### 2.4.2.1. LITHIUM DRIFTED DETECTORS(\*)

Lithium is a donor atom. The diffusion coefficient is about  $10^7$  higher than that for phosphorus and therefore, deep diffused junctions can be prepared. First, lithium is coated onto single crystals into which it is diffused by heating. In the second step, the sample is heated and a strong reverse

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(\*) Detailed explanations about these detectors can be obtained from the given references, such as [De-63, Pr-64, Ou-75, So-72].

bias(\*) is applied. This helps the lithium atoms to diffuse deeper into the crystal. There are three region; the p region, the n region and an intrinsic region. Figure(2.10) shows these regions.

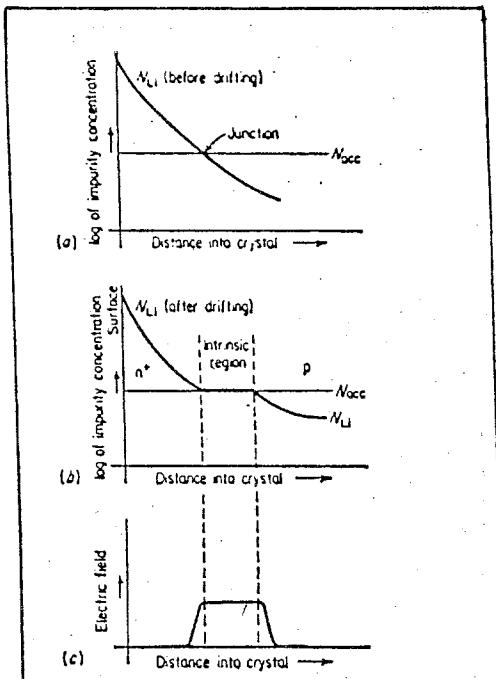
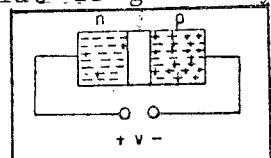


Fig. 2.10. Concentration profile for acceptor impurities ( $N_{acc}$ ) and for lithium donor impurities ( $N_{Li}$ ) in a diffused junction diode. (a) Before the drifting process; (b) after the drifting process; (c) electric field distribution with applied reverse bias [Pr-64].

When lithium atoms diffuse onto a surface, the donor - acceptor profile of the junction diode will be as shown in the figure 2.10 (a). If the resulting junction is reverse - biased and the temperature is raised for a short time, the donor-acceptor profile changes to that shown in fig. 2.10 (b). The donor and acceptor impurities in equal numbers compensate each other and effectively produce an intrinsic region bet-

(\*) Reverse bias is given by the following figure.



ween the p and the n regions. When the material is returned to room temperature and operated as a detector with a reverse bias, the residual carriers are swept from the intrinsic region and a space charge is developed at either edge, as indicated by the electric field plot in fig. 2.10 (c).

Intrinsic regions over 1 cm thick have been produced by this technique and further developments will lead to thicker sensitive regions. But when one goes to larger and larger sensitive regions, the pulse rise time lengthens.

## 2.5. GAMMA RAY SPECTROMETRY

The detection of gamma rays is mostly performed by means of a NaI(TL) scintillator or with a Ge(Li) junction. As the output of these detectors is proportional to the amount of energy absorbed, integral counting as well as spectrometry is possible. The NaI(TL) and the Ge(Li) detectors are made in different shapes, according to the purposes for which they will be used such as planar, coaxial etc.

Although gamma rays are monoenergetic, their energy spectra are complex, as illustrated in Fig.(2.11),

According to the size and the absorbing properties of the detector used and depending on the energy of the gamma ray, total or partial absorption can occur.

With NaI(TL) detectors, the escape of the detector X ray by photoelectric effect can be observed at 28 keV. At higher energies the escape peak disappears under the photo-

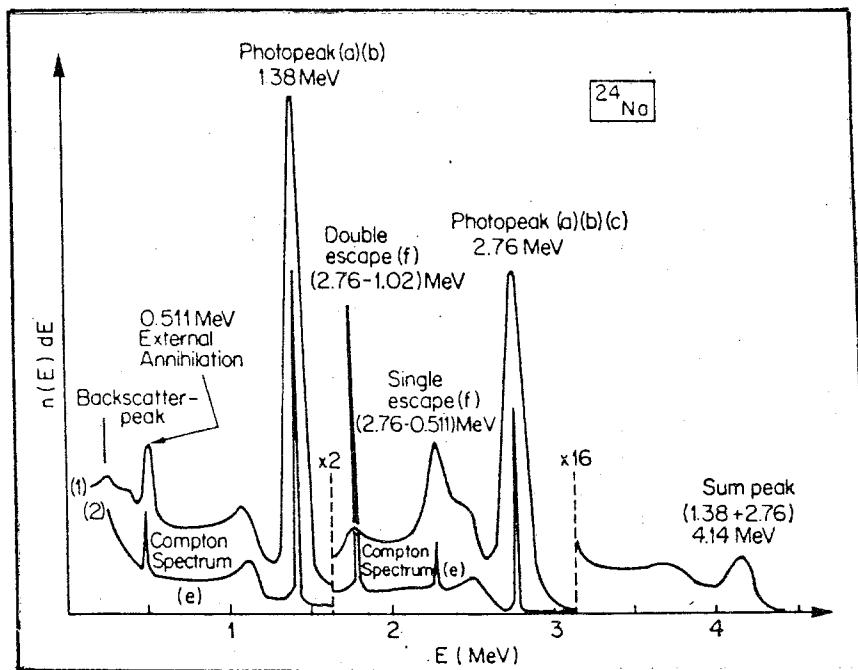


Fig. 2.11. Gamma spectrum of  $^{24}\text{Na}$  [SO-72].

peak due to the poor detector resolution. In Ge(Li) detectors the escape peak should appear at about 10 keV below the photopeak, and should be observed up to energies of approximately 1 MeV.

When dealing with gamma rays with energies higher than 1.02 MeV single and double escape of the positron annihilation quanta produce peaks at energies respectively 0.511 and 1.02 MeV below the gamma ray energy. In this case an annihilation peak also occurs at 0.511 MeV due to positron escape and subsequent annihilation in the surrounding materials. When positron emitters are measured, the typical annihilation gamma ray of 0.511 MeV appears in the spectrum and in good geometry also the 1.02 MeV sumpeak.

In order to achieve gamma spectrometric measurements, pulse height discrimination becomes necessary, which can be

done either with a single channel or a multichannel pulse height analyzer.

The resolution of a gamma spectrometer varies with the gamma ray energy and is normally given for the 0.662 MeV peak of  $^{137}\text{Cs}$ . With a NaI(TL) detector, the resolution R is expressed in percent using the expression, [SO-72],

$$R_{\%} = \frac{(\text{FWHM}) \times 100}{E} \quad (2.19)$$

where, FWHM is full width at half maximum of the photopeak and E is the peak energy.

When dealing with Ge(Li) detectors, the resolution is normally expressed as the FWHM in keV of the 0.662 MeV  $^{137}\text{Cs}$ . Typical resolution of these detectors are between 5 and 2 keV.

The detector resolution  $R_D$  is energy dependent, and can be expressed as follows:

$$R_D^2 = 2.355 FEE \quad (2.20)$$

where,  $R_D$  and the gamma energy E are given in keV,  $\epsilon$  is the energy needed to create an electron-hole pair and is approximately equal to  $3.10^{-3}$  keV for Ge, for Ge(Li) detectors, F is the Fano factor which is variance to yield factor (The true value of fano factor for Si and Ge is still unknown. However it is assumed as 0.1 for both Si and Ge [Or-80]).

Then the resolution of the spectrometer R is composed of the electronic line broadening, for which the main factor is noise produced by the detector and the amplifying instruments, and of the detector resolution as,

$$R^2 = R_E^2 + R_D^2 \quad (2.21)$$

The energy of the unknown gamma ray can be determined by the pulse height of the photopeak maximum. The calibration of the spectrometer is performed by means of isotopes emitting gamma rays of known energies. Sets of calibration sources are commercially available or can be prepared by irradiation of the stable isotopes. As a Ge(Li) detector shows a very good resolution, gamma ray energies can be determined within a few tenths of a keV. Table 2.2 shows some calibration sources for gamma-ray spectrometry.

Table 2.2. Calibration sources for gamma-ray spectrometry  
 [SO-72]

Isotope	Energy (keV)	Isotope	Energy (keV)
$^{241}\text{Am}$	$59.568 \pm 0.017$	$^{85}\text{Nb}$	$765.83 \pm 0.07$
$^{131}\text{I}$	$80.166 \pm 0.009$	$^{54}\text{Mn}$	$834.84 \pm 0.07$
$^{154}\text{Gd}$	$97.43 \pm 0.02$	$^{88}\text{Y}$	$898.01 \pm 0.07$
$^{158}\text{Gd}$	$103.18 \pm 0.02$	$^{107}\text{Bi}$	$1063.82 \pm 0.28$
$^{177}\text{Lu}$	$112.97$	$^{60}\text{Co}$	$1173.13 \pm 0.04$
$^{141}\text{Ce}$	$145.44 \pm 0.05$	$^{60}\text{Co}$	$1332.39 \pm 0.05$
$^{188}\text{Ce}$	$185.84 \pm 0.03$	$^{14}\text{Na}$	$1368.40 \pm 0.04$
		$^{60}\text{Co(D.E.)}$	$1576.9 \pm 0.32$
$^{177}\text{Lu}$	$208.36$	$^{108}\text{Tl(ThC'')}(D.E.)$	$1592.3 \pm 0.13$
$^{203}\text{Hg}$	$279.12 \pm 0.05$	$^{24}\text{Na (D.E.)}$	$1731.6 \pm 0.16$
$^{131}\text{I}$	$364.47 \pm 0.005$	$^{88}\text{Y}$	$1836.1 \pm 0.07$
		$^{60}\text{Co}$	$2035.2 \pm 0.50$
		$^{60}\text{Co(D.E.)}$	$2232.2 \pm 0.67$
$^{198}\text{Au}$	$411.776 \pm 0.01$	$^{24}\text{Na (S.E.)}$	$2242.6 \pm 0.14$
		$^{60}\text{Co}$	$2598.9 \pm 0.30$
Annihilation	$511.006 \pm 0.02$	$^{108}\text{Tl (ThC'')}$	$2614.3 \pm 0.09$
$^{107}\text{Bi}$	$569.65 \pm 0.10$	$^{24}\text{Na}$	$2753.6 \pm 0.12$
$^{137}\text{Cs}$	$661.59 \pm 0.07$	$^{56}\text{Co}$	$3202.4 \pm 0.65$
		$^{56}\text{Co}$	$3254.2 \pm 0.65$
		$^{56}\text{Co}$	$3273.6 \pm 0.4$
		$^{56}\text{Co}$	$3452.5 \pm 0.75$

S.E. = single escape      D.E. = double escape.

Quantitative data of the gamma ray intensity can be obtained from the area or the height of the photopeak. The photopeak can be described as a Gaussian error curve, with an area S, given by

$$S = 1.06 \text{ (FWHM)} h \quad (2.22)$$

where,  $h$  is the peak height.

When peaks are superimposed on Compton continuum of higher energy or when poor counting statistics are obtained, it is difficult to determine the peak height. There are some other methods to calculate the peak areas, such as the method of Covell (which will be examined in chapter 3 in detail), spectrum stripping, etc.

Linearity of a detector is another important subject. This property of semiconductor detector is excellent, and deviations from linearity in existing spectrometers can be traced back to amplification and analysis equipment except for very low energies, [H0-71].

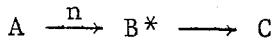
## 2.6. QUANTITATIVE ANALYSIS

### 2.6.1. Basic Principles and Concepts

The technique of activation analysis is based on the formation of radioactive nuclides as a result of reactions between nuclear particles and the isotopes of the trace elements of interest. These isotopes are transformed into different isotopes of either the same or a different element. There are many nuclear reactions for this purpose. In the great majority of cases two-particle reactions are utilized; one particle being a reactant and the other being a product. The particles for general use as reactants are neutrons, protons, deuterons, alpha particles and photons.

As an example, when a target material is exposed to

neutrons, photons or charged particles, the resulting nuclear reaction and the product decay may be represented by,



The stable isotope A being bombarded is transmuted to radionuclide  $B^*$  which decays with its characteristic decay constant  $\lambda_B$  to the stable isotope C. (or unstable isotope  $C^*$  which will also decay with  $\lambda_C$ , etc.). These subjects are examined in 2.1.1 and 2.1.2 in detail.

The rate of formation,  $R_F$ , of a particular activation product B in a given sample is proportional to the intensity of the flux or beam of incident particles, to the concentration of the target nuclide in the sample, and to the cross-section for the nuclear reaction. Thus, for the case of neutron irradiation  $R_F$  is given as,

$$R_F = \phi N_A \sigma V \quad (2.23)$$

where  $N_A = Avfp/M_A$  or for unit volume,  $N_A = Avmf/M_A$  and  $R_F$  is assumed as constant (the case of  $R_F \neq$  constant, was examined in subchapter 2.1.2). Then,

$$R_F = \frac{\phi m Avf\sigma}{M_A} \quad (2.24)$$

where,

$N_A$  = the number of target atoms

$\phi$  = the neutron flux ( $n/cm^2\text{-sec}$ )

$m$  = the mass of the trace element in the specimen  
(gm)

$M_A$  = the atomic weight of the trace element.

$f$  = the fractional isotope abundance of the target nuclide

$A_V$  = Avagadro's number (atom/gm. atom)

$\sigma$  = the reaction cross-section ( $\text{cm}^2/\text{atom}$ )

The decay rate expressed in atomic disintegrations per second of the product radionuclide in the specimen was given by the equation 2.3, as

$$\frac{dN}{dt} = -\lambda N$$

Therefore, the rate of change of the quantity of the activation product in the sample during the irradiation is given as,

$$\frac{dN_B}{dt} = R_F - N_B \lambda_B \quad \text{or,}$$

$$\frac{dN_B}{dt} = \frac{\phi m A_V f \sigma}{M_A} - N_B \lambda_B \quad (2.25)$$

The solution of this differential equation will be given in the appendix B. The result is,

$$N_B = \frac{\phi m A_V f \sigma}{\lambda_B M_A} (1 - e^{-\lambda_B t}) \quad (2.26)$$

The number of disintegrations per second of the product represented as the activity after an irradiation time  $t$  sec is,

$$A = N_B \lambda_B = \frac{\phi m A_V f \sigma}{M_A} (1 - e^{-\lambda_B t}) \quad (2.27)$$

The equation (2.27) can be used to estimate the activation levels for the various elements in the sample under varying conditions of flux, irradiation time and sample size. This equation is rearranged for M and is given as, [KO-60],

$$M(\text{gm}) = \frac{M_A A}{\phi A_V f \sigma (1 - e^{-\lambda_B t})} \quad (2.28)$$

$$M(\text{gm}) = \frac{M_A A}{6.02 \times 10^{23} \phi f \sigma (1 - e^{-\lambda_B t})} \quad (2.29)$$

The maximum or saturation activity is attained when the irradiation time is long compared to the half-life of the product and the rate of formation is equal to the rate of disintegration  $[1 - e^{-\lambda_B t}]$  approaches unity and,

$$A_s = N_B \lambda_B = \frac{\phi M A_V f \sigma}{M_A} \quad (2.30)$$

Assuming the sample has been irradiated to saturation and no significant decay has occurred in the interval between the end of bombardment and counting time  $t$ , a formula can be obtained to calculate the weight of the element by reducing the eq. (2.30) to,

$$M(\text{gm}) = \frac{M_A A}{6.02 \times 10^{23} \phi f \sigma} \quad (2.31)$$

Besides, the sensitivity expressed in terms of the minimum weight of a target element that will produce the minimum detectable activity after a certain bombarding time  $t$  will be given by,

$$\text{Sensitivity in micrograms} = \frac{M_A A \times 10^6}{6.02 \times 10^{23} \phi f \sigma (1 - e^{-\lambda_B t})} \quad (2.32)$$

### 2.6.2. Methods of Analysis

When determining a large number of elements in one sample, the comparison of samples is very troublesome and time consuming. Besides, it is often impossible to irradiate a large number of comparison samples together with the unknown samples because of the restricted volumes of irradiation containers. Moreover, when performing multielement determinations, the presence of one or several elements in the sample is often only realized during the evaluation of the gamma spectra. When no comparison standards for these elements were irradiated a semiquantitative guess is all that can be derived concerning the concentrations.

Several techniques have been put forward to eliminate the above mentioned shortcomings, such as absolute, single or multicomparator methods [H0-71].

Absolute Method: This direct method performed by Girardi, [Gi-64], based on the determination of weights by means of the activation relationship is generally considered as a semiquantitative technique. It deals with absolute gamma-ray counting and direct calculation of weights from an estimation of the activation formula. The reliability of that method depends on the accuracy with which the absolute of the thermal cross-section, the resonance integral and the decay schemes are known. But most of these are not sufficiently well known to allow their use for accurate absolute calculations.

**Comparator Method:** Many sources of error can be eliminated by irradiating the sample with a standard of similar composition. When the composition of a substance is unknown, a preliminary irradiation can be used as a qualitative determination, and a suitable standard can be fabricated for simultaneous irradiation with the sample. The sample and standard should be approximately the same weight, shape and thickness. Thus, effects due to variations in flux and self attenuation during the irradiation will not influence the analysis.

If the activities are measured in an identical manner, comparing the counting rates in the sample and the standard will give the weight of the element in the sample by the following simple relation, [Ad-70],

$$\text{Weight of the element in sample} = \frac{\text{(Activity in sample)} \cdot \text{(Weight of element in standard)}}{\text{(Activity in standard)}}$$

**Single Comparator(\*):** The use of Ge(Li) detectors allows the simultaneous determination of an important number of elements after a single irradiation. The classical comparator method requires one standard for every element to be determined; but this method uses only one comparator consisting of known amounts of elements to be determined.

## 2.7. USE OF COMPUTERS IN NAA

With the development of modern methods of radionuclide measurement, the ability to record vast amounts of data reliably and automatically has led to the use of computers. Many computer programs have been developed up to now, to interpret and evaluate that data. Some of these programs have been pre-  
(\*) This method will be discussed in appendix C in detail.

pared for big computers; some others are for small ones, which are particularly for the routine processing of spectrometric data.

The large computers allow, of course, the most sophisticated and complete analysis of that data. The computing programs can easily be written and the hardware problems for data collection and transfer to the large computer system have been solved for several years. This data analysis system keeps its full validity, particularly when large batches of samples must be analysed in a similar way [Be-73].

On the other hand, the small computers are used at the laboratory site for both data acquisition and analysis, requiring the small amounts of memory locations. However, the programs prepared for these computers could not define the location of photopeaks and the computation of the peak areas as reliably as those prepared for the big ones [Ci-81].

As a result of this short discussion, it can be concluded that; the choice of a data-handling system is a rather cumbersome task since the money involved is important and the information available on the real performances of the various systems are often incomplete.

Modern gamma-spectrometers collect their data simultaneously in a large number of energy channels. When NaI(Tl) scintillators are used, a few hundred energy channels were sufficient for adequate representation of the spectrum. But, the introduction of the Ge(Li) type detector with its excellent energy resolution, pushed the number of energy channels required for an adequate spectral response, up into the thousands. For the relevant information from the enormous amount of digital data comprised in a Ge(Li) type spectrum,

"data-reduction system" has been used. The purpose of such a system is to recognize valuable data and to reject useless information.

The following five steps can be distinguished in the course of a data-reduction procedure, as in Gretel which will be discussed in chapter 3, [HO-71];

- a) the preliminary treatment of all data
- b) the location of possible photopeaks
- c) the determination of the peak limits
- d) the application of statistical and peak shape tests,
- e) the evaluation of exact peak centroid location,  
determination of net peak area with corresponding  
standard deviation and detection limit.

a) In general, the preliminary treatment of data involves the application of smoothing techniques and the computation of the first or higher derivatives of the spectral data. Smoothing, as will be discussed in 3.3.2, is used to minimize the influence of the statistical counting fluctuations First or second derivatives which can be calculated according to the least squares method, detect the location of the photopeaks [So-72, Sa-64].

b) For the detection of exact photopeak location, the calculation of the maxima that belong to true photopeaks is the second problem. When a preliminary data treatment has produced a first derivative, then the maxima correspond to points where this function goes from a positive value to a negative one.

c) The most critical point in the data-reduction system is the determination of the left and right boundaries of the

photopeaks. This will determine the separation that is to be made between the peak area and underlying continuum. This will also determine both accuracy and precision of any quantitative interpretation of the spectra.

d) Once a maximum has been detected and its boundaries have been established, some further tests are required to make sure that a real photopeak has been found. There are different tests used for that purpose. Some of them used in Gretel will be studied in 3.3.3.

e) Once a peak has been detected and accepted, the spectral data contributing to the photopeak should be interpreted in terms of energy and intensity of the corresponding gamma radiation. This is the classical problem of NAA and it is usually the last step of many computer programs.

Besides these, another important subject of some programs is the analysis of detection limits for the peaks actually found or for those not detected but expected at specified location.

Up to now some analysts have used minimum data-reduction without any qualitative interpretation. Others used a very extensive data reduction but only a limited amount of qualitative analysis, mainly to interpret the standard spectra in order to define the elements to be determined [Ho-71].

The program examined in this thesis is one of these programs which involves data-reduction, interpretation of the activation process and standard spectra quantitatively, which will be examined in the following chapter in detail.

### 3. GRETEL

#### A COMPUTER PROGRAM FOR GAMMA RAY SPECTROMETRY WITH Ge(Li) DETECTORS

##### 3.1. INTRODUCTION OF THE COMPUTER CODE

Gretel performs the quantitative analysis of gamma-ray spectra obtained by Ge(Li) detectors, using special "oriented libraries" which are prepared for each particular problem (Table 3.1 shows such an oriented library).

The scheme of the Gretel program is the following: An energy calibration source is counted as the first spectrum of the series; then the unknown neutron activated samples are successively counted. The counting equipment consists of a 4096 channel analyzer for high resolution spectrometry with Ge(Li) detectors, equipped with sample changers to allow the automated acquisition of gamma-ray data from successive specimen. The data coming from the analyzer, are first punched on paper tapes, then transferred on to magnetic tapes. These tapes are then read by one of the subroutines (TAPE, TAPEAS or TAPEGA), according to the punching code adopted; such as IBM, ASCII or ASCII with no parity. These routines transform the data in a suitable format, either by the functions CONV or CONVB.

The analysis is carried out by the single comparator method as will be seen in the appendix C.

TABLE 3.1- EXAMPLE OF "ORIENTED LIBRARY" FOR LONG LIVED  
RADIOISOTOPES

[Gu-74]

Radioisotope	Energy (keV)	Resolution (keV) FWHM	Decay Constant (minutes)	Specific Activity <sup>(1)</sup> (cpm)	Molecular Weight
Ag 110 M	657.8	3.0	$1.85 \times 10^{-6}$	$6.911 \times 10^8$	107.87
Ca 47	489.5	2.9	$1.01 \times 10^{-4}$	$5.761 \times 10^{13}$	40.08
Ca 47	807.4	3.1	$1.01 \times 10^{-4}$	$9.274 \times 10^{13}$	40.08
Ca 47	1296.4	4.2	$1.01 \times 10^{-4}$	$1.13 \times 10^{14}$	40.08
Co 60	1173.2	4.1	$2.497 \times 10^{-7}$	$2.612 \times 10^7$	58.9
Co 60	1332.4	4.2	$2.497 \times 10^{-7}$	$2.893 \times 10^7$	58.9
Cs 134	604.7	3.0	$5.98 \times 10^{-7}$	$4.1 \times 10^7$	132.91
Cs 134	795.0	3.1	$5.98 \times 10^{-7}$	$5.683 \times 10^7$	132.91
Hg 203	279.1	2.5	$1.035 \times 10^{-5}$	$1.018 \times 10^9$	200.61

(1) Calculated from irradiation of one  $\mu\text{g}$  of element in a thermal flux of  $10^{13} \text{n/cm}^2 \cdot \text{sec}$  at saturation and at decay time equal zero.

The program is essentially composed of a MAIN part which controls the various subroutines, also involving those mentioned above, thirteen subroutines and three functions.

These routines which detect and evaluate peak areas perform the following operations:

- a) Local smoothing of the spectrum for minimizing the influence of the statistical counting fluctuations.
- b) First derivative of the smoothed spectrum.
- c) Detection of peak location according to the change of sign of the first derivative.
- d) Computation of the net area of each peak found.
- e) Possibility of detection and computation of double peak.

f) Computation of the minimum counting rates that could have had a photopeak to be detected over the existing background in case no peaks are found in the interval indicated by the oriented library [Gu-74, Gu-67].

All those subjects will be discussed in the following subchapters in more detailed form. Description of the routines will also be given in appendix G.

Results in ppm or sensitivity limits for the elements not detected, are obtained in the form of digital lists.

At first, the original raw spectrometric data are collected on punched tapes which are then processed at the Scientific Information Processing Center, Ispra-Italy, by an IBM 370/165 computer with fortran IV level G and assembly languages. It also has possibility of obtaining analog outputs as results given in digital lists, using a CALCOMP unit. One request, a graphical representation of the spectrum could be produced, showing the way in which the spectrum has been processed. The code has been updated by the author for UNIVAC-1106, by deleting all the plotting subroutines from the main program because a Univac plotting unit was not available in BU. The updated form of the code is recorded on a new magnetic tape for further studies by BU-NE Department. This tape(\*) contains four files:

1. file: UNIVAC-1106 version of GRETEL source program containing main and subprograms.
2. file: sample problem input data
3. file: spectra for sample problem
4. file: sample problem output data

(\*) This tape covering the UNIVAC version of Gretel and input and output data is labelled as "SAGLAM" for further studies by the NE Department.

### 3.2. THEORY OF NAA USED IN GRETEL

In this chapter, the theory of neutron activation analysis, NAA, used in Gretel is given in a summary form as follows:

The neutron activation analysis in subchapter 1.3 and the basic principles of this method in 2.6 were examined in detail. The equation (2.27) derived in the same subchapter 2.6 was given

$$A = N_B \lambda_B = \frac{\Phi m A_v f \sigma}{M_A} (1 - e^{-\lambda_B t})$$

where, A represents the amount of radioactivity of the daughter nuclei  $N_B$  which is present at the end of the activation time  $t$ . Since the activity also decays exponentially with time, according to the equation (2.5), the activity  $A_d$  that will be detected, will depend on the decay time  $\tau$  after irradiation,

$$A_d = A e^{-\lambda_B \tau} = \frac{\Phi m A_v f \sigma}{M_A} (1 - e^{-\lambda_B t}) e^{-\lambda_B \tau} \quad (3.1)$$

This equation can be rearranged for the weight of the element as,

$$g(\mu\text{gm}) = \frac{M_A A_d \times 10^6}{6.02 \times 10^{23} \Phi f \sigma (1 - e^{-\lambda_B t}) e^{-\lambda_B \tau}} \quad (3.2)$$

Besides the basic activation formulas given above the analysis of the spectra with computers will be discussed in the following chapters in the detailed form.

### 3.3. ANALYSIS OF GAMMA-RAY SPECTRA WITH DIGITAL COMPUTERS

#### 3.3.1. Introduction

With the development of modern methods of radionuclide measurement, as discussed in subchapter 2.7, the ability to record vast amounts of data automatically has led to the use of computers. Many computer programs have been derived up to now, to interpret that data.

Gretel is one of these programs prepared for gamma-ray spectra obtained with high resolution Ge(Li) detectors. The program is used for the quantitative analysis of trace elements from gamma-spectra of neutron activated materials. As mentioned before, it is composed of three main parts as follows:

First part introduces the smoothing procedure by taking 5, 7 or 9 point segments of the spectrum. This procedure is used to minimize the influence of the statistical counting fluctuations. The smoothed spectrum is then examined to define the location of a peak where the sign of the derivative changes from a positive value to a negative one. This subject will be discussed in the subchapter 3.3.2 in more detail.

In the second part, the peaks are searched and located exactly. To avoid the statistical fluctuations from being kept as analytical peaks, the absolute values of the maximum and minimum of the derivative must be larger than a confidence band chosen suitably. The criteria for the choice of confidence band will be explained in the subchapter 3.3.3. Besides this procedure, some other tests for recognizing the peaks as single or double will also be introduced in the same subchapter.

Third part examines the computation methods of peak

areas. There are two different methods used in the program.

1) Computation of the areas of the peaks observed over the background: If the peaks found are above the Compton continuum, their left and right limits are examined according to Covell, [Co-59], in the subsection 3.3.4.1.

2) Searching of detection limits: As mentioned in the 3.1 briefly, in case the peak is not detected in the interval given by the library, the minimum counting rates due to the hidden peaks are calculated by a particular subroutine, subroutine SENSIT. That procedure will be given in the 3.3.4.2 in more detail.

Finally, the results in ppm or sensitivity limits for the elements not detected are obtained in the form of a digital list. The errors due to statistical counting fluctuations, as percentages, are also estimated in the program. That data is also given in the appendix K.

### 3.3.2. Smoothing and Differentiating Procedures

The majority of published literature on the uses of computers in activation analysis relates to the unscrambling of gamma-ray spectra. This may be achieved in a variety of ways, such as spectrum stripping, the method of least squares fitting, vector analysis and iterative methods, etc [Gi-65]. One of these ways is the spectrum smoothing procedure.

The primary output of any experiment is information which measures the phenomenon under observation. The random errors which are indistinguishable from this information are

characteristically described as noise. It is important for an analyst, to remove as much of this noise as possible without unduly degrading the underlying information. There are some mathematical methods for handling such problems in the processing of analytical data.

One of the simplest ways to smooth the fluctuating data is by a moving average based on the concept of a convolute and of a convolution function(\*) [Sa-64].

In summarized form, it can be said that the method of data convolution is to fit a polynomial to such data by use of the method of least squares. Assuming that  $f$ 's represent any set of convoluting integers, and  $S_n$  is the smoothed value in the  $n$ th channel, the mathematical description of this process is given by [Sa-64, Gu-74],

$$S_n = \frac{1}{N} \sum_{i=m}^{+m} (f_i S_{n+i}) \quad (3.3)$$

where the index  $n$  indicates that  $(2n+1)$  points are used for that procedure. For the calculation of these convolution coefficients, a set of experimental points is to be fitted to a curve, as given in the eq. (3.3), and then the square of the differences between the computed values and the observed values are to be minimum for the total of the observations.

There is also an associated normalizing or scaling factor. These coefficients and factors are given in the tabular form [Sa-64]. The table 3.2 gives the convoluting integers and normalizing factors.

---

(\*) Convolution method will be discussed in the appendix D.

TABLE 3.2 [Sa-64]

CONVOLUTES	SMOOTHING	QUADRATIC	CUBIC	A20	A30						
POINTS	25	23	21	19	17	15	13	11	9	7	5
-12	-253										
-11	-138	-42									
-10	-33	-21	-171								
-09	62	-2	-76	-136							
-08	147	15	9	-51	-21						
-07	222	30	84	24	-6	-78					
-06	287	43	149	89	7	-13	-11				
-05	322	54	204	144	18	42	0	-36			
-04	387	63	249	189	27	87	9	9	-21		
-03	422	70	284	224	34	122	16	44	14	-2	
-02	447	75	309	249	39	147	21	69	39	3	-3
-01	462	78	324	264	42	162	24	84	54	6	12
00	467	79	329	269	43	167	25	89	59	7	17
01	462	78	324	264	42	162	24	84	54	6	12
02	447	75	309	249	39	147	21	69	39	3	-3
03	422	70	284	224	34	122	16	44	14	-2	
04	387	63	249	189	27	87	9	9	-21		
05	322	54	204	144	18	42	0	-36			
06	287	43	149	89	7	-13	-11				
07	222	30	84	24	-6	-78					
08	147	15	9	-51	-21						
09	62	-2	-76	-136							
10	-33	-21	-171								
11	-138	-42									
12	-253										
NORM	5175	8059	3059	2261	323	1105	143	429	231	21	35

Increase in the number of data points used causes better smoothing but decreases the peak amplitudes at the same time. The minimum distortion occurs when the polynomial accurately describes the analytical data. The best results are obtained when the data are digitized at high densities, i.e., points very close together and the number of points used in the convolution is chosen to be small enough so that no more than one inflection in the observed data is included in any convolution interval. As an example, equation (3.4) can be illustrated for 5 points as, [Gi-65, Gu-74].

$$S_n = \frac{1}{35} \left[ -3S_{n-2} + 12S_{n-1} + 17S_n + 12S_{n+1} - 3S_{n+2} \right] \quad (3.4)$$

Another important subject in the use of this method is the degree of polynomial. High degree polynomials represent less smoothing than the others. This is especially important when there are double peaks found. Therefore, it is shown that, quadratic and cubic functions are the best for that convolution process. [Ci-81].

This type of data processing, as far as computers are concerned requires a relatively small amount of programming and relatively little use of the computer memory.

As mentioned in the previous subchapters, the first selection of possible peaks is done by considering the change of sign of the first derivative from a positive value to a negative value. The zero point can be considered as the location of a peak.

Therefore after smoothing procedure, this smoothed spectrum is differentiated by the following formula [Gu-74],

$$d_n = \frac{s_{n-1} + s_{n+1}}{2} \quad (3.5)$$

where  $d_n$  is the differentiated value of the content of the nth channel.  $s_n$ 's represent the smoothed values in the channels (n-1) and (n+1).

These smoothing and derivation processes are carried out by the subroutines SMOOS and DERIV which are given in the appendices G, I.

### 3.3.3. Search of the Peaks

After the smoothing procedure, the second problem con-

sidered by Gretel is the search of peak locations. As mentioned in the previous subchapter, a first selection of possible peaks is made by considering the change of sign of the first derivative from a positive value to a negative value. Therefore, one needs the values of maxima and minima of the spectrum. Many authors use different methods, [Ho-71], to obtain these values with or without preliminary data treatment as explained in the subchapter 2.7. The most simplified system of all is used by Anders [An-69], by just taking any set of consecutive data points that are higher than their neighboring points as a possible peak.

A similar method is used in Gretel which can be explained briefly as follows:

A possible maximum in channel  $n$ , is given by the condition below [Gu-67],

$$C_{n-2} < C_n - P \sqrt{C_n} > C_{n+2} \quad (3.6)$$

when its content  $C_n$  satisfies that condition. Where  $P$  is chosen empirically (presently  $P = 1$ ).

The minima on both sides of the maxima are chosen as the channels  $(n-k)$  and  $(n+k')$  for which:

$$C_{n-k-1} \geq C_{n-k} - P \sqrt{C_{n-k}} \quad (3.7)$$

and,

$$C_{n+k'+1} \geq C_{n+k'} - P \sqrt{C_{n+k'}} \quad (3.8)$$

The point  $n$  is considered as the location of a peak.

For the determination of the exact photopeak locations, besides the conditions stated, two conditions must be satisfied simultaneously:

1. The absolute values of the maximum and the minimum of the derivative must be larger than a confidence band suitably chosen. That band is calculated by multiplying standard deviations of data in each channel with a factor chosen, [Gu-74]. Data is taken from the smoothed spectrum instead of the original one. As a result of that process, the counting fluctuations are reduced and statistical fluctuations are kept as analytical peaks are avoided.

2. The ratio between maximum and minimum values of the spectrum must be less than or equal to 1.5. This also avoids unsymmetrical peaks being considered.

After having made these tests, the center of a peak where the sign of the first derivative changes from a positive value to a negative value, is determined by linear interpolation by taking the negative and positive differentiated data in the nearest channels to the center.

In the cases in which these two conditions are not fulfilled, a further examination of the shape of the derivative is performed to ascertain if a double peak is present in the considered interval. For two successive peaks to be considered as a doublet, the distance between the summit of each peak should be less than  $(2.0 \times \text{FWHM})$  [Gu-67, Gu-74].

According to the tests performed on the ratios between the maxima (AMAX) and the minima (AMIN) of the derivatives, three different cases are possible according to Guzzi, [Gu-74]. These are shown in the figure (3.1).

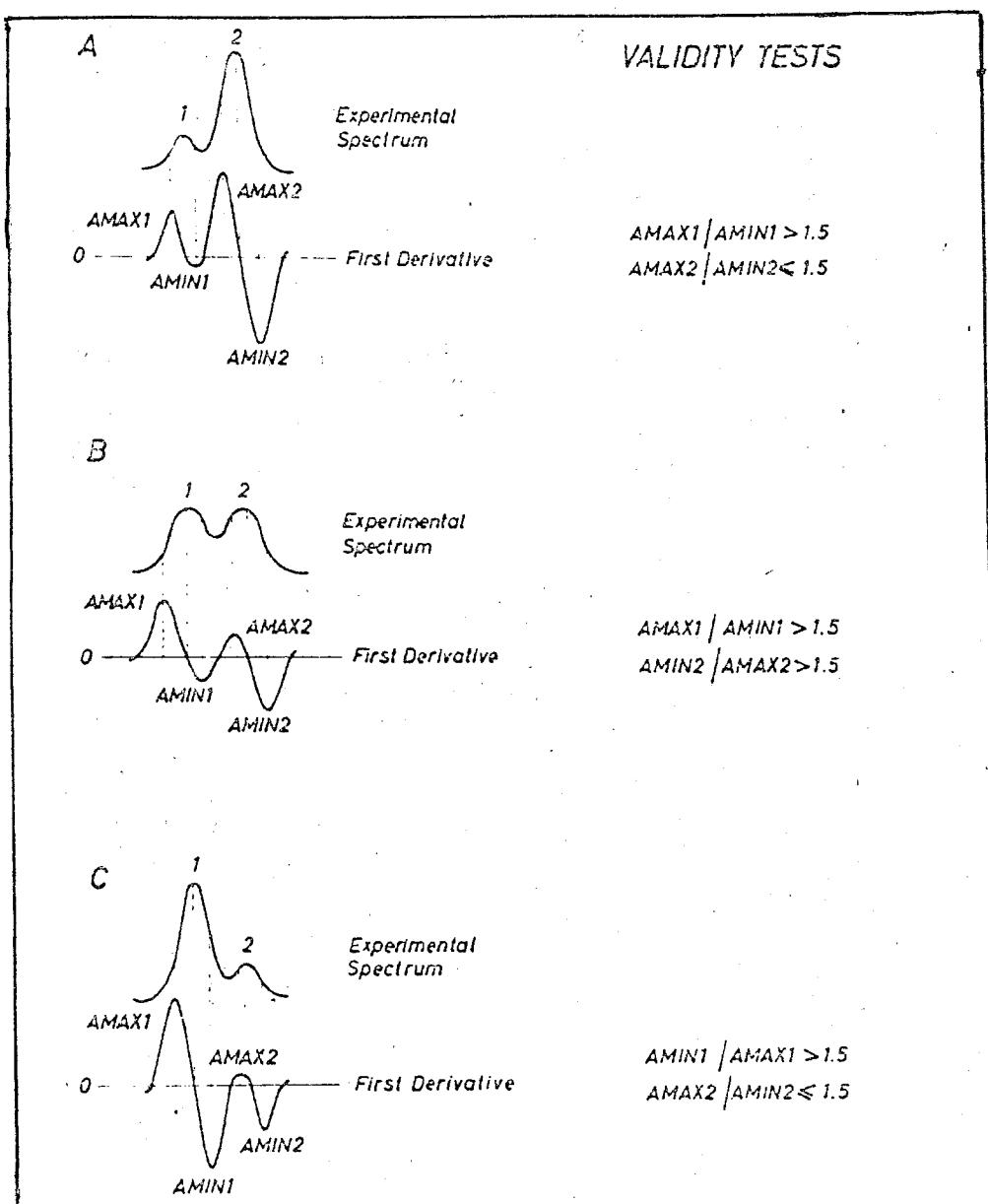


Figure 3.1

where,

A.  $AMAX1 / AMIN1 > 1.5 \quad AMAX2 / AMIN2 \leq 1.5$

Peak 1 is considered as belonging to a doublet, peak 2 is treated as a single peak.

B.  $AMAX1 / AMIN1 > 1.5 \quad AMIN2 / AMAX2 > 1.5$

Both 1 and 2 are treated as a doublet

C.  $AMIN1 / AMAX1 > 1.5 \quad AMAX2 / AMIN2 \leq 1.5$

Peak 1 is considered as single peak, peak 2 is treated as being a doublet.

On the other hand, the other most critical point in searching of peak locations is the determination of the left and right boundaries of the photopeaks. This will indeed determine the separation that is to be made between the peak area and underlying continuum. Many authors follow different ways for the determination of the peak boundaries [Ho-71]. That used in Gretel can be given in a brief form as follows:

The below figure, fig.(3.2), shows a small photopeak which is assumed as Gaussian, superimposed on a high constant

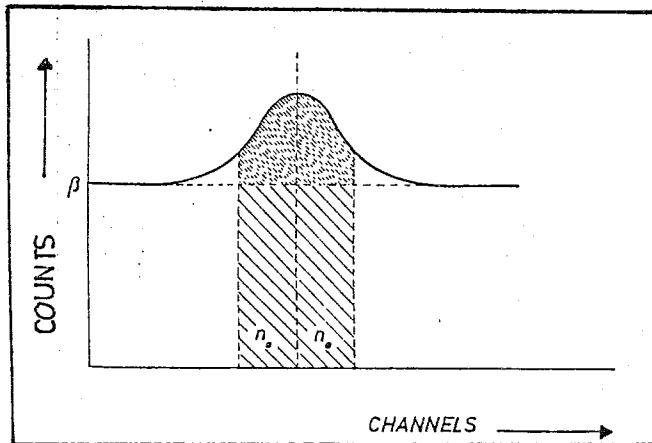


Fig.3.2. Schematic representation of a photopeak [Pa-66].

background such as it would be obtained after a very long measurement. The area of the background under the photopeak as seen in the above figure is given by J.Pauly et al. [Pa-66], by the relation, ( $2n_o = 1.2 \times \text{FWHM}$ ). Where FWHM is the full width at half maximum. If the background counting rate is small, as often happens when a lithium drifted germanium detector is used, the optimum value of  $n_o$  increases slightly.

But approximate value is taken as  $2n_0 = 1.2 \times \text{FWHM}$  for all values of the background [Pa-66, Gu-74].

Under this consideration the left and right limits of the peaks are determined in the program by the relations given below;

$$H_1 = n - 1.2 \times \text{FWHM} \quad (3.9)$$

$$H_2 = n + 1.2 \times \text{FWHM} \quad (3.10)$$

where,  $H_1$  and  $H_2$  represent left and right boundaries of a peak. FWHM is the energy resolution.

All these procedures described above are carried out by the subroutines ANALYS and PKF.

### 3.3.4. Computation of Peak Areas

One of the classical problems of qualitative and quantitative interpretation of gamma spectra for NAA is the calculation of peak areas found by some tests described before.

The procedure employed by Gretel can be explained in two subsections as follows:

1. Computation of the areas of the peaks observed over the existing background. These may be single or double peaks.

2. Computation of the minimum counting rates in case no peaks are found in the given interval.

### 3.3.4.1. Computation of the Areas of Observed Peaks

#### a) Computation of the area S of a single photopeak:

There are several methods, in the literature, used for the separation of a peak from its underlying continuum. Seven different methods, [Co-59, Yu-68, Qu-69], were especially studied up to now. Five of them use a straight line to separate the peak from the underlying continuum. Two use a nonlinear procedure, [Ho-71]. One of them which is known as Covell's method, [Co-59], is more common than the others. The method used in Gretel is derived from that method and it can be summarized as follows:

This method describes a procedure which utilizes the digital nature of pulse height distribution data to apply statistical methods of data reduction, [Co-59]. As the response of a pulse height analyzer is stated in counts per unit increment of amplitude, individual channel responses may be represented graphically as rectangles whose areas bear direct proportionality to the number of counts observed in the channel. A graphical representation is given in the figure (3.3).

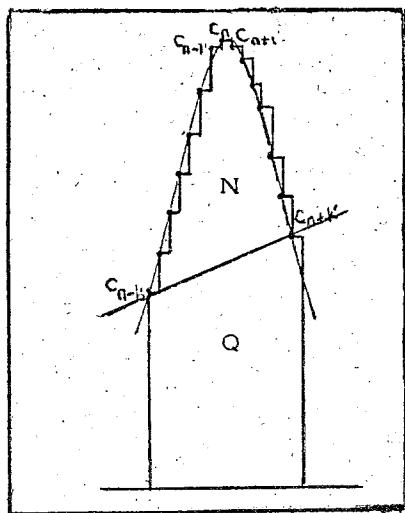


Fig.3.3. Fraction, N, of total counts contained in peak channel,  $a_2$  and  $n$  channels on either side.

Here, the response of the channel containing the greatest number of counts is defined as  $C_n$  and succeeding channel responses, progressing down the low amplitude side of the peak as  $C_{n-1} \dots C_{n-k}$ , similarly channel responses on the high amplitude side of the peak are defined as  $C_{n+1} \dots C_{n+k}$  (where  $C_{n-k}$  and  $C_{n+k}$  are defined by the intercept points of the rising and falling traces of the curve).

If the contributions from the  $C_n$  channel and the channels on either side are added, the sum is a value representing the total counts contained in these channels. This value is graphically represented as the area  $P$  in the above figure. If this area  $P$ , were divided by a line connecting the ordinate values of  $C_{n-k}$ ,  $C_{n+k}$  as seen in the figure (3.3), the area above this line can be defined as follows:

$$N = P - Q \quad (3.11)$$

where,  $N$  may be used under a wide variety of observational conditions to estimate the total peak area.

Although this method due to Covell, [Co-59], is the most common one, it is especially used for NaI(TL) detector peak area computations. For the Ge(Li) detector peak area computations, many authors use different methods, [Ho-71].

The method used in Gretel is the one which is based on smoothing and differentiating procedures of the spectra. Yule, [Yu-68], gives the principles of that method which is derived from the Covell's method. This method can be explained briefly as follows:

The method known as the smoothed first derivative method employs the simplified least squares data convolution

technique(\*) to generate, from the observed spectrum, a new spectrum which has essentially all the statistical scatter removed. The new spectrum defines a smooth curve through the observed data. The data convolution techniques can also generate a spectrum which is the smoothed first derivative of the observed data. The total peak area is then computed from the equation given by P.H. Yule as, [Yu-68]

$$\text{Total peak area} = \sum_{n=n-k}^{n+k'} C_n \quad (3.12)$$

where,  $C_n$  is the number of counts in channel  $n$ , and the boundary channels are  $(n-k)$ ,  $(n+k')$ . The base area is the area of the trapezoid below the peak, similar to the figure 3.3.

$$\text{Base Area} = \frac{C_{n-k} + C_{n+k'}}{2} (k-k'-1) \quad (3.13)$$

and the net peak area is given by the difference between them, [Yu-68, Gu-74]

$$\text{Net peak area} = \text{Total Peak Area} - \text{Base Area}$$

or,

$$S = \sum_{n=n-k}^{n+k'} C_n - \frac{C_{n-k} + C_{n+k'}}{2} (k-k'-1) \quad (3.14)$$

where, the quantity  $(k-k'-1)$  is the number of channels included in the peak or, in other words, it represents the width of the peak.

---

(\*) This subject will be discussed in the appendix D as mentioned in subchapter 3.2.

The associated errors in the evaluation of the peak areas are also calculated and given as digital lists.

b) Computation of the area of a double peak:

For the computation of the area of a double peak several assumptions are made by the authors. One that is used in Gretel is given as: The area of a doublet is approximated by considering the left half of the first peak and the right half of the second peak as being symmetrical with respect to the remaining portions of each peak. Then these halves are doubled to obtain the total area. The underlying continuum is subtracted as explained in the previous subchapter. Standard

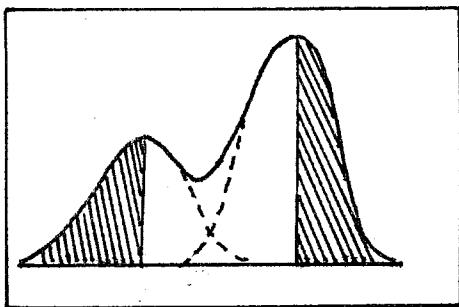


Fig. 3.4. Computation of the area of a doublet.

devitaion is approximated by doubling the standard deviation calculated for each half of each peak of the doublet.

All these operations are performed by the routines SURF and SURF2.

### 3.3.4.2. Search of Detection Limits

In the case where no peaks are found by the tests described in the subsection 3.3.4.1, in the indicated interval, the minimum counting rates that could have had a photo-

peak over the existing background, are also calculated in Gretel. This procedure is performed by the subroutine SENSIT. Theory of that calculation can be explained briefly as follows:

As known, many properties of materials depend on their impurity content. There always exists a lower limit of concentration beyond which the effect of an impurity becomes negligible. Therefore, in an analytical study it is usually sufficient to demonstrate that the concentration is smaller than a detection limit chosen to be low enough, so that the effects on the properties of the substance can be neglected.

As a result of this idea, in many problems it is important to know the concentration, or an upper limit for it for as large a number of elements as possible [Pa-66].

In NAA, the gamma spectra obtained from the experiments contain a small number of visible photopeaks which can be used to determine the exact concentration of the corresponding impurities. The other elements produce peaks too small to appear above the background due to their activities and it is then possible only to evaluate "an upper limit of the concentration, which is the sensitivity or detection limit for that particular gamma-spectrum. The operation for the evaluation of detection limits can be summarized as follows: If the element to be determined does not give a visible photopeak in the gamma-ray spectrum, whether a chemical separation has been applied or not, a detection limit is deduced by considering in the zone in which the photopeak should occur.

For this procedure, a gamma sensitivity spectrum is derived from the experimental gamma-ray spectrum by means of a mathematical treatment which is based on the statistical

laws. This is done as; taking a detection limit for each spectrometer channel, the whole set of detection limits constitute the sensitivity spectrum. This spectrum is one in which the channel contents represent the minimum detectable activity of an isotope having a peak centered on the channel. The principles on which the derivation of the gamma sensitivity spectrum is based differ according to the configuration of the part of the spectrum which is considered. A typical gamma spectrum obtained with a NaI(Tl) scintillation detector is given in the figure (3.5).

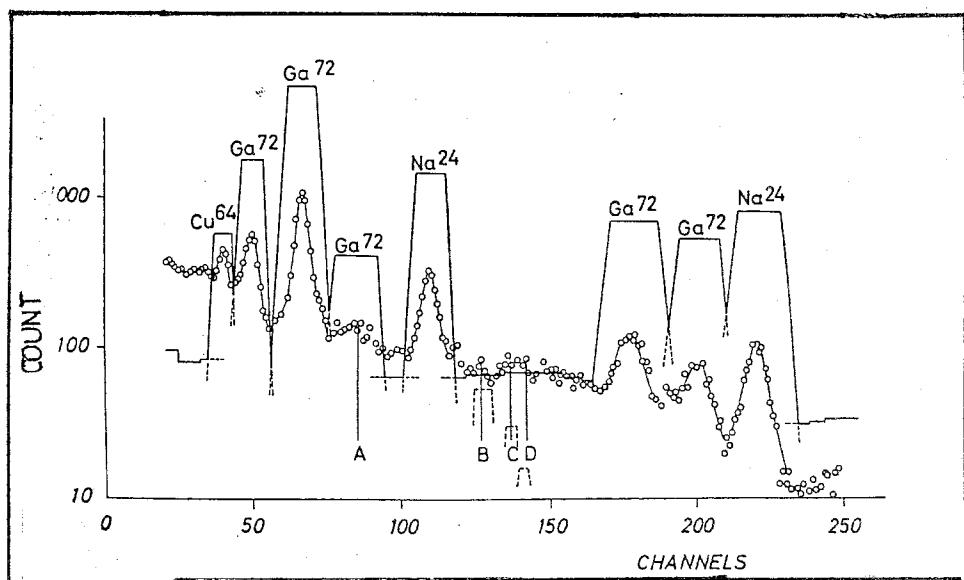


Fig. 3.5. Derivation of the sensitivity spectrum from an original one. [Pa-66].

(The detection limits corresponding to the spectrum are seen in the above figure. The part of the curve corresponding to the photopeaks have a form which retains the aspect of the original peak, but the top is flattened. Between these peaks the region corresponding to the background shows a detection limit which varies rather smoothly as a function of the channel number).

As seen, it consists of rather smoothly varying continuous distribution on which several gamma peaks of different radioisotopes are superimposed. For the regions of the spectrum which are far from the visible photopeaks, and where the difference in the counting rates of different isotopes, for adjacent channels is small, the detection limit is calculated from the counting statistics.

In the zone where the counting rates vary smoothly between successive channels, the minimum detectable activity is obtained by considering the activity in the spectrum to be a background and calculating an upper limit of the statistical fluctuations as given below:

If  $v_1$  is the counting rate of the background, it is given by [Se-64, Di-57, Se-59],

$$v_1 = \frac{n_1}{t_1} \pm \frac{n_1^{1/2}}{t_1} \quad (3.15)$$

Similarly, for the observed effect, , it is given as,

$$v = \frac{n}{t} \pm \frac{n^{1/2}}{t} \quad (3.16)$$

where, n and  $n_1$  represent counts; t and  $t_1$  represent counting times. The expressions following the ± sign are always standard deviations.

For the net activity the below equation is given,

$$\text{Net activity} = v - v_1 \quad (3.17)$$

Since the minimum detectable activity is obtained by taking the activity to be background due to this method described above, it can be  $v_1 = v - v_1 \Rightarrow v = 2v_1$  Then using

the formula of propagation of errors,

$$\sigma(v) = \left[ \sigma^2(v_1) + \sigma^2(v) \right]^{1/2}, \text{ one obtains the standard}$$

deviation of the measurement as,

$$\sigma(v) = \left[ \frac{n}{t^2} + 2 \frac{n_1}{t_1^2} \right]^{1/2} = \left[ \frac{v}{t} + 2 \frac{v_1}{t_1} \right]^{1/2} \quad (3.18)$$

Assuming the counting times  $t$  and  $t_1$  are the same, and considering a confidence level required for the problem,  $\sigma(v)$  is given by, [Pa-66]

$$\sigma(v) = k \left[ \frac{2v_1 + v}{t} \right]^{1/2} \quad (3.19)$$

where the constant  $k$  can be taken as 2 corresponding to a confidence level of 95% [Pa-66, Gu-74]

The minimum detectable effect is then derived from this equation by assuming equal to its standard deviations, which finally gives,

$$v = \left( \frac{1}{2} k^2 / t \right) \left[ 1 + (1 + 8tv_1/k^2)^{1/2} \right] \quad (3.20)$$

From the curve representing the gamma detection limits, in fig. 3.5, and from the value given by equation (3.20), the minimum detectable weights of the elements are calculated. First, from fig. 3.5, it is easy to derive the minimum detectable absolute activity by dividing by the efficiency of the counter. By means of these limits, the minimum detectable weights for each element are then derived by comparing the results to the specific activity which is calculated from the given experimental conditions. Since an element can give several radioisotopes upon irradiation, e.g.  $^{72}\text{Ga}$ , a certain

number of different values are obtained for the minimum detectable weight of the element. Among these values, the smallest one is selected for that element.

### 3.4. MODIFICATION OF THE CODE

As mentioned in the previous subchapter 3.1, the computer code examined in this thesis was prepared originally by using an IBM 370/165 computer with fortran IV level G and assembly languages of the computer used, at the Scientific Information Processing Center, Ispra-Italy. It was then adopted for use with the UNIVAC-1106 at BU. However, since a Calcomp plotting unit was not available in BU and the assembly language depends on the computer used, it was impossible to modify it in the original form to UNIVAC-1106. Therefore, all the plotting subroutines (assembler) which were given as two files, were deleted from the source program. The remaining part of the code which still consists of a main part and thirteen subroutines, was run by using the UNIVAC-1106. This listing is given in the appendix I.

The modified form of the code then was recorded on a new tape for further studies by BU-NE Department.

Some examples of the updating programs(\*) used during the procedure mentioned above, are given as follows:

The first program is used to read the original tape and the second is used to record the content of that tape to the main storage of a UNIVAC-1106 computer used in BU. First,

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(\*) These updating programs are prepared according to EXEC level 36R2 (1978) manual, [EXEC-78], SPERRY UNIVAC, Series 1100, Executive System, Vol.2.

main program and input data were recorded on the same file, and they were then loaded separately into three different files; one being the program file, second being the input data for sample problem, and the third one as spectra for sample problem. To rerun the main program by adding these data files, many corrections were necessary. Programs 3,4,5 and 6 given in the following pages, represent some examples for updating procedure. Program 6 is also used for the rerun of the main program. Finally, program 7 is used for recording all these processes and output data on a new tape and program 8 is for getting a listing of that tape.

Program 1 Reads the tape

/ RUN,  
/ ASG, TJ T., 6C9, D80218  
/ COB, ISE

IDENTIFICATION DIVISION.

PROGRAM-ID. TEYP-OKUMA.

ENVIRONMENT DIVISION.

CONFIGURATION SECTION.

SOURCE-COMPUTER. U-1106.

OBJECT-COMPUTER. U-1106.

INPUT-OUTPUT SECTION.

FILE-CONTROL.

SELECT T ASSIGN TO UNISERVO T.

DATA DIVISION.

FILE SECTION.

F D T

LABEL RECORDS OMITTED

RECORDING MODE IS F.

O 1 T-REC PIC X (80).

PROCEDURE DIVISION.

AC. OPEN INPUT T WITH NO REWIND.

OPEN OUTPUT F.

OKU. READ T AT END GO TO SON.

DISPLAY T-REC UPON PRINTER.

GO TO OKU.

SON. CLOSE T WITH NO REWIND.

STOP RUN.

/ MAP, IN  
/ XQT  
/ FIN

Program 2      Records the tape on the mass-storage

@RUN,  
@ASG, TJ T., 6C9, D80218  
@DELETE, C GAMMA.  
@ASG, UP GAMMA.  
@USE F., GAMMA.  
@COB, ISE

IDENTIFICATION DIVISION.  
PROGRAM-ID. TEYP-OKUMA.  
ENVIRONMENT DIVISION.  
CONFIGURATION SECTION.  
SOURCE-COMPUTER. U-1106.  
OBJECT-COMPUTER. U-1106.  
INPUT-OUTPUT SECTION.

FILE-CONTROL.  
SELECT T ASSIGN TO UNISERVO T.  
SELECT F ASSIGN TO MASS-STORAGE F.

DATA DIVISION.  
FILE SECTION.

FD T  
LABEL RECORDS OMITTED  
RECORDING MODE IS F.

01 T-REC PIC X(80).

FD F  
RECORDING MODE IS SDF.

01 F-REC PIC X(80).

PROCEDURE DIVISION.  
AC. OPEN INPUT T WITH NO REWIND.

OPEN OUTPUT F.

OKU. READ T AT END GO TO SON.

MOVE T-REC TO F-REC.

WRITE F-REC

GO TO OKU.

SON. CLOSE T WITH NO REWIND.

CLOSE F.

STOP RUN.

a MAP, IN  
a XQT  
a DATA, L SAGLAM.  
a FIN

Program 3 Updating of main program

a RUN,  
a ASG, UP DATA1.  
a ASG, A SAGLAM.  
a COPY SAGLAM., DATA1.  
a ASG, A GAMMA.  
a FTN, US GAMMA. MAIN  
-183,183  
-184  
IF (NPK.LE.1) GO TO 333  
a PREP GAMMA.  
a MAP, I GAMMA.MAIN  
IN GAMMA. MAIN  
LIB GAMMA.  
a XQT GAMMA. MAIN  
a ADD DATA 1.  
a FIN

Program 4      Updating of the data file

```
@RUN,  
@ASG,A     DATA 1.  
@ASG,UP    DATA 1 (+1).  
@DATA,L    DATA 1., DATA (+1).  
-10,10  
     21  
@END  
@FIN
```

Program 5      Evaluation of a new program and updating of it

```
@RUN,  
@ASG,A    GAMMA.  
@ASG,A    DATA 1.  
@ASG,A    DATA 2.  
@USE II, DATA 2.  
@ASG,UP   SPECTRA., F //1000 , UD105  
@COPY     GAMMA., SPECTRA.  
@DELETE, SR   .SPET  
@DELETE, SR   .FIGURE  
@FTN,S     .KAL  
@FTN,S     .SMOOS
```

•            •  
•            •  
•            •

```
a MAP,I SPECTRA.MAIN  
IN SPECTRA.MAIN  
LIB SPECTRA.  
a XQT SPECTRA.MAIN  
a ADD DATA 1.  
a ADD DATA 2.  
a FIN
```

Program 6 Rerun of the main program with data

```
a RUN,  
a ASG,A SPECTRA.  
a ASG,A TKR.  
a USE 11, TKR.  
a ASG,A INPUTX.  
a ASG,UP INPUTX(+1).  
a DATA,L INPUTX., INPUTX(+1).  
-10,10
```

22

SCX 1119.0 3.12 5.675E-06 3.900E+00

```
a END  
a XQT SPECTRA. MAIN  
a ADD TKR.  
a ADD INPUTX.  
a FIN
```

Program 7      Records to a new tape from the mass-storage

@RUN,  
@ASG,A    SPECTRA.  
@ASG,T    T.,16N,SAGLAM  
@MOVE    T.,1  
@COPY,GM    SPECTRA.,T.  
@FIN

Program 8      Taking the listing of the tape

@RUN,  
@ASG,T    T.,16N,SAGLAM  
@UNIVAC\*TTOC.TTOC T.  
@FIN

#### 4. COMPARISON OF GRETEL WITH ANOTHER CODE, CORGAM

The importance and use of digital computers in NAA was mentioned in the previous subchapters. It was also mentioned that there are many computer codes dealing with this problem. Each of these codes have their own techniques in analysing, in unfolding complex gamma-ray spectra. Some of them study the estimating of intensity coefficients, as Corgam. There are many methods for estimating these coefficients. These methods are stripping, least squares, iterative methods, vector analysis and stepwise regression [Ec-68, Le-65].

One of these codes mentioned above, prepared by NEA-CPL in the experimental data processing field is Corgam. Corgam was studied before as a subject of another thesis introduced at NE Department. Since these two codes, Corgam and Gretel, deal with NAA, but their logics for the approaching to the problems are quite different from each other, a short comparison of these two computer codes will be given in this chapter. Therefore first, Corgam will be introduced in a summary form in the following subchapter.

##### 4.1. INTRODUCTION OF CORGAM

Corgam, a correlation algorithm for gamma-ray spectra, allows the reference gamma-ray spectra to be correlated with a complex gamma-ray spectrum [Ec-69]. This correlation algorithm is based on a least squares procedure which is a logical method for determining the intensity coefficients for NAA.

The analysis used by Corgam is described as the least squares procedure for fitting a dependent variable, e.g., a complex spectrum, to a set of independent variables, e.g., a set of reference spectra.

Corgam sets up a mathematical model in order to make an analysis by using least squares procedure. The formulation of Corgam can be summarized as follows:

The gamma-ray spectrum of a complex sample containing several isotopes ( $m$  in number) may be represented by [Ec-69],

$$Y_i = \sum_{j=1}^m B_{ij} \quad i = 1, 2, \dots, n \quad (4.1)$$

where,

$Y_i$  = the counts registered in channel  $i$  of a multi-channel analyzer.

$B_{ij}$  = the counts registered in channel  $i$  from the  $j^{\text{th}}$  constituent isotope.

The reference gamma-ray spectra of each of the  $m$  constituent isotopes are related to the complex gamma-ray spectrum by,

$$Y_i = \sum_{j=1}^m X_{ij} B_j + e_i \quad i = 1, 2, \dots, m \quad (4.2)$$

where,

$X_{ij}$  = the intensity coefficient for isotope,  $j$ , i.e., a coefficient proportional to the quantity of isotope  $j$  in the complex sample.

$x_{ij}$  = the counts registered in channel i from the  $j^{\text{th}}$  isotope of known quantity.

$e_i$  = the deviation at point i of the estimated value of  $Y_i$ ,  $\sum x_{ij} B_j$ , from the observed value  $Y_i$ .

There are some difficulties in applying least squares technique to the unfolding of gamma-ray spectra. One of them is that some calculated intensity coefficients may have negative sign. For physical reasons, they must be non-negative. Besides, the least squares method may yield positive intensity coefficients for all reference spectra, but some of these may not be significant according to the tests applied. The problem is to determine which reference spectra are not significant.

In order to overcome these difficulties, some statistical tests are applied such as t value for the null hypothesis which is calculated for each intensity coefficient. These values are used in the correlation algorithm to eliminate those reference spectra for which the calculated intensity coefficients are negative or non-significant.

As a summary, it can be stated that Corgam,

- a) compensates for electronic instabilities in the multichannel analyzer,
- b) corrects for the background, subtracts it from the complex spectrum,
- c) normalizes the data to a fixed neutron flux level,
- d) represents a mathematical model in matrix form for reference spectra and allows a choice of weighting factors,
- e) allows a choice of methods for the calculation of standard deviations.

- f) it corrects for decay time,
- g) may also consider time dependent spectra for those isotopes which have isomers.

Finally, Corgam is a novel method of unfolding complex gamma-ray spectra because the variance calculations include contributions from both the complex and reference spectra. Also, only reference spectra that have intensity coefficients which are significant at a preselected level are retained in the output.

#### 4.2. COMPARISON OF THE TWO CODES

As mentioned in the previous chapters, Gretel and Corgam are two computer programs prepared for NAA problems. However, their mathematical approach to these problems are quite different. One of the reasons for these differences is that they are prepared to analyze data from different kinds of detectors; Gretel uses data from a Ge(Li) detector, Corgam from a NaI(Tl) scintillator. Therefore, their data handling procedures are different from each other. Besides that, many authors apply their own techniques to unfold gamma-ray spectra. For the comparison of these two codes, this sub-chapter gives the main specifications in the following form:

CORGAM is a computer code of unfolding complex gamma-ray spectra by using reference spectra. In the analysis, intensity coefficients of the isotope spectra which are significant at a preselected level are retained in the output and the variance calculations include contributions both from the reference and the complex spectra [Bö-82, Ec-69]. Its specifications can be given in a brief form as follows:

1. Corgam is based on estimating the intensity coefficient. It uses the least squares procedure for fitting a dependent variable, i.e., a complex spectrum, to a set of independent variables, i.e., a set of reference spectra [Ec-68].

2. Corgam sets up a mathematical model and by using the least squares procedure, correlates the reference gamma-ray spectra with a complex one.

Example: The program multiplies any spectrum of a reference isotope with a coefficient and similarly other spectra with other coefficients. These coefficients are defined as intensity coefficients. Then, adding the contents of these spectra channel by channel, a third spectrum is obtained. Subtracting the complex spectrum due to an unknown sample from this third one, their difference is obtained. By using the least squares procedure the program tries to calculate these coefficients for the minimization of that difference. Those intensity coefficients are proportional to the quantity of isotope in the complex spectrum. Finally, the quantity of the isotope in the complex can be given in terms of ppm.

3. The reference spectra and the complex one required for Corgam are collected for the fixed counting time, using the scintillation detectors.

4. Before the analysis of the spectra, Corgam compensates for electronic instabilities in the spectrometer system used, because these instabilities can cause shifts in these spectra. To compensate for these inconsistencies, the gamma ray photopeaks of the spectra are fit to a Gaussian function using the least squares method.

5- Corgam corrects for the background and decay times. It normalizes the data to a fixed neutron flux level.

6- Corgam in the standard form is restricted to a problem of 400 channels and 15 reference spectra.

7- Corgam requires less than 1 minute of execution time with the restrictions mentioned above, on the computer IBM 360/50.

8- Corgam also considers time dependent spectra for those isotopes which have isomers.

9- The program was recorded originally for IBM 360/50 using fortran IV level G. It was then updated by Bögrün, [Bö-82], for UNIVAC-1106. The updated form of the code was recorded on to a magnetic tape for further use in BU-NE department.

10- An intermediate disk storage is required for Corgam. The source deck contains 1303 cards.

GRETEL is a computer program which is set up for routine batchwise processing of spectrometric data [Gu-74]. The characteristics of Gretel can be given as follows:

1- Gretel performs the quantitative analysis of gamma-ray spectra using special oriented libraries which are prepared for each particular problem.

2- The gamma-ray spectra needed for Gretel, are obtained by Ge(Li) detectors.

3- For the analysis of the spectra, a preliminary data handling procedure required was discussed in detail in the

chapter 3. As a summary, this procedure can be given as:  
First, smoothing of the spectra is done. Then, the peak locations are searched by using some tests to avoid the statistical fluctuations being kept as analytical peaks. Computation of the peak areas is the third step of the program. Two different methods are used for that purpose. Since Gretel examines any spectrum peak by peak, for the visible peaks a method derived by Yule, [Yu-69], and for hidden peaks new detection limits are determined.

4- In Gretel, compton continuum at the fixed level is subtracted from the computed areas of the photopeaks. Also, decay time corrections are made.

5- The restrictions for Gretel in the standard form, are given as; 50 elements as the maximum number for the oriented library which corresponds the reference isotopes in Corgam, and 4096 channels as the maximum number of the spectrometer used.

6- For a typical analysis, on the average, of 30 spectra of 2048 channels (a calibration spectrum plus 29 unknowns) with a library of 30 elements the running time is about 30 seconds.

7- The memory requirements are not much for Gretel.

8- Gretel was recorded originally for IBM 370/165 using fortran IV level G. The code was then updated by the author for UNIVAC-1106, by deleting all the plotting subroutines since there was not available a Univac plotting unit. The modified form of the code is recorded on a new magnetic tape for further studies by BU-NE department.

As a result of these specifications and others given in 4.1, one can conclude that Corgam is a more comprehensive program prepared for the activation analysis by using a NaI(Tl) scintillation detector and a small channel region in the spectrometer used. On the other hand, Gretel is one of first ones prepared for NAA problems by using a Ge(Li) detector which has a better energy resolution than a scintillator. The program also gives analog outputs with a Calcomp unit and it performs the quantitative analysis.

## 5. DISCUSSION AND CONCLUSIONS

The basic principles, the use and importance of neutron activation analysis, NAA, was discussed in the previous subchapters. It was also mentioned that the determination of the microconstituents of an unknown sample was possible down to the ppm (parts per million) level or even to the ppb (parts per billion) level. As also discussed in the previous chapter, determination of a large number of elements in one sample and the treatment of the comparison samples are very troublesome and time consuming. Therefore, instrumental activation analysis has been improved as one of the major techniques for the control and measurement of the trace element distribution in a large number of samples. The speed of this technique is based to a large extent on the availability of nuclear reactors with a high and reliable neutron flux. It also depends on the development of the high resolution gamma-ray spectrometers with the computer hardware and software. The computer programs for NAA problems are usually prepared for the spectra obtained especially by two types of detectors, such as NaI(Tl) scintillators and Li drifted Ge or Si semiconductors. Recently, semiconductor detectors with excellent energy resolution pushed the number of energy channels required for an adequate spectral response up into the thousands.

As an example, a computer code for NAA based on a GE(Li) spectra was studied in this thesis as a part of it. The program which is set up for routine batchwise processing of spectrometric data, was first prepared in 1966 as one of

the earliest codes developed for Ge(Li) spectra. This program has then been revised and rewritten to follow the continuous development of the analytical instrumentation, such as multi-channel analyzer, calcomp unit of the computer used, etc. The new program, called Gretel, performs the quantitative analysis of gamma-ray spectra obtained by a Ge(Li) detector which has a better energy resolution than a scintillator. The data-reduction system required for Ge(Li) spectra is used in Gretel. This system involves the smoothing of the spectra, differentiation of these data, the determination of peak locations and peak boundaries, the computation of peak areas and the associated errors. The program gives the results in terms of ppm in the form of digital lists. In addition, with some modifications in the main program, analog outputs can also be obtained by means of a Calcomp unit if it is available. Also, Gretel performs the search of the small peaks not detected over the background and gives the minimum detectable activity.

However, one can not conclude that Gretel is an integral program. Because the program fails in the identification of isotopes when there are interferences coming from different isotopes, e.g., Sc and Zn. To avoid this problem, the preparation of the libraries for each kind of problem, which is a responsibility of the analyst, is very important. Some suggestions can be made to correct this shortcoming. First, for the preparation of any library, "analytical peaks" should be chosen. These peaks are those given the best sensitivity and the highest chance of being free from interference within a range of energy which depends on the resolution of the detector. Second, when there are interfering isotopes, some modifications can be applied to the main program such as control peaks. Introducing other peaks due to interfering isotopes, one can check whether these isotopes are present or not. Third, the energy range in which the interfering peaks are

searched could be restricted considerably by using a pre-amplifier with a high resolution power. Fourth, since the single Ge(Li) measurements are not adequate so the coincidence measurements may be offered for analysis of gamma-ray spectra free of interference. However, coincidence technique is not much successful for Ge(Li) detectors because the reduced detector efficiency seems to be a serious obstacle.

The other program, Corgam, described briefly in the Chapter 4 to make a comparison, examines the spectra obtained by a NaI(Tl) scintillation detector. As mentioned in the above subchapters, Corgam has a more comprehensive mathematical model; so it can be stated that it is one of the better programs for the resolution of gamma-ray spectra with the correlation algorithm. Besides, the program can be applied to other kinds of analysis problems, such as the analysis of a spectrum in the ultraviolet light region, etc. On the other hand, Corgam is restricted to a problem of 400 channels and 15 reference spectra due to the level of accuracy desired. Also, the computer memory requirements are large for the correlation algorithm.

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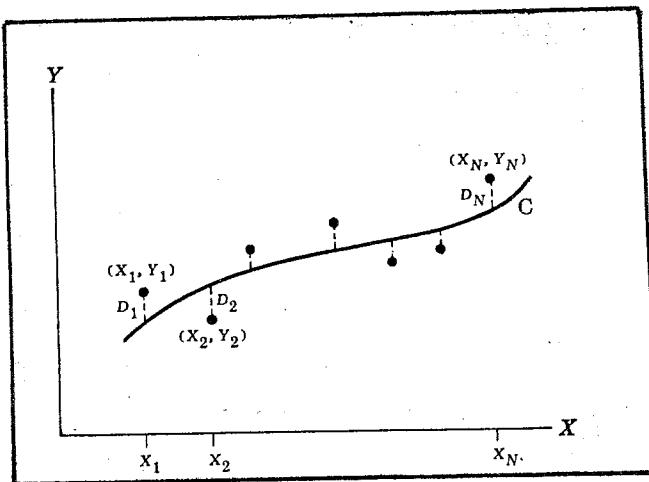
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## APPENDIX A THE METHOD OF LEAST SQUARES

A measure of the fit for the curve C given in the figure, to the given data is provided by the quantities  $D_1^2 + D_2^2 + \dots + D_N^2$ . Those D's are denoted as deviations or errors.



If D's are small, it is said that the fit is good, if they're large, the fit is bad.

Of all the curves approximating a given set of data points, the curve having the property that  $D_1^2 + D_2^2 + \dots + D_N^2$  is a minimum is called a best fitting curve in the sense of least squares. It is also called a least square curve. Thus a line having this property is called a least square line; a parabola with this property is called a least square parabola, etc. [Mu-61].

The least square line: The least square line approximating the set of points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  has the equation, [Ec-68],

$$y_i = A + Bx_i + e_i \quad i = 1, 2, \dots, n \quad (1)$$

where  $e_i$  is the deviation at point  $i$  of the estimated value, from its observed value  $y_i$ ,  $A$  and  $B$  are the true values of the intercept and slope respectively. The estimators  $a$  and  $b$  for  $A$  and  $B$ , can be obtained by minimizing the sum of squared errors. If each data point has a different, statistical accuracy, then each residual is multiplied by a proper weight,  $w_i$ . Therefore the sum of squared errors is given by, [Ec-68, So-41],

$$S = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n [y_i - (A+Bx_i)]^2 w_i \quad (2)$$

For this problem  $w_i$  are equal to 1. Then,

$$S = \sum_{i=1}^n [y_i - (A+Bx_i)]^2 \quad (3)$$

$S$  is minimized by differentiating with respect to  $A$  and  $B$ , and equating the results to zero. Then  $a$  and  $b$  the estimators are substituted for  $A$  and  $B$ . The resulting equations are,

$$\sum_{i=1}^n [y_i - (a+bx_i)] = 0 \quad (4)$$

$$\sum_{i=1}^n \{x_i [y_i - (a+bx_i)]\} = 0 \quad (5)$$

Equations (4) and (5) are rearranged into a form called the normal equations [Mu-61],

$$a n + b \sum_{i=1}^n x_i = \sum_{i=1}^n y_i \quad (6)$$

$$a \sum_{i=1}^n x_i + b \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i \quad (7)$$

Solution of these equations for a and b, results in,

$$b = \frac{\sum_{i=1}^n x_i y_i - ((\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i))/n}{\sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2/n} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (8)$$

$$a = \bar{y} - b\bar{x} \quad (9)$$

where

$$\bar{y} = (\sum_{i=1}^n y_i)/n \quad \text{and,} \quad (10)$$

$$\bar{x} = (\sum_{i=1}^n x_i)/n \quad (11)$$

Then, equation (1) can also be rewritten in terms of the estimators b and mean value  $\bar{x}$ ,  $\bar{y}$  through the use of equation (9) as,

$$y_i = \bar{y} + b(x_i + \bar{x}) \quad (12)$$

## APPENDIX B

### ISOTOPE BUILD-UP AND DECAY

Considering  $N_1$ , the number of parent and  $N_2$ , the number of daughter nucleus as functions of decay constants and time, it is possible to write the decay rate of the parent nuclei as,

$$\frac{dN_1}{dt} = -\lambda_1 N_1 \quad (1)$$

or

$$\frac{dN_1}{dt} = \lambda_1 N_{1,0} e^{-\lambda_1 t} \quad (2)$$

where,

$N_{1,0}$ : number of parent nuclei initially present

$\lambda_1$  : decay constant of parent

The analogous equation for the daughter nuclei is given by,

$$\frac{dN_2}{dt} = R_T - \lambda_2 N_2 \quad (3)$$

Since  $R_T$  represents the rate of formation of the daughter, it is also given as,

$$\frac{dN_2}{dt} = \lambda_1 N_{1,0} e^{-\lambda_1 t} - \lambda_2 N_2 \quad (47)$$

which is a 1<sup>st</sup> order linear differential equation.

For the solution of that equation, choosing  $y = N_2$ ,  $x = t$ ,  $P(x) = \lambda_2$  and the integrating factor as,

$$e^{\int P(x) dx} = e^{\int \lambda_2 dt} = e^{\lambda_2 t}$$

then, multiplying both sides of the original differential equation, eg.(4), with this factor, it is obtained as, [Wy-66]

$$e^{\lambda_2 t} \frac{dN_2}{dt} + e^{\lambda_2 t} \lambda_2 N_2 = \lambda_1 N_{1,0} e^{\lambda_2 t} e^{-\lambda_1 t}$$

where the sum of two terms on the left side are equal to the term  $\frac{d}{dt}(e^{\lambda_2 t} N_2)$ .

Then,

$$\frac{d}{dt}(N_2 e^{\lambda_2 t}) = \lambda_1 N_{1,0} e^{(\lambda_2 - \lambda_1)t}$$

Integrating both sides from  $t=0$  to  $t=t$  and rearranging it for  $N_2$ ,

$$N_2 = \frac{\lambda_1}{\lambda_2 - \lambda_1} N_{1,0} (e^{-\lambda_1 t} - e^{-\lambda_2 t}) + C e^{-\lambda_2 t} \quad (5)$$

If the amount of daughter is initially zero, i.e., at  $t = 0$ ,  $N_2 = N_{2,0} = 0$ , then the second term of the equation (5) at the right side which represents the decay of daughter vanishes.

Finally, one obtains

$$N_2 = \frac{\lambda_1}{\lambda_2 - \lambda_1} N_{1,0} (e^{-\lambda_1 t} - e^{-\lambda_2 t}) \quad (6)$$

## APPENDIX C

### SINGLE COMPARATOR METHOD

Neutron activation analysis usually consists of 5 steps, such as 1. irradiation, 2. purification, 3. measurement, 4. comparison, 5. verification [Ad-70].

For the first step, suitable amounts of the sample and standard are weighted and irradiated simultaneously for a predetermined time. The sample and standard sizes should be chosen so that the intensity of radiation emitted from the desired radioelement will be approximately the same in both sources. There are three methods for the analysis such as a) absolute method, b) comparator or relative method, c) single comparator method. Single comparator method is used in Gretel so it will be described briefly in the following:

The use of germanium-lithium drifted detectors allows the simultaneous determination of an important number of elements after a single irradiation. The classical comparator method requiring one comparator for each element to be determined hence becomes less appropriate for routine work. These operations are time-consuming and can also introduce sources of error. On the other hand, the absolute method which performs direct calculation of weights of the isotopes from an estimation of the activation formula, suffers from the inaccurate knowledge of several constants.

In the single comparator method, the known weights of the elements are irradiated together with a suitable flux monitor under specified conditions (A known weight of a reference element is taken as flux monitor). The unknown sample is then irradiated with a similar flux monitor which is used

as a single comparator for different elements [Gu-65]. This method is suitable especially for routine or automated determinations; mainly when dealing with isotopes with a very short half-life, when a large number of elements is determined or when standards and samples could not be irradiated together.

There is also a very similar method which utilizes elements present in known quantities in the matrix itself as internal standard (as in Gretel), with the advantage of correcting flux perturbations within the matrix.

Principle of the method can be summarized as follows:

The weight,  $w$ , of an irradiated element is related to the photopeak counting rate,  $A_p$ , of the radioisotope measured by the relation, [Gu-65],

$$w = \frac{A_p}{\phi S D} \frac{M}{\sigma N E a \delta} \quad (1)$$

where,

M: atomic weight of the irradiated element

$\delta$ : isotopic abundance of the target nuclide.

$\sigma$ : effective activation cross section for the neutron energy spectrum used

N: Avagadro's number

E: efficiency of the detector for the gamma ray measured

a: gamma-ray abundance in decay scheme

$\phi$ : neutron flux

S: saturation factor  $(1-e^{-\lambda T})$  depending on irradiation time  $T$  and decay constant  $\lambda$

D: decay factor  $(e^{-\lambda t})$ , where  $t$  is decay time

When the neutron flux is measured by irradiating a known weight of a reference element (neutron flux monitor) and measuring the induced radioactivity by gamma-ray spectrometry and using the other known quantities due to this element, the same relation holds:

$$\phi = \frac{Ap^*}{S^* D^* W^*} \frac{M^*}{\sigma^* \delta^* NE^* a^*} \quad (2)$$

where the asterisks refer to the neutron flux monitor which is also used as single comparator for the elements to be determined in a sample. By substituting  $\phi$  taken from eg.2 in eg.1 one obtains,

$$W = k \frac{Ap}{Ap^*} \frac{S^* D^*}{S D} W^* \quad (3)$$

where

$$k = \left( \frac{\sigma^* \delta^* NE^* a^*}{M^*} \right) / \left( \frac{\sigma \delta NE a}{M} \right) \quad (4)$$

## APPENDIX D

### CONVOLUTION METHOD

In much experimental work, the information may be obtained in the form of a two-column table of numbers, e.g. A vs. B. There are some methods for handling of this type of data [Sa-64].

One of the simplest ways to smooth fluctuating data is by a moving average. In this procedure, one takes a fixed number of points, adds their ordinates together, and divides by the number of points to obtain the average ordinate at the center abscissa of the group. Next, the point at one end of the group is dropped, the next point at the other end added, and the process is repeated.

Table (1) illustrates how the moving average might be obtained. According to this table, the set of numbers on the right are the data or ordinate values, those on the left, the abscissa information. The outlined block in the center may be considered to be a separate piece of paper on which a new set of abscissa numbers are written ranging from -2 through 0 to +2. The C's at the right represent the convoluting integers. For the moving average, each C is numerically equal to one. To perform a convolution of the ordinate numbers in the table of data with a set of convoluting integers  $C_i$ , each number in the block is multiplied by the corresponding number in the table of data, the resulting products are added and this sum is divided by five. The set of ones is the convoluting function and the number by which we divide, in this case 5, is the normalizing factor. To get the next point in the moving average, the center block is slid down one line and process repeated.

1800.0		705	Table 1. Convolution opera-
1799.8		712	tion.
1799.6		717	Abscissa
1799.4		718	point on the left, tabular
1799.2	$x_o$ -2	C <sub>-2</sub>	data on the right. Opera-
1799.0	$x_o$ -1	C <sub>-1</sub>	tion is the multiplication
1798.8	$x_o$	C <sub>0</sub>	of the data points by the
1798.6	$x_o$ +1	C <sub>1</sub>	corresponding C <sub>i</sub> , summa-
1798.4	$x_o$ +2	C <sub>2</sub>	tion of the products and
1798.2			division by a normalizer,
1798.0		736	resulting in a single
1797.8		741	convolute at point $x_o$ .
1797.6		746	
		750	

The concept of convolution can be generalized beyond a simple moving average. In the general case the C's represent any set of convoluting integers. There is an associated normalizing factor. The mathematical description of the process described above, is given as;

$$y_j = \frac{\sum_{i=-m}^{+m} c_i y_{j+i}}{N} \quad (1)$$

The index j represents the running index of the ordinate data in the original data table. For the moving average, each C<sub>i</sub> is equal to one and N is the number of convoluting integers. However, for many types of data, the set of all 1's which yields the average, is not particularly useful. For example, on going through a sharp peak, the average would tend to degrade the end of the peak. There are different types of smoothing functions. Figure (1) illustrates these functions.

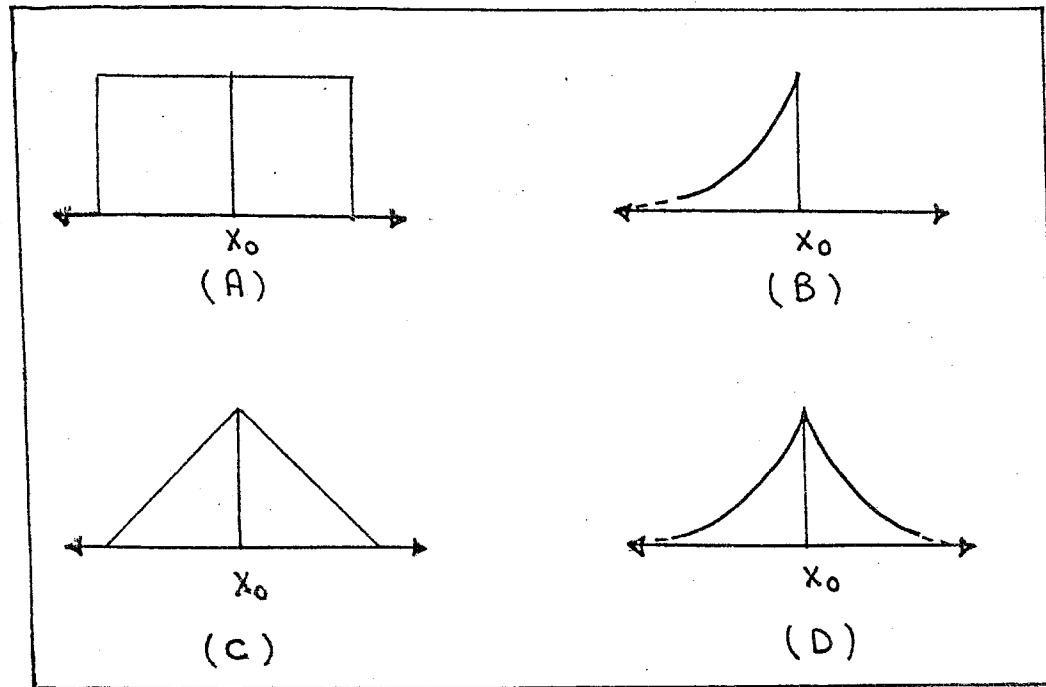


Fig.1- Various convolute functions

A. Moving average. B. Exponential function. C. Symmetrical triangular function. D. Symmetrical exponential function.

The function in the figure 1.B is an exponential set which simulates the exponential law. The usual spectrum from a spectrophotometer is the resultant of two convolutions of the actual spectrum of the material; first with a function representing the slit function of the instrument which is given in the figure 1.C, and then this first convolute spectrum is further convoluted with a function representing the time constant of the instrument.

## APPENDIX E

### LISTING OF COMMON VARIABLES USED IN GRETEL

The common variables used in Gretel can be given in the following form:

ELI	: Symbol of the radioelement in calibration library
ENI	: Energy of this isotope in keV
ICAN	: Channel in which the calibration peak falls
INT	: Interval for the search of the calibration peak (in channels)
ELEM	: Symbol of the radioelement in oriented library
EN	: Energy of this isotope in keV
FWT	: Full width at half maximum in keV (oriented lib.)
XLAM	: Decay constant of the radiosotope in minutes (oriented lib.)
AA	: Specific activity (oriented lib.)
COUNT	: Counts in each channel
SPSM	: The smoothed values in each channel
DER	: Differentiated values of the contents in each channel
ISTAR	: First channel of the spectrum
IEND	: Last channel of the spectrum
INDEX	: Index indicating the kind of the peak found
JMAX	: Number of peaks found by PKF
FMEDIO	: Average value of the geometrical correction factor
AREA	: Area of the photopeak calculated by SURF
ERR	: Error calculated during the evaluation of peak areas
FWHM	: Full width at half maximum
LS	: Left limit of the peak found
CENTR	: Center of the peak found by PKF

LD : Right limit of the peak found  
PMOL : Molecular weight of the element given in the oriented library  
DECAY : Decay constant of the radioisotope (calibration lib.)  
VALA : Specific activity for a  $\mu$ gram sample irradiated in a thermal flux of  $10^{13}$  neutrons/cm $^2$ sec (calib.lib.)  
PESO : Weight of the element in grams (calib. lib.)  
TDEC1 : Decay times of radioisotopes calculated by TDEC  
TIRR : Irradiation duration in minutes  
TCON : Counting duration in minutes  
ALFA : Slope of the calibration line  
BETA : Intercept of the calibration line  
FLUX : Neutron flux during irradiation  
WEIGHT : Weight of the sample in grams  
STAND(6,K):Area zero/microgram of the element  
NELST : Number of standards in standard library  
IREL : A switch indicating the way which is followed by the program  
NIRR : Irradiation number  
MO : The beginning of the measurement being year, month, day, hour and minute  
ANOME : The name of the problem involved  
ASAMPL : Identification of the sample  
EL4 : Symbol of the radioisotope found by FIRST for the calibration line  
CKK : Center of the peak found by FIRST  
VKK : Energy of the peak found by FIRST  
VMAX : Counts due to the peak found by FIRST  
NPK : Number of the peaks in the calibration lib.  
EL3 : Symbol of the radioisotope found by SENSIT  
VS : Counts due to that peak  
P2 : Energy of that peak in keV  
CS : Center of that peak

VS2 : Right limit of that peak  
VD2 : Left limit of that peak  
CLS2 : Channel contents at the right limit of the peak  
CLD2 : Channel contents at the left limit of the peak  
ISENS : Number of peaks found by SENSIT  
EL2 : Symbol of the radioisotope found by PKF  
VC : Counts due to the single peak found by PKF  
PI : Energy of that peak in keV  
VS1 : Right limit of that peak  
VD1 : Left limit of that peak  
CC : Center of that peak  
CLSI : Channel contents at the right limit of that peak  
CLDI : Channel contents at the left limit of that peak  
IPICK : Number of single peaks found by PKF  
FDEC : Decay factor calculated as  $e^{\lambda t_{dec}}$  by ANALYS  
FSAT : Saturation factor calculated as  $(1-e^{\lambda t_{irr}})$  by ANALYS  
DENS : Density of the sample  
EL2D : Symbol of the radioisotope found by PKF  
VCD : Counts due to double peaks found by PKF  
PID : Energy of the doublet in keV  
CCD : Center of one of the doublet  
VID : Left limit of that peak (or right limit according to peak)  
CLID : Channel contents at the limit of that peak  
IPCD : Number of doublet  
EL2REL : Symbol of the radioisotope found by PKF when there is a standard library  
EL3REL : Symbol of the radioisotope found by SENSIT when there is a standard library  
EL2RDRE: Symbol of the radioisotope which gives a doublet when there is a standard library

## APPENDIX F

### LISTING OF THE INPUT DATA AND INPUT OPTIONS

Input for Gretel consists of:

i) IME: One card for the computation of decay times (in minutes) of the radioisotopes after irradiation in the reactor. (It indicates the days in each month of the year)

FORMAT (12I6)

ii) LIBST: One card indicating the number of peaks of the calibration library.

FORMAT (I6)

iii) One card for each gamma peak of the calibration library. This card contains:

ELI	:	Symbol of the radioelement
ENI	:	Energy in keV
ICAN	:	Channel in which the calibration peak falls
INT	:	Interval for the search of the calibration peak (in channels)
DECAY	:	Decay constant of the isotope to which the peak belongs ( $\lambda = 0.693/T_{1/2}$ in minutes)
VALA	:	Specific activity for a g sample irradiated in a thermal flux of $10^{13}$ neutrons/cm <sup>2</sup> sec
PESO	:	Weight of the element in grams

where the formats are given as,

FORMAT (A6, F7.2, 2I4, 2E10.4, F12.8)

iv) NLIB: One card indicating the number of peaks of the "oriented analytical library".

FORMAT (I6)

v) One card for each gamma peak of the above mentioned library.

This card contains:

ELEM : Symbol of the radioelement of the oriented library  
EN : Energy in keV  
FWT : Full width at half maximum in keV  
XLAM : Decay constant of the radioisotope in minutes  
AA : Specific activity  
PMOL : Molecular weight of the element

Where the format is given as,

FORMAT (A8, 2F10.3, 2E10.4, F10.5)

vi) One card giving irradiation and problem characteristics:

FLUX : Neutron flux during irradiation in neutrons/  
cm<sup>2</sup> sec  
TIRR : Irradiation duration in minutes  
IO : End of the irradiation stating its year, month  
day, hour and minute  
NIRR : Irradiation number  
ANOME : The name of the problem involved  
DENS : Density of the sample, to compute atoms/cm<sup>3</sup>  
for each element

Put 1 if not requested.

FORMAT (E10.4, F10.3, 5I4, I5, 5A4, F7.3)

vii) One card with a set of figures and switches allowing the program to flow in different ways:

NSPT : Number of spectra to elaborate  
NCH : Number of channels for each spectrum. In the case in which a partial data-out has been performed,  
  
NCH = 2048  
  
NSMO : Number of points to be used for the smoothing of the spectra  
NSMO = 5 five point smoothing  
NSMO = 7 seven point smoothing  
NSMO = 9 nine point smoothing  
  
IPDO : Indicates if a partial data-out has been used:  
IPDO = 0 the whole spectrum has been punched  
IPDO = 1 partial data-out  
  
IASCI : Indicates the perforation code used:  
IASCI = 1 IBM code  
IASCI = 2 ASCII code  
IASCI = 3 ASCII code, no parity

where the format is given as,

FORMAT (6I6)

viii) In the case of partial data-out (IPDO = 1) one card for each measurement, containing:

MO : year, month, day, hour and minute of the beginning of the measurement  
ASAMPL : identification of the sample  
WEIGHT : weight of the sample in grams  
TCON : counting duration in minutes  
ISTAR : first channel of the partial spectrum  
IEND : last channel

ITR : switch indicating whether to elaborate the spectrum or not

ITR = 1 elaboration

ITR = 0 no elaboration

IS : switch indicating whether the area of the peaks must be computed with the original spectrum or with the smoothed one

IS = 0 original spectrum

IS = 1 smoothed spectrum

Where the format is given as,

FORMAT (5I4, 3A4, F10.6, F10.3, 2I5, 3I2)

ix) According to the values of IASCI, one of the following cards is read for each measurement:

a) IASCI = 1 or 2; the card contains:

MO, ASAMPL, WEIGHT, ITR, IS

FORMAT (5I4, 3A4, F10.6, f0X, 2I2)

b) IASCI = 3; the card contains:

MO, ASAMPL, WEIGHT, TCON, ITR, IS

FORMAT (5I4, 3A4, F10.6, F10.3, 10X, 2I2)

## APPENDIX G

### DESCRIPTION OF GRETEL

Gretel, as mentioned in the chapter 3.1, performs the quantitative analysis of gamma-ray spectra obtained by Ge(Li) detectors. The program is composed of a MAIN part which controls the various subroutines and allows the reading of the input data and library from punched cards, a number of subroutines and three functions.

As also mentioned in the same subchapter and in the 3.4, some modifications due to elimination of some subroutines belong to plotting procedure were required on original Gretel in order to adopt it to UNIVAC 1106. After having eliminated these routines, the program reran. These thirteen subprograms called by the main program are given in the following pages in detail.

The gamma-ray spectra of up to 4096 channels obtained by the multichannel analyzer, are first punched on paper tapes and read by one of the routines, TAPE, TAPEAS or TAPEGA, according to the punching code adopted, such as IBM, ASCII or ASCII with no parity. The routines transform the data in a suitable format, either by the function CONV or CONVB.

The routines used in Gretel, except the five mentioned above, are listed in the order called:

- 1- Function TDEC
- 2- Subroutine SMOOS
- 3- Subroutine DERIV
- 4- Subroutine FIRST
- 5- Subroutine KAL

- 6- Subroutine ANALYS
- 7- Subroutine PKF
- 8- Subroutine SURF
- 9- Subroutine SURF2
- 10- Subroutine SENSIT
- 11- Subroutine PRINT

The following is the description listing of the main and subprograms called by the main part. These descriptions are given with their options.

#### MAIN PROGRAM

The main part of the program reads the data of the calibration source, the oriented or standard libraries and some other input parameters, such as weight of samples and neutron flux. It also controls the various subroutines and functions.

It contains a number of common statements at the beginning of the program. These are described in the appendix E.

#### 1. Function TDEC

```
FUNCTION TDEC (MO, IO, IME)
DIMENSION MO(5), IO(5), IME(12)
```

Where MO, IO and IME are defined in the appendix F. MO and IO are in terms of year, month, day, hour and minute so they are given as MO(5), IO(5).

This function calculates the decay times of isotopes in minutes.

## 2. Subroutine SMOOS

SUBROUTINE SMOOS (NSMO)

NSMO : number of points to be used for the smoothing  
of the spectra

NSMO = 5 five point smoothing

NSMO = 7 seven point smoothing

NSMO = 9 nine point smoothing

This routine performs the smoothing of the spectra on five, seven or nine points in order to reduce the influence of the statistical fluctuations.

## 3. Subroutine DERIV

SUBROUTINE DERIV (NSMO)

NSMO : it is explained in the above routine

It gives the first derivative of the smoothed spectrum. The shape of this spectrum is then analyzed in each given interval.

## 4. Subroutine FIRST

SUBROUTINE FIRST (LIBST, NCH, III, JS)

DIMENSION CK(10), VK(10), FCOR(10)

LIBST : number of peaks of the calibration library

NCH : number of channel of the spectrum

III : number of spectra to elaborate

JS : switch indicating whether the area of the peaks must be computed with the original spectrum or with the smoothed one

JS = 0 original spectrum

JS = 1 smoothed spectrum

CK : centers of the peaks found  
VK : energies of these peaks  
FCOR : correction factor for counting geometry to  
the specific activities of the elements  
belonging to the oriented library and  
finally the calibration line equation.

It is given as,  $\frac{\text{exp. specific activity}}{\text{theoretical specific activity}}$

Subroutine FIRST treats the first spectrum of the series that is calibration spectrum. There is a certain number of known peaks in that spectrum. The calibration spectrum is always the first one in the set.

### 5. Subroutine KAL

SUBROUTINE KAL (N,C,E,A,B)  
DIMENSION C(10), E(10)

N : number of measurement  
C : number of channel used as abscissa for the calibration line  
E : gamma-ray energies used as ordinate for the calibration line  
A : slope of the calibration line  
B : intercept of that line

Subroutine KAL calculates the calibration by least squares fitting, according to the data given in the calibration library.

The maximum number of the calibration peaks is 10, so C and E are given as C(10) and E(10).

## 6. Subroutine ANALYS

SUBROUTINE ANALYS(NLIB,NCH,III,JS)

NLIB : number of peaks of the oriented library which  
is prepared for each particular problem.  
NCH : as defined in FIRST  
III : as defined in FIRST  
JS : as defined in FIRST

Subroutine ANALYS analyses all the spectra except that which belongs to calibration library, according to the information given in the oriented library in each interval calculated from the FWHM value given in that library. The program also performs the calculation of the concentration of the elements present in the sample in terms of ppm.

## 7. Subroutine PKF

SUBROUTINE PKF (JJJ,III,IRIG)

DIMENSION SIGMA(50)

DIMENSION IND(50)

JJJ : number of channels of the spectrum  
III : number of spectrum to be analyzed  
IRIG : number of write statements used  
SIGMA : standard deviation for each element  
IND(JMAX): indexes indicating the kinds of the peaks found by the routine.

The search of the peaks based on the change of the sign of the first derivative of the spectrum is carried out by this routine, PKF. It also searches the possible double peaks in the spectrum. The mathematical tests used for that purpose are given in the subchapter 3.3.3 in detail.

The maximum number of elements of the oriented library is given as 50 so it is used as dimensions for SIGMA and IND in the routine.

#### 8. Subroutine SURF

SUBROUTINE SURF (NCH, JS)

DIMENSION POUNT (4096)

NCH : defined in FIRST

JS : defined in FIRST

POUNT : number of counts detected in each channel

This routine computes the area of the peaks found by the routine PKF. The method for the computation of areas is discussed in the subchapter 3.3.4.

#### 9. Subroutine SURF2

SUBROUTINE SURF2 (IRIG)

DIMENSION SIGMA (50)

IRIG : defined in PKF

SIGMA : defined in the same routine.

Subroutine SURF2 computes the areas of doublet when they are recognized by the routine PKF.

#### 10. Subroutine SENSIT

SUBROUTINE SENSIT (RAD)

RAD : minimum detectable effect observed.

If no peaks are observed in the interval indicated by the oriented library, the minimum counting rates that could have had a photopeak over the existing background are calculated by this routine, SENSIT.

11. Subroutine PRINT

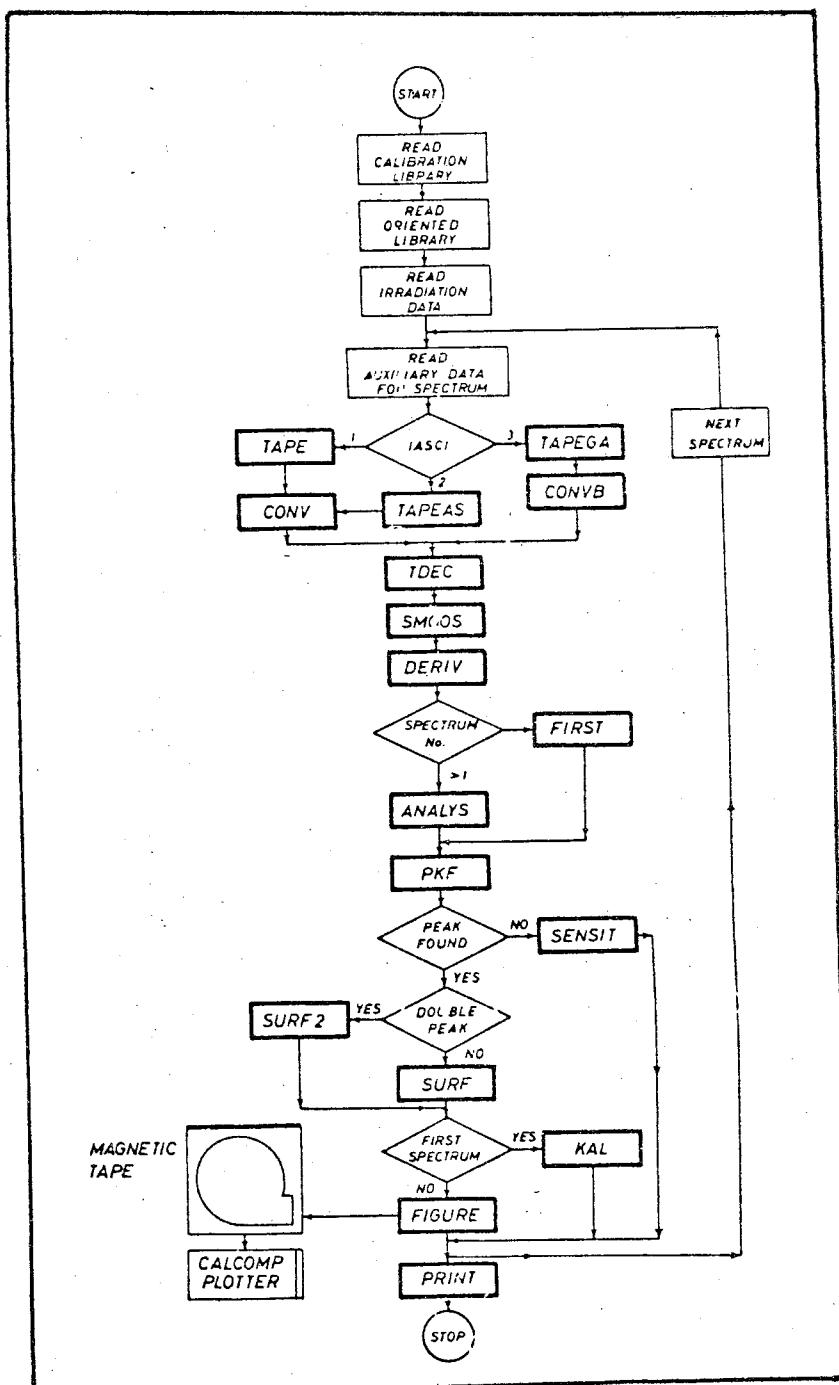
SUBROUTINE PRINT (IWR, IRIG)

IWR : an integer indicating what are printed  
according to the routines

IRIG : it is defined in PKF

This routine is used for the printing of the results obtained.

## APPENDIX H



Flow chart for the GRETEL code

APPENDIX I

LISTING OF THE UNIVAC VERSION OF  
GRETEL

```

1. C CON QUESTO PROGRAMMA SI TROVANO I PICCHI DOPPI
2. C
3. C
4. C
5. C
6. C
7. C REAL*8 EL1,ELEM
8. C REAL*8 EL2,EL3,EL4,EL2D
9. C
10. C COMMON EL1(10),EN1(10),TCAN(10),INT(10)
11. C COMMON ELEA(50),EN(50),FWT(50),XLAM(50),AA(50)
12. C COMMON COUNT(4096),SPSM(4096),DER(4096)
13. C COMMON ISTAR,IEJD,INDEX,JMAX,FMEDIO
14. C COMMON AREA(50),FRR(50),FWHM(50)
15. C COMMON LS(50),CENTR(50),LD(50),PMOL(50)
16. C COMMON DECAY(10),VALA(10),PESO(10)
17. C COMMON TDEC1,TIRR,TCON,ALFA,BETA,FLUX,WETGHT
18. C COMMON STAND(6,50),NEILST,IREL
19. C
20. C COMMON/ET1/NTRR,I0(5),MO(5),AHOME(5),ASAMPL(3)
21. C COMMON /ET4/ FL4(10),CKK(10),VKK(10),VMAX(10),NPK
22. C COMMON /ET5/ EL3(50),VS(50),P2(50),CS(50),VS2(50),VD2(50),CLS2(50)
23. C 1,CLD2(50),TSFNS
24. C COMMON /ET6/ EL2(50),VC(50),P1(50),CC(50),VS1(50),VD1(50),CLS1(50)
25. C 1,CLD1(50),TPICK
26. C COMMON/ET8/EDFC,FSAT,DFNS
27. C COMMON/ET9/EL2D(50),VCD(50),P1D(50),CCD(50),V1D(50),CL1D(50),IPICD
28. C COMMON/ET10/EL2REL(50),EL3REL(50),FL2DPE(50),
29. C
30. C DIMENSION TIME(12)
31. C DATA STAN//,STAN,/
32. C
33. C FLUX=0.
34. C DENS=0.
35. C DO 777 J=1,50
36. C AA(J)=0.
37. C PMOL(J)=0.
38. C CONTINUE
39. C READ(5,999) (IME(I),I=1,12)
40. C READ(5,1000) LIBST
41. C DO 9 K=1,LIBST
42. C 9 READ(5,998) EL1(K),EN1(K),TCAN(K),INT(K),DECAY(K),VALA(K),PESO(K)
43. C READ(5,1000) NSPT,NCH,NSMO,IPDO,TASCI,IREL
44. C IF(IREL) 200,200,201
45. C 201 READ(5,1000) NEILST
46. C
47. C *****
48. C
49. C STAND(1,K)=SIMBOLO ELEMENTO (4 LETTERE)
50. C STAND(2,K)=ENERGIA PICCO IN KEV
51. C STAND(3,K)=RESOLUZIONE RIVELATORE IN KEV
52. C STAND(4,K)=CONSTANTE DECADIMENTO 0.693/TDEC IN MINUTI

```

53. STAND(5,K)=PPM DI ELEMENTO DELLO STANDARD  
 54. STAND(6,K)=AREA PICCO AL TEMPO ZERO/MICROGRAMMT ELEMENTO (CALCOLATA  
 55. DA DAL PROGRAMMA E MESSO IN LIBERTA' DELLO STANDARD)  
 56. \*\*\*\*\*  
 57. \*\*\*\*\*

```

    58. DO 202 K=1,NELST
    59. 202 READ(5,1030) STAND(1,K),STAND(2,K),STAND(3,K),STAND(4,K),STAND(5,
    60. 1K)
    61. READ(5,1031) (IO(K),K=1,5),NTRR,TIPR,(ANOME(K),K=1,5)
    62. GO TO 500
    63. 200 READ(5,1000) NLIB
    64. DO 10 J=1,NLIR
    65. 10 READ(5,1001) ELEM(J),EN(J),FWT(J),XLAM(J),AA(J),PMOL(J)
    66. READ(5,1003) FLUX,TIRR,(IO(K),K=1,5),NTRR,(ANOME(K),K=1,5),DENS
    67. C
    68. C
    69. WRITE(6,1014) NSPT
    70. IF(IASCI-2) 70,80,60
    71. 60 WRITE(6,1012) IASCI
    72. GO TO 90
    73. 70 WRITE(6,1015) IASCI
    74. GO TO 90
    75. 80 WRITE(6,1016) IASCI
    76. 90 WRITE(6,1013)
    77. DO 50 K=1,NLIR,2
    78. K1=K+1
    79. 50 WRITE(6,1019) ELEM(K),EN(K),FWT(K),XLAM(K),AA(K),PMOL(K),ELEM(K1),
    80. 1,EN(K1),EN(K1),XLAM(K1),AA(K1),PMOL(K1)
    81. C
    82. 500 TCON=1
    83. DO 1 I=1,NSPT
    84. ITIETT
    85. IF(IPDO.EQ.1) GO TO 444
    86. ISTAPE=1
    87. TEND=NCH
    88. IF(IASCI-2) 20,30,33
    89. C
    90. *** LETTURA CON CODICE ASCII NO PARITY ***
    91. C
    92. 33 READ(5,1003)(MO(K),K=1,5),(ASAMPL(K),K=1,3),WEIGHT,TMTS,ITR,TCALC,
    93. 1JS
    94. IF(ASAMPL(1).NE.STAN) GO TO 7770
    95. 7771 STAND(5,IJK)=WEIGHT*STAND(5,IJK)
    96. 7770 CALL TAPEGA(NCH,COUNT)
    97. TCON=TMTS
    98. GO TO 40
    99. C
    100. *** LETTURA CON CODICE IBM ***
    101. C
    102. 20 READ(5,1004)(MO(K),K=1,5),(ASAMPL(K),K=1,3),WEIGHT,ITR,TCALC,JS
    103. IF(ASAMPL(1).NE.STAN) GO TO 7772
    104. 7773 IJK=1,NELST
    105. 7773 STAND(5,IJK)=WEIGHT*STAND(5,IJK)
    106. CALL TAPE(NUCH,COUNT)
    107. IF(COUNT(1).LE.1.) GO TO 40
    108. TCON=COUNT(1)/240.
    109. GO TO 40
    110. C
    111. *** LETTURA CON CODICE ASCII ***
    112. C
    113. 30 READ(5,1004)(MO(K),K=1,5),(ASAMPL(K),K=1,3),WEIGHT,ITR,TCALC,JS
    114. IF(ASAMPL(1).NE.STAN) GO TO 7774
    115. 7775 IJK=1,NELST
    116. 7775 STAND(5,IJK)=WEIGHT*STAND(5,IJK)
    117. CALL TAPEAS(NCH,COUNT)
    118. IF(COUNT(1).LE.1.) GO TO 40
    119. TCON=COUNT(1)/60.
    120. C
    121. GO TO 40
    122. 444 READ(5,1011)(MO(K),K=1,5),(ASAMPL(K),K=1,3),WEIGHT,TCON,ISTAR,TEND
    123. 1,ITR,TCALC,JS
    124. IF(ASAMPL(1).NE.STAN) GO TO 7776
    125. 7777 IJK=1,NELST
    126. 7777 STAND(5,IJK)=WEIGHT*STAND(5,IJK)
    127. 7776 NCH=TEND-ISTAR+1
    128. IF(IASCI-2) 445,446,447
    129. C
    130. *** LETTURA CON CODICE ASCII NO PARITY ***
    131. C
    132. 447 CALL TAPEGA(NCH,COUNT)
    133. C
    134. C
  
```

135. C GO TO 40  
 136. C \*\*\* LETTURA CON CODICE ASCII, \*\*\*  
 137. C  
 138. C 446 CALL TAPEAS(NCH,COUNT)  
 139. C GO TO 40  
 140. C  
 141. C \*\*\* LETTURA CON CODICE IBM \*\*\*  
 142. C  
 143. C 445 CALL TAPE(NCH,COUNT)  
 144. C 440 CONTINUE  
 145. C IF(IRR.EQ.0) GO TO 1  
 146. C  
 147. C TDEC1=TDEC(M0,10,IMF)  
 148. C IF(ICALC.EQ.1) GO TO 9999  
 149. C WRITE(6,1005) TT,NCH,TCON,(M0(K),K=1,5),TDEC1  
 150. C GO TO 9998  
 151. C 9999 WRITE(6,1020) TT,NCH,TCON,(M0(K),K=1,5),TDEC1  
 152. C 9998 CONTINUE  
 153. C  
 154. C  
 155. C IF(IPDO.EQ.1) GO TO 448  
 156. C WRITE(6,1006) (I,I=1,10)  
 157. C IMX=NCH/10+1  
 158. C DO 2 I=1,IMX  
 159. C  
 160. C IPE=I-1  
 161. C ILE=IP+10+1  
 162. C THEMIN(I\*10,NCH)  
 163. C 2 WRITE(6,1007) IP,(COUNT(J),J=I,ILE)  
 164. C GO TO 449  
 165. C  
 166. C 448 WRITE(6,1009) (I,I=1,8)  
 167. C DO 336 JE=1,NCH  
 168. C IE=J+ISTAR-1  
 169. C COUNT(I)=COUNT(J)  
 170. C DO 337 IE=ISTAR,IEND,8  
 171. C IPE=I-1  
 172. C ILE=IP+1  
 173. C JHETL=I+7  
 174. C 337 WRITE(6,1010) IP,(COUNT(J),J=I,ILE)  
 175. C  
 176. C 449 WRITE(6,109)  
 177. C  
 178. C CALL SMOOS(NSMO)  
 179. C CALL DERIV(NSMO)  
 180. C IF(IT.GT.1) GO TO 11  
 181. C  
 182. C CALL PRINT(1,0)  
 183. C  
 184. C CALL FIRST(LIBST,NCH,TTI,JS)  
 185. C IF(JMAX.LE.1) GO TO 333  
 186. C IF(NPK.LE.1) GO TO 333  
 187. C WRITE(6,1013) ALFA,BETA  
 188. C GO TO 1  
 189. C  
 190. C 11 CALL PRINT(2,0)  
 191. C  
 192. C INELSTENELST  
 193. C IF(IREL.EQ.1) NLIB=INFLST  
 194. C CALL ANALYS(NLIB,NCH,TTI,JS)  
 195. C IF(ICALC.EQ.0) GO TO 1  
 196. C 1 CONTINUE  
 197. C 199 FORMAT(1H1)  
 198. C 998 FORMAT(A6,F7.2,2I4,2E10.4,F12.8)  
 199. C 999 FORMAT(12I6)  
 200. C 1000 FORMAT(6I6)  
 201. C 1001 FORMAT(A8,2E10.3,2E10.4,F10.5)  
 202. C 1002 FORMAT(10F8.3)  
 203. C 1003 FORMAT(F10.4,F10.3,5I4,I5,5A4,F7.3)  
 204. C 1004 FORMAT(5I4,3A4,F10.6,20X,3I2)  
 205. C 1005 FORMAT(1H1,SPETTRO N,,I5,, CANALI,,I5,, TCON,,F10.3,, MTNUTT  
 206. C 1 DATA ,,5I4,, DECAD,,F12.3,, MIN,/)  
 207. C 1006 FORMAT(1H0,10(8X,I2)/)  
 208. C 1007 FORMAT(1H,,I3,10F10.0)  
 209. C 1008 FORMAT(5I4,3A4,F10.6,F10.3,10X,3I2)  
 210. C 1009 FORMAT(1H0,8(8X,I2)/)  
 211. C 1010 FORMAT(1H,,I4,3F10.0)  
 212. C 1011 FORMAT(5I4,3A4,F10.6,F10.3,2I5,3I2)  
 213. C 1012 FORMAT(1H+,45X,, PERFORATI CON CODICE ASCII NO PARITY)  
 214. C 1013 FORMAT(1H0,,CALIBRAZIONE Y=,F7.3,,\*X+,F8.3)  
 215. C 1014 FORMAT(1H0,,TH QUESTO PROGRAMMA CI SONO ,I4,, SPETTRI,)  
 216. C 1015 FORMAT(1H4,45X,, PERFORATI CON CODICE IBM,)  
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217. 1016 FORMAT(1H+,45X,'PERFORATI CON CODICE ASCITI.')  
 218. 1017 FORMAT(1H0,'NON CI SONO PICCHI DI CALIBRAZIONE')  
 219. 1018 FORMAT(1H0,5X,'LIBERTA',//,FLEM,,5X,FN(KEY) RES(KEY) DEC(MTN)  
 220. 1019 1,,3X,,VALORE A,,3X,,P.MOL.,,5X,,ELEM,,5X,,EN(KEY) PFS(KEY) DEC(M  
 221. 2IN,,3X,,VALORE A,,3X,,P.MOL.,,5X,,ELEM,,5X,,EN(KEY) PFS(KEY) DEC(M  
 222. 1019 FORMAT(1H0,A3,3X,F7.2,F7.2,3X,1PE9.3,2X,E9.3,2X,0PF7.3,5X,A8,2X,F  
 223. 1020 17.2,F7.3,3Y,1PE9.3,2X,F9.3,2X,0PF7.3)  
 224. 1020 FORMAT(1H1,,SPETTRO N,,I5,,CANALI,,I5,, TCON,,F10.3,, MTNUIT  
 225. 1 DATA ,,'5T4',,DECAD,,#12.3,, MIN,,14X,,CALCOMP,/)  
 226. 1030 FORMAT(A4,PF7.2,2E9.3)  
 227. 1031 GO TO 334  
 228. 333 FORMAT(5I4,I5,F10.3,5A4)  
 229. 334 STOP  
 230. END  
 231.  
 IN 405 IRANK 330 DBANK 14800 COMMON  
 S SPECTRA.TDEC  
 R1 \*06/16/82-22:12(2,  
 1. FUNCTION TDEC(M0,I0,IME)  
 2. DIMENSION M0(5),I0(5),IME(12)  
 3. I1=MO(2)  
 4. I2=I0(2)  
 5. TDEC=((MO(1)-I0(1))\*365+IME(I1)-IME(I2)+MO(3)-I0(3))\*24+MO(4)-I0(4)  
 6. +MO(5)-I0(5)  
 7. RETURN  
 8. END  
 IN 52 IRANK 18 DBANK  
 S SPECTRA.KAL  
 R1 \*06/16/82-22:12(2,  
 1. SUBROUTINE KAL(N,C,E,A,B)  
 2. DIMENSION C(10),E(10)  
 3. C  
 4. FN=0.  
 5. C1=0.  
 6. E1=0.  
 7. C2=0.  
 8. CE=0.  
 9. DO 1 J=1,N  
 10. C1=C1+C(J)  
 11. E1=E1+E(J)  
 12. C2=C2+C(J)\*\*2  
 13. CE=CE+C(J)\*E(J)  
 14. 1 CONTINUE  
 15. DEN=FN\*C2-C1\*\*2  
 16. A=(FN\*CE-C1\*E1)/DEN  
 17. B=(C2\*E1-C1\*CE)/DEN  
 18. RETURN  
 19. END  
 FTN 85 IRANK 26 DBANK  
 S SPECTRA.TAPE  
 R1 \*06/16/82-22:12(7,  
 1. SUBROUTINE TAPE(NPT,Y)  
 2. DIMENSION Y(4096)  
 3. INTEGER A(64)  
 4. J=0  
 5. 2 CONTINUE  
 6. IF (J.EQ.NPT) GO TO 3  
 7. READ(11,1,END=4) (A(I),I=1,60)  
 8. 1 FORMAT(6X,60A1)  
 9. J=J+1  
 10. Y(J)=CONV(A,1,5)  
 11. IF(Y(J).NE.0.) GO TO 2  
 12. Y(J)=1.  
 13. GO TO 2  
 14. 3 UPTO J  
 15. RETURN  
 16. 4 WRITE(6,5)  
 17. 5 FORMAT(1H1, '\*\* END OF FILE ON PAPER TAPE \*\*)  
 18. STOP  
 19. END  
 FTN 48 IRANK 103 DBANK  
 S SPECTRA.TAPEAS  
 R1 \*06/16/82-22:12(7,  
 1. SUBROUTINE TAPEA'(NPT,Y)  
 2. DIMENSION Y(4096)  
 3. INTEGER A(64)  
 4. INTEGER UN0/-1 //  
 5. J=0

```

6. 22 CONTINUE
7. IF(J.EQ.NPT) GO TO 3
8. READ(11,1,END=4) K,(A(I),I=1,60)
9. 1 FORMAT(3X,I3,60A1)
10. IF(K=57) 2,101,102
11. 2 IF(K=1) 22,22,103
12. 103 DO 100 I=1,60
13. A(I)=UNO
14. 100 CONTINUE
15. 101 DO 5 K=1,8
16. J=J+1
17. L1=EK*7-6
18. L2=L1+5
19. Y(J)=CONVB(A,L1,L2)
20. IF(Y(J).NE.0.) GO TO 5
21. Y(J)=1.
22. 5 CONTINUE
23. GOTO 22
24. 102 DO 6 K=1,8
25. J=J+1
26. L1=EK*7-5
27. L2=L1+5
28. Y(J)=CONVB(A,L1,L2)
29. IF(Y(J).NE.0.) GO TO 6
30. Y(J)=1.
31. 6 CONTINUE
32. GOTO 22
33. 3 NPT=J
34. RETURN
35. 4 WRITE(6,15)
36. 15 FORMAT(1H1, '**END OF FILE ON PAPER TAPE**')
37. STOP
38. END

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IN 117 IBANK 116 DBANK  
 SPECTRA.TAPEGA  
 R1 \*06/16/82-22:12(3.)  
 1. SUBROUTINE TAPEGAG(NPT,Y)  
 2. DIMENSION Y(4096)  
 3. INTEGER A(64)  
 4. INTEGER UNO/,1 ,/  
 5. J=0  
 6. 22 CONTINUE  
 7. IF(J.EQ.NPT) GO TO 3  
 8. READ(11,1,END=4) K,(A(I),I=1,64)
 9. 1 FORMAT(3X,I3,10X,64A1)
 10. IF(K=71) 2,101,101
 11. 2 IF(K=12) 22,22,103
 12. 103 DO 100 I=1,64
 13. A(I)=UNO
 14. 100 CONTINUE
 15. 101 DO 5 K=1,8
 16. J=J+1
 17. L1=EK\*8-7
 18. L2=L1+7
 19. Y(J)=CONVB(A,L1,L2)
 20. IF(Y(J).NE.0.) GO TO 5
 21. Y(J)=1.
 22. 5 CONTINUE
 23. GO TO 22
 24. 3 NPT=J
 25. RETURN
 26. 4 WRITE(6,15)
 27. 15 FORMAT(1H1, '\*\*END OF FILE ON PAPER TAPE\*\*')
 28. STOP
 29. END

30. FUNCTION CONVB(A,L1,L2)
 31. C
 32. INTEGER A(1),TAB(11)
 33. DATA TAB /1,0 ,,,1 ,,,2 ,,,3 ,,,4 ,,,5 ,,,6 ,,,7 ,,,8 ,,
 34. \* ,,,9 ,,,1 /
 35. \* CONVB=0.
 36. DO 2 I=L1,L2
 37. IF(A(I).EQ.TAB(11)) A(I)=TAB(1)

```

38:      DO 1 J=1,10
39:      1 IF(A(J).EQ.TAB(J)) GO TO 3
40:      1 CONTINUE
41:      1 CONV=0.
42:      1 RETURN
43:      3 FJ=J
44:      3 CONV=CONV*10.+FJ-1.
45:      2 CONTINUE
46:      2 RETURN
47:      END

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- GREF0648
- GREF0649
- GREF0650
- GREF0651
- GREF0652
- GREF0653
- GREF0654
- GREF0655
- GREF0656
- GREF0657

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48:      FUNCTION CONVR(A,L1,L2)
49:      C
50:      INTEGER A(1),TAB(11)
51:      DATA TAB /0 , 1 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 1 /
52:      *CONVR=0.
53:      DO 2 I=L1,L2
54:      IF(A(I).EQ.TAB(11)) RETURN
55:      DO 1 J=1,10
56:      IF(A(I).EQ.TAB(J)) GO TO 3
57:      1 CONTINUE
58:      CONVR=0
59:      RETURN
60:      3 FJ=J
61:      3 CONVR=CONVR*10.+FJ-1.
62:      2 CONTINUE
63:      RETURN
64:      END

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- GREF0658
- GREF0659
- GREF0664
- GREF0665
- GREF0666
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- GREF0674
- GREF0675

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N 216 TBANK 164 DBANK
SPECTRA SMOOS
*06/16/82-22:12(2)
1      SUBROUTINE SMOOS(NSMO)
2      C
3      REAL*8 EL1,ELEM
4      COMMON EL1(10),EN1(10),ICAN(10),INT(10)
5      COMMON ELEM(50),EN(50),FWT(50),XLAM(50),AA(50)
6      COMMON COUNT(4096),SPSM(4096),PER(4096)
7      COMMON ISTAR,IEND,INDPX,JMAX,FMEDTO
8      COMMON AREA(50),ERR(50),FWHM(50)
9      COMMON LS(50),CENTR(50),LD(50),PMOL(50)
10     COMMON DECAY(10),VALA(10),PESO(10)
11     COMMON TDEC1,TIRP,TCON,ALFA,BETA,FLUX,WETGHT
12
13      C
14      IF(NSMO-7) 30,40,50
15      C
16      *** SMOOTHING A 9 PUNTI ***
17
18      50 N1=ISTAR+4
19      N2=IEND-4
20      C0=50.
21      C1=54.
22      C2=30.
23      C3=14.
24      C4=-21.
25      CNORM=231.
26      GO TO 60
27
28      C
29      *** SMOOTHING A 7 PUNTI ***
30
31      40 N1=ISTAR+3
32      N2=IEND-3
33      C0=7.
34      C1=6.
35      C2=3.
36      C3=-2.
37      C4=0.
38      CNORM=21.
39      GO TO 60
40
41      C
42      *** SMOOTHING A 5 PUNTI ***
43
44      30 N1=ISTAR+2

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- GREF0678
- GREF0679
- GREF0680
- GREF0681
- GREF0682
- GREF0683
- GREF0684
- GREF0685
- GREF0686
- GREF0687
- GREF0688
- GREF0689
- GREF0690
- GREF0691
- GREF0692
- GREF0693
- GREF0694
- GREF0695
- GREF0696
- GREF0697
- GREF0698
- GREF0699
- GREF0700
- GREF0701
- GREF0702
- GREF0703
- GREF0704
- GREF0705
- GREF0706
- GREF0707
- GREF0708
- GREF0709
- GREF0710
- GREF0711
- GREF0712
- GREF0713
- GREF0714
- GREF0715
- GREF0716
- GREF0717

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43.      N2=IEEND-2
44.      C0=17.
45.      C1=12.
46.      C2=-3.
47.      C3=0.
48.      C4=0.
49.      CNORM=35.
50.
51.      DO 1 K=N1,N2
52.      SPSM(K)=C0*COUNT(K)+C1*(COUNT(K+1)+COUNT(K-1))+C2*(COUNT(K+2)+COUNT(K-2))+C3*(COUNT(K+3)+COUNT(K-3))+C4*(COUNT(K+4)+COUNT(K-4))
53.      1 T(K)=SPSM(K)/CNORM
54.      RETURN
55.      END
56.

N 105 IRANK 39 DBANK 13030 COMMON
SPECTRA DERTV
*06/16/82-22:12(2,)

1.      SUBROUTINE DERTV(NSMO)
2.      REAL*8 EL1,ELEM
3.      COMMON EL1(10),EN1(10),ICAN(10),INT(10)
4.      COMMON ELEM(50),FN(50),FWT(50),XLAM(50),AA(50)
5.      COMMON COUNT(4096),SPSM(4096),DER(4096)
6.      COMMON ISTAR,TEND,INDEX,JMAX,FMEDIO
7.      COMMON AREA(50),FRR(50),FWHM(50)
8.      COMMON LS(50),CENTR(50),LD(50),PMOL(50)
9.      COMMON DECAY(10),VALA(10),PESO(10)
10.     COMMON TDEC1,TIRR,TCON,ALFA,BFTA,FLUX,WEIGHT
11.
12.     IF(NSMO-7) 10,20,30
13.     30 ISE=ISTAR+5
14.     IE=IEEND-5
15.     GO TO 40
16.     20 ISE=ISTAR+4
17.     IE=IEEND-4
18.     GO TO 40
19.     10 ISE=ISTAR+3
20.     IE=IEEND-3
21.
22.     40 DO 1 I=IS,IE
23.     IP=I+1
24.     IN=I-1
25.     DER(I)=(SPSM(IP)-SPSM(IN))/2.
26.     1 CONTINUE
27.     RETURN
28.     END

N 56 IRANK 15 DBANK 13030 COMMON
SPECTRA FIRST
*06/16/82-22:12(2,)

1.      SUBROUTINE FIRST(LIBST,NCH,ITT,JS)
2.      REAL*8 EL1,ELEM
3.      REAL*8 EL4
4.      COMMON EL1(10),EN1(10),ICAN(10),INT(10)
5.      COMMON ELEM(50),FN(50),FWT(50),XLAM(50),AA(50)
6.      COMMON COUNT(4096),SPSM(4096),DER(4096)
7.      COMMON ISTAR,TEND,INDEX,JMAX,FMEDIO
8.      COMMON AREA(50),FRR(50),FWHM(50)
9.      COMMON LS(50),CENTR(50),LD(50),PMOL(50)
10.     COMMON DECAY(10),VALA(10),PESO(10)
11.     COMMON TDEC1,TIRR,TCON,ALFA,BFTA,FLUX,WEIGHT
12.     COMMON STARD(6,50),NEIST,IPER
13.     COMMON /ET4/ EL4(10),CKK(10),VKK(10),VMAX(10),NPK
14.
15.     DIMENSION CK(10),VK(10),FCOR(10)
16.
17.     NPKE=0
18.     JJJ=0
19.     CALL PKF(JJJ,ITT,TRIG)
20.     IF(JMAX.LE.1) RETURN
21.     CALL SURF(NCH,JS)
22.
23.     WRITE (6,1998)
24.     WRITE (6,1999)
25.     DO 3 J=1,JMAX
26.     DO 4 I=1,LIBST
27.     TDELTA=ICAN(I)-INT(I)
28.     KDELTA=ICAN(I)+INT(I)
29.     TF(CENTR(J)-TDELTA) 4,6,6
30.     6 IF(CENTR(J)-KDELTA) 7,7,4
31.     7 NPKE=NPKE+1
32.     CK(NPK)=CENTR(J)

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33.      VK(NPK)=EN1(I)
34.      EL1(NPK)=EL1(I)
35.      FDEC=EXP(DECAY(I)*TDEC1)
36.      FSAT=1.-EXP(-DECAY(I)*TIRR)
37.      CPM=AREA(J)/TCON
38.      AZERO=CPM*FDEC
39.      ASPEP=0.
40.      FCOR(NPK)=0.
41.      TF(TREL,FQ,I) GO TO 100
42.      ASPEREFLUX*FSAT*PESO(I)*1.F+06/AZERO
43.      FCOR(NPK)=ASPER/VALA(I)
44.
45.      C      **** I SEGUENTI VALORI VANNO NEL COMMON /ET4/ E SERVONO PER ,ETGUR
46.
47.      100 TK=ECK(NPK)+0.5
48.      VMAX(NPK)=ECOUNT(TK)
49.      EL4(NPK)=EFL1(NPK)
50.      CKK(NPK)=ECK(NPK)
51.      VKK(NPK)=EVK(NPK)
52.      C      WRITE (6,2000) NPK,EL1(NPK),VK(NPK),PESO(I),CK(NPK),CPM,AZERO,ASPE
53.      1R,VALA(I),FCOR(NPK)
54.      4 CONTINUE
55.      3 CONTINUE
56.      IF(NPK.LE.1) RETURN
57.      C      CALL KAL(NPK,CK,VK,ALFA,BETA)
58.      FMEDIO=0.
59.      DO 5 K=1,NPK
60.      5 FMEDIO=FMEDIO+FCOR(K)
61.      FMEDIO=FMEDIO/NPK
62.      WRITE (6,2002)
63.      WRITE (6,2001) NPK,FMEDIO
64.
65.      C      1998 FORMAT (1H0)
66.      1999 FORMAT (1H0,3X,,N,,4X,,ELFM,,7X,,FN,,6X,,PESO (6),,5X,,CENTR,,5X,
67.      1,C P M,,4X,,AREA ZERO,,3X,,A SPER,,5X,,A TEOF,,4X,,FATT CORR,///)
68.      2000 FORMAT (1H,,T5,2X,A8,2X,F7.2,2X,F11.8,3X,F7.2,5(2X,1PE9.3))
69.      2001 FORMAT (1H,,5X,,VALORE MEDIO DEL FATTORE CORRETTIVO SU ,,T4,, PIICK
70.      1H1,,30X,1PE9.3//))
71.      2002 FORMAT (1H0,9.3X,-----//)
72.      RETURN
73.      END
74.
75.

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IN 198 IBANK 213 DBANK 13383 COMMON  
SPECTRA ANALYS

\*06/16/82-22:12(2)

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1.      SUBROUTINE ANALYS(NLIB,NCH,ITI,JS)
2.      INTEGER H1,H2
3.      REAL*8 EL1,ELEM
4.      REAL*8 EL2,EL3,EL2D
5.
6.      C      COMMON EL1(10),EN1(10),ICAN(10),INT(10)
7.      COMMON ELEM(50),EN(50),FWT(50),XLAM(50),AA(50)
8.      COMMON COUNT(4096),SPSM(4096),PER(4096)
9.      COMMON TSTAR,IEEND,INDEX,JMAX,FMEDIO
10.     COMMON AREA(50),FRR(50),FWHM(50)
11.     COMMON LS(50),CENTR(50),LD(50),PMOL(50)
12.     COMMON DECAY(10),VALA(10),PESO(10)
13.     COMMON TDEC1,TIRR,TCON,ALFA,BETA,FLUX,WEIGHT
14.     COMMON STAND(6,50),NELST,IPREL
15.     COMMON FWHT
16.     C      COMMON /ET1/ NIRR,TO(5),MO(5),ANOME(5),ASAMPL(3)
17.     COMMON /ET2/ PPM,ATOM1,PERC,AKEV,CPM,AREAO,UGM,LARG,H1,H2,U1
18.     COMMON /ET5/ EL3(50),VS(50),P2(50),CS(50),VS2(50),VD2(50),CLS2(50)
19.     1,CLD2(50),ISENS
20.     1,CLD2(50),IPICK
21.     COMMON /ET7/ C1,C2,JDOUR,KKK,INN2
22.     COMMON /ET8/ FDEC,FSAT,DFNS
23.     COMMON /ET9/ EL2D(50),VCD(50),P1D(50),CCD(50),V1D(50),CL1D(50),IPICD
24.     COMMON /ET10/ EL2RFL(50),EL3REL(50),EL2DRE(50)
25.     DATA STAN/,STAN,/
26.     DATA BLANK/,/
27.
28.
29.      C      IPICD=0
30.      IPICK=0
31.      ISEN=0
32.      IRIG=0
33.      FAEP=
34.      FBFL=1.2
35.

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36.      CALL PRINT(3,IRIG)
37.      C 200 IF(IREL.EQ.1) NLIRENLIST
38.          IF(ASAMPL(1).NE.STAN) GO TO 204
39.          DO 201 K=1,NFLST
40.              XLA(M(K))=STAND(4,K)
41.              EN(K)=STAND(2,K)
42.              FWT(K)=STAND(3,K)
43.          201 DO 3 J=1,NLIR
44.              JJ(J)=J
45.              J1E(J)
46.              FDEC=EXP(XLA(M(J))*TDEC1)
47.              FSATE1=-EXP(-XLA(M(J))*TIRR)
48.              FNCH=(EN(J)-BETA)/ALFA
49.              FWHT=FWT(J)/ALFA
50.              ISTAR=(FNCH-FWHT*FA)
51.              IEND=(FNCH+FWHT*FA)
52.              H1=(FNCH-FWHT*FB)-0.5
53.              H2=(FNCH+FWHT*FB)+0.5
54.              L=1
55.              IF(ISTAR.GT.L.AND.IEND.LT.NCH) GO TO 7
56.
57.      C CALL PRINT(4,IRIG)
58.
59.      C 60 TO 3
60.          7 CALL PKF(JJJ,ITI,IRIG)
61.          IF(JMAX.GT.0) GO TO 9
62.          IF(JDOUR.GT.0) GOTO 3
63.          IF(ASAMPL(1).NE.STAN) GO TO 10
64.          STAND(6,J)=BLANK
65.          PPM=BLANK
66.          GO TO 301
67.      10 CALL SENSIT(RAD)
68.          SENSE=RAD/TCON
69.          AREA0=SENS*TDEC
70.          IF(ASAMPL(1).EQ.1) STAND(6,J)=AREA0/STAND(5,J)
71.          IF(IREL.EQ.1) GO TO 300
72.          UGM=AA(J)*AREA0/(FLUX*FSAT)
73.          PPM=(UGM/WEIGHT)
74.          ATOMI=6.02E17*UGM*DENS/(PMOL(J)*WEIGHT)
75.          GO TO 301
76.
77.      C 300 IF(STAND(6,J).NE.BLANK) GO TO 299
78.          PPM=BLANK
79.          GO TO 301
80.      299 PPM=(1./STAND(6,J))*(AREA0/WEIGHT)
81.      301 CONTINUE
82.      C **** I SEGUENTI VALORI VANNO NEL COMMON /ET5/ E SERVONO PER FIGUR
83.      C
84.      TIN=H1+(H2-H1)/2
85.      TSENS=SENS+1
86.      VS(TSENS)=COUNT(TIN)
87.      P2(TSENS)=EN(J)
88.      CS(TSENS)=TIN+0.5
89.      IF(IPEL.EQ.1) GO TO 400
90.      EL3(TSENS)=ELEM(J)
91.      GO TO 401
92.      400 EL3RFL(TSENS)=STAND(1,J)
93.      401 VS2(TSENS)=H1+0.5
94.      VD2(TSENS)=H2+0.5
95.      CLS2(TSENS)=COUNT(H1)
96.      CLD2(TSENS)=COUNT(H2)
97.
98.      C CALL PRINT(5,IRIG)
99.
100.     C 101 GO TO 3
101.     C 9 CALL SURF(NCH,JS)
102.         DO 1 K=1,JMAX
103.             IF(AREA(K).GT.0) GO TO 8
104.             GO TO 10
105.         8 CPM=AREA(K)/TCON
106.             ERR1=ERR(K)/TCON
107.             PERC=ERR1*100./CPM
108.             AREA0=CPM*TDEC
109.             IF(ASAMPL(1).EQ.1) STAND(6,J)=AREA0/STAND(5,J)
110.             IF(IPEL.EQ.1) GO TO 302
111.             UGM=AA(J)*AREA0/(FLUX*FSAT)
112.             PPM=(UGM/WEIGHT)
113.             ATOMI=6.02E17*UGM*DENS/(PMOL(J)*WEIGHT)
114.             GO TO 303
115.             302 IF(STAND(6,J).NE.BLANK) GO TO 299
116.                 PPM=BLANK
117.

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118.      GO TO 303
119. 298  PME(1,J) STAND(6,J)) * (AREAO/WEIGHT)
120. 303  CONTINUE
121.     AKEV=CENTR(K)*ALFA+BETA
122. ENDIF
123.     H1=LS(K)
124.     H2=LD(K)
125.     LARGELD(K)=LS(K)+1
126.     TK=CENTR(K)+0.5
127. C     **** I SEGUENTI VALORI VANNNO NEL COMMON /ET6/ E SERVONO PER ,ETGUR
128. C
129.     IPICK=IPICK+1
130.     IF(IREL.EQ.1) GO TO 402
131.     EL2(IPICK)=ELEM(J)
132.     GO TO 403
133. 402  EL2RFL(IPICK)=STAND(1,J)
134. 403  CONTINUE
135.     VC(IPICK)=COUNT(TK)
136.     P1(IPICK)=AKEV
137.     CC(IPICK)=CENTR(K)
138.     VS1(IPICK)=LS(K)
139.     VD1(IPICK)=LD(K)
140.     CLS1(IPICK)=COUNT(H1)
141.     CLD1(IPICK)=COUNT(H2)
142. C
143.     IF(PERC.GT.50.) GO TO 40
144. C
145.     CALL PRINT(9,IRIG)
146. C
147.     GO TO 1
148. C
149. 40  CALL PRINT(10,IRIG)
150. 1  CONTINUE
151. 3  CONTINUE
152. C
153.     IF(ASAMPL(1).NE.STAN) GO TO 202
154.     WRITE(6,2001)
155.     DO 3000 K=1,NELST
156.     IF(STAND(6,K).NE.BLANK) GO TO 297
157.     WRITE(6,2002) STAND(1,K),STAND(2,K),STAND(3,K),STAND(4,K),STAND(5
158.     1,K),STAND(6,K)
159.     GO TO 3000
160. 297  WRITE(6,2000) STAND(1,K),STAND(2,K),STAND(3,K),STAND(4,K),STAND(5
161.     1,K),STAND(6,K)
162. 3000  CONTINUE
163. C
164. 2000  FORMAT(1H0,A4,6X,F7.2,F7.3,3X,1PE9.3,2(2X,E9.3))
165. 2001  FORMAT(1H1,,LIBRERIA METODO RELATIVO,///, ELEM,,5X,,EN(KEV) RFS
166. 1(KEV) DEC(MIN),,5X,,UGM,,6X,,CPM0/UGM,/)
167. 2002  FORMAT(1H0,A4,6X,F7.2,F7.3,3X,1PE9.3,2X,E9.3,7X,A4)
168. 202  RETURN
169. END
170.

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IN 485 IRANK 211 DBANK 14774 COMMON

SPECTRA.PKF  
\*06/16/82-22:12(2)

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1.      SUBROUTINE PKF(JJJ,IIT,IRIG)
2.      REAL*8 EL1,ELEM,EL2D
3.      INTEGER H1,H2
4.      COMMON EL1(10),EM1(10),ICAN(10),INT(10)
5.      COMMON ELEM(50),FN(50),FWT(50),XLAM(50),AA(50)
6.      COMMON COUNT(4096),SPSM(4096),PER(4096)
7.      COMMON ISTAR,IFND,TNDFX,JMAX,FMEDIO
8.      COMMON AREA(50),ERR(50),FWHM(50)
9.      COMMON LS(50),CENTR(50),LD(50),PMOL(50)
10.     COMMON DECAY(10),VALA(10),PESO(10)
11.     COMMON TDEC1,TIRP,TCON,ALFA,RFTA,FLUX,WEIGHT
12.     COMMON STAND(6,50),NELST,IREL
13.     COMMON FWHT
14.     COMMON/ET2/PPM,ATOMT,PERC,AKEV,CPM,AREAO,UGM,LARG,H1,H2,J1
15.     COMMON/ET3/ENERG(50)
16.     COMMON/ET7/C1,C2,JDOUB,KKK,IND2
17.     COMMON/ET8/FDEC,FSAT,DFNS
18.     COMMON/ET9/EL2D(50),VCD(50),P1D(50),CCD(50),V1D(50),CL1D(50),TPICD
19.     DIMENSION SIGMA(50)
20.     DTIMENSION TND(50)
21.
22.
23. C
24.     J1=JJJ
25.     JDOUB=0
26.     TTOUTR=0

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26.    ITTOUPE=0          GPF1035
27.    CONF=1.5           GPF1036
28.    TESTAR             GPF1037
29.    JMAX=0              GPF1038
30.    10 TI=I
31.    ISW=-1
32.    1 IF(I.GE.TEND) GOTO 6      GPF1039
33.    IF(DFR(I).LT.0) 3,3,2      GPF1040
34.    2 IF(ISW.GT.0) 60 TO 1      GPF1041
35.    ISW=1
36.    GO TO 1
37.    3 IF(ISW.LT.0) GO TO 1      GPF1042
38.    ISW=-1
39.    AMAX=-10.E+30
40.    AMINE=+10.E+30
41.    JEI=1
42.    7 IF(DFR(J).LE.AMAX) GO TO 4      GPF1043
43.    AMAX=DFR(J)
44.    JLEJ
45.    JEJ=1
46.    GO TO 7
47.    4 CONTINUE
48.    JEI
49.    8 IF(DFR(J).GE.AMIN) GO TO 5      GPF1044
50.    AMIN=DFR(J)
51.    JREJ
52.    JEJ+1
53.    GO TO 8
54.    5 CONTINUE
55.    A1=SPSM(JL+1)+SPSM(JL-1)      GPF1045
56.    A2=SPSM(JR+1)+SPSM(JR-1)      GPF1046
57.    IF(A1.LE.0.OR.A2.LE.0) GO TO 10      GPF1047
58.    SDEV1=CONF*SORT(A1)/2.0      GPF1048
59.    SDEV2=CONF*SORT(A2)/2.0      GPF1049
60.    AMIN=AMIN(AMIN)      GPF1050
61.    IF(AMIN.EQ.0.OR.AMAX.EQ.0) GOTO 10      GPF1051
62.    VALMAX=AMAX1(AMAX,AMIN)      GPF1052
63.    VALMIN=AMIN1(AMAX,AMIN)      GPF1053
64.    RATIO=VALMAX/VALMIN      GPF1054
65.    IF(AMAX.LE.SDEV1.AND.AMIN.LE.SDEV2) GO TO 10      GPF1055
66.    JMAX=JMAX+1
67.    C POUR CHAQUE PIC RECHERCHE LE L,INDICE TND(JMAX)
68.    C IF((AMAX.GT.SDEV1.AND.AMIN.GT.SDEV2).AND.(RATIO.LE.1.5)) GOTO 97      GPF1056
69.    C IF(AMAX.GT.SDEV1.AND.AMAX.GE.AMIN) GOTO 98      GPF1057
70.    C IF(AMIN.GT.SDEV2.AND.AMIN.LE.AMAX) GOTO 99      GPF1058
71.    C 97 TND(JMAX)=0      GPF1059
72.    C GOTO 100
73.    C 98 IND(JMAX)=1      GPF1060
74.    C GOTO 100
75.    C 99 IND(JMAX)=2      GPF1061
76.    C CALCUL DES PARAMETRES
77.    C 100 FL=JL+(DER(JL-1)-DER(JL+1))*0.5/(DFR(JL+1)-2.*DER(JL)+DFR(JL-1))      GPF1062
78.    C FREJR=(DER(JR-1)-DER(JR+1))*0.5/(DFR(JR+1)-2.*DER(JR)+DFR(JR-1))      GPF1063
79.    C IM=I-1
80.    C CENTR(JMAX)=IM-DER(IM)/(DER(I)-DER(IM))      GPF1064
81.    C CENTR1=CENTR(JMAX)
82.    C SIGMA(JMAX)=(FR-FL)/2.0      GPF1065
83.    C SIGMA1=SIGMA(JMAX)
84.    C FWHM(JMAX)=SIGMA(JMAX)*2.355      GPF1066
85.    C FWHM1=FWHM(JMAX)
86.    C INDICE=IND(JMAX)
87.    C I=JR
88.    C VALABLE POUR LE PREMIER SPECTRE DE CALIBRATION
89.    C EXCLUSION DES PICS DOUBLANTS
90.    C 101 IF(ITT-1)102,103,102
91.    C 102 IF(IND(JMAX).EQ.1.OR.IND(JMAX).EQ.2)JMAX=JMAX-1      GPF1067
92.    C IF(JMAX.LT.0) JMAX=0
93.    C GOTO 10
94.    C 102 ENERG(JMAX)=CENTR(JMAX)*ALFA+BETA      GPF1068
95.    C ENERG1=ENERG(JMAX)
96.    C
97.    C
98.    C
99.    C
100.   C
101.   C
102.   C
103.   C
104.   C
105.   C
106.   C
107.   C

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108.      IF(IND(JMAX).EQ.2) GOTO 400
109.      IF(IND(JMAX).EQ.1) GO TO 900
110.      IF(IND(JMAX).EQ.0) FAIT PARTIE D'UN DOUBLLET
111.      RECHERCHE SI LE PIC AVEC IND(JMAX)=0 FAIT PARTIE D'UN DOUBLLET
112.      IF(IND(JMAX-1).EQ.1) GO TO 200
113.      IF((CENTR(JMAX)-CENTR(JMAX-1)).GE.(2.0 * FWHT)) GOTO 300
114.      C1=CENTR(JMAX-1)
115.      C2=ISTAR
116.      JDOURE=1
117.      CALL SURF2(IRIG)
118.      GOTO 301
119. 300  IF(ITOUR.EQ.1) GOTO 800
120. 301  JMAX=JMAX-1
121.      CENTR(JMAX)=CENTR1
122.      FWHM(JMAX)=FWHM1
123.      SIGMA(JMAX)=STGMA1
124.      IND(JMAX)=INDICE
125.      ENERG(JMAX)=ENERG1
126.      IF(ITOUR.EQ.1) GOTO 60
127.      GOTO 10
128.      ETUDE DU PTC AVEC IND(JMAX)=2
129.      RETOUR EN ARRIERE DU CANAL DE DEPART DE L'INTERVALLE
130.      C 400  IF(JMAX.GT.1) GOTO 500
131.      IF(ITOUR.GT.0) GOTO 303
132.      ISTARE=CENTR1-5*FWHT
133.      ITOUR=ITOUR+1
134.      GOTO 12
135.      RECHERCHE DU PTC DOUBLLET
136.      1) FORME UN PIC DOUBLLET AVEC PTC NORMAL IND(JMAX)=0
137.      C 500  IF(IND(JMAX-1).EQ.1) GO TO 700
138.      IF((CENTR(JMAX)-CENTR(JMAX-1)).GE.(2.0 * FWHT)) GOTO 310
139.      C2=CENTR(JMAX)
140.      C1=TFEND
141.      JDOURE?
142.      CALL SURF2(IRIG)
143.      302  IF(ITOUR.NE.1) GOTO 303
144.      JMAX=JMAX-1
145.      ITOUR=ITOUR+1
146.      GOTO 10
147. 310  IF(ITOUR.NE.1) GOTO 303
148.      JMAX=JMAX-2
149.      ITOUR=ITOUR+1
150.      GOTO 10
151. 303  JMAX=JMAX-1
152.      GO TO 10
153.      2) FORME UN PIC DOUBLLET AVEC PIC IND(JMAX)=1
154.      C 700  IF((CENTR(JMAX)-CENTR(JMAX-1)).GE.(2.0 * FWHT)) GOTO 801
155.      C1=CENTR(JMAX-1)
156.      C2=CENTR(JMAX)
157.      JDOURE=3
158.      CALL SURF2(IRIG)
159.      801  IF(ITOUR.NE.1) GOTO 800
160.      JMAX=0
161.      ITOUR=ITOUR+1
162.      GOTO 10
163. 800  JMAX=JMAX-2
164.      IF(ITOUR.EQ.1) GOTO 60
165.      GO TO 10
166.      ETUDE DU PTC AVEC IND(JMAX)=1
167.      900  IF(JMAX.EQ.1) GO TO 10
168.      IF(IND(JMAX-1).EQ.1) GO TO 1000
169.      GO TO 11
170. 1000 JMAX=JMAX-1
171.      CENTR(JMAX)=CENTR1
172.      FWHM(JMAX)=FWHM1
173.      SIGMA(JMAX)=STGMA1
174.      IND(JMAX)=INDICE
175.      ENERG(JMAX)=ENERG1
176.      GOTO 10
177. 6  IF(JMAX.EQ.0) GOTO 60
178.      IF(IND(JMAX)-1) 60,62,60

```

190. C BOND EN AVANT DU CANAL FINAL DE L'INTERVALLE  
 191. C  
 192. 62 IF(ITOURE.GT.0) GOTO A1  
 193. TEND=CENTR1+5\*FWHT  
 194. ITOURE=ITOURE+1  
 195. TEUR  
 196. GOTO 10  
 197. 61 JMAX=JMAX-1  
 198. 60 CONTINUE  
 199. RETURN  
 200. END

201. C

485 TBANK 157 DBANK 13753 COMMON  
 SPECTRA SURF

\*06/16/82-22:13(2)

SUBROUTINE SURF(IICH,JS)  
 1. REAL\*8 EL1,ELEM  
 2. COMMON EL1(10),EN1(10),ICAN(10),INT(10)  
 3. COMMON ELEM(50),EN(50),FWT(50),XLAM(50),AA(50)  
 4. COMMON COUNT(4096),SPSM(4096),DER(4096)  
 5. COMMON ISTAR,IEID,INDEX,JMAX,FMEDIO  
 6. COMMON AREA(50),ERR(50),FWHM(50)  
 7. COMMON LS(50),CENTR(50),LD(50),PMOL(50)  
 8. COMMON DECAY(10),VALA(10),PESO(10)  
 9. COMMON TDENC1,TIRR,TCON,ALFA,BETA,FLUX,WETGHT  
 10. DIMENSION POUNT(4096)  
 11.  
 12. C  
 13. 1 IF(JS.EQ.1) GO TO 20  
 14. DO 30 J=1,NCH  
 15. 30 POUNT(J)=COUNT(J)  
 16. GO TO 40

17. C  
 18. 20 DO 10 I=1,NCH  
 19. 10 POUNT(I)=SPSM(I)

20. C  
 21. 40 DO 1 JE1,JMAX  
 22. IC=CENTR(J)+0.5  
 23. ILEIC-1  
 24. TREIC+1  
 25. W=POINT(POUNT(IC))  
 26. WEPOINT(IC)=W  
 27. TND=0  
 28. ARE=POINT(IC)  
 29. IF(POINT(IC-1).LT.W) GO TO 2  
 30. IND=1  
 31. 2 IF(POINT(IC+1).LT.W) GO TO 3  
 32. IF(IND.EQ.1) GO TO 4  
 33. ARE=ARE+POINT(IC+1)  
 34. TR=TR+1  
 35. 3 IF(IND.EQ.0) GO TO 4  
 36. ARE=ARE+POINT(IC-1)  
 37. TL=IL-1  
 38. 4 CONTINUE  
 39. ARE=POINT(IL)+POINT(TR)  
 40. INTV=CENTR(J)+FWHM(J)\*2.1231+0.5  
 41. DO 5 I=IC,INTV  
 42. ARE=ARE+A  
 43. TR=TR+1  
 44. IL=IL-1  
 45. A1=POINT(TR)+POINT(TL)  
 46. IF(A1.GT.A) GO TO 6  
 47. A=A1  
 48. 5 CONTINUE  
 49. 6 HM=TR-TL-1  
 50. A2=(POINT(TR-1)+POINT(TL+1))/2.  
 51. FONDO=A2\*HM  
 52. LD(J)=TR-1  
 53. LS(J)=TL+1  
 54. AREA(J)=AR=FONDO  
 55. ERR(J)=SORT(AR+HM\*FONDO/2.0)

56. 1 CONTINUE  
 57. RETURN  
 58. END

TN 186 TBANK 4137 DBANK 13030 COMMON  
 SPECTRA SURF?

R1 \*06/16/82-22:13(4)

SUBROUTINE SURF2(TRTG)

1. REAL\*8 EL1,ELEM,EL2D  
 2.  
 3. INTEGER H1,H2  
 4. COMMON EL1(10),EN1(10),ICAN(10),INT(10)

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 GRF1 1 887  
 GRF1 1 88

```

5.      COMMON ELEM(50),FN(50),FWT(50),XLAM(50),AA(50)
6.      COMMON COUNT(4096),SPSM(4096),DER(4096)
7.      COMMON ISTAR,IEEND,INDEX,JMAX,EMENDO
8.      COMMON AREA(50),ERR(50),FWHM(50)
9.      COMMON LS(50),CFNTR(50),LD(50),PMOL(50)
10.     COMMON DECAY(10),VALA(10),PESO(10)
11.     COMMON TDEC1,TIRR,TCON,ALFA,BETA,FLUX,WEIGHT
12.     COMMON STAND(6,50),NELST,IREL
13.     COMMON FWT
14.     COMMON/ET1/NTPR,IO(5),MO(5),ANOME(5),ASAMPL(3)
15.     COMMON/ET2/PPM,ATOMI,PFRC,AKEV,CPM,AREAO,UGM,LARG,H1,H2,J1
16.     COMMON/ET3/ENERG(50)
17.     COMMON/ET7/C1,C2,JDOUB,KKK,IND2
18.     COMMON/ET8/FDEC,ESAT,DENS
19.     COMMON/ET8/EL2D(50),VCD(50),P1D(50),CCD(50),V1D(50),CL1D(50),IPICD
20.     COMMON/ET10/EL2PEL(50),EL3PEL(50),EL2DRE(50)
21. DIMENSION SIGMA(50)
22. DATA STAN//,STAN//,STAN//,STAN//,STAN//,STAN//,STAN//,STAN//,STAN//,STAN//
23. DATA BLANK//,BLANK//,BLANK//,BLANK//,BLANK//,BLANK//,BLANK//,BLANK//,BLANK//,BLANK//
24. C
25.     JJJ=J1
26.     IC1=I1
27.     IC2=I2
28.     JC1=IC1+1
29.     JC2=IC2+1
30.     ASPM1=AMAX1(SPSM(IC1),SPSM(JC1))
31.     ASPM2=AMAX1(SPSM(IC2),SPSM(JC2))
32.     IF(ASPM1.NE.SPSM(IC1)) IC1=JC1
33.     IF(ASPM2.NE.SPSM(IC2)) IC2=JC2
34.     INDE=1
35.     GOTO(10,20,30),JD0UB
36. 30  JD0URE?
37.     D01 K1=1,JD0UR
38.     KKKE=K1
39.     GOTO (11,21),KKK
40. 10  D01 K2=1,JD0UR
41.     KKKE=K2
42.     ARE=SPSM(IC1)
43.     WEAR
44.     IL=IC1+1
45.     IPICD=IPICD+1
46.     GOTO 4
47. 20  D01 K3=2,JD0UR
48.     KKKE=K3
49.     21 ARE=SPSM(IC2)
50.     WEAR
51.     IL=IC2+1
52.     INDE=1
53.     IPICD=IPICD+1
54.     4 IF(W=SPSM(IL))2,3,3
55.     3 TND=TND+1
56.     ARE=ARE+SPSM(IL)
57.     W=SPSM(IL)
58.     GOTO (40,50),KKK
59. 40  IL=IL-1
60.     GOTO 4
61. 50  IL=IL+1
62.     GOTO 4
63.     2 ARE=AR?
64.     IF(KKK.NE.1) GOTO 60
65.     IL=IL+1
66.     AR=AR-SPSM(IC1)
67. C
68.     IF(IREL.EQ.1) GO TO 202
69.     EL2D(IPICD)=ELEM(JJJ)
70.     GO TO 203
71. 202  EL2DRE(IPICD)=STAND(1,JJJ)
72. 203  VCD(IPICD)=COUNT(IC1)
73.     P1D(IPICD)=ENERG(JMAX-1)
74.     CCD(IPICD)=C1
75.     V1D(IPICD)=E1
76.     CL1D(IPICD)=COUNT(IL)
77. C
78.     GOTO 70
79. 60  ARE=AR-SPSM(IC2)
80.     IL=IL-1
81. C
82.     IF(IREL.EQ.1) GO TO 200
83.     EL2D(IPICD)=ELEM(JJJ)
84.     GO TO 201
85. 200  EL2DRE(IPICD)=STAND(1,JJJ)
86. 201  VCD(IPICD)=COUNT(IC2)

```

```

87: P1D(TPTCD)=ENERG(JMAX)
88: CCD(TPTCD)=EC2
89: V1D(TPTCD)=TL
90: CL1D(TPTCD)=COUNT(TL)
91: C
92: 70 FIND=IND*2
93: FINDFTD=1
94: FOND=IND*FIND
95: ARESEAR=FOUND
96: CPMEARES/TCON
97: FRSESOFT(AP=FIND+FOND/2,0)
98: ERR1EERS/TCON
99: PERCEERR1(100./CPM
100: AREA0=CPM*FDEC
101: IF(ASAMPL(1))EQ-STAN) STAND(6,JJJ)=AREA0/STAND(5,JJJ)
102: IF(IRET.EQ.1) GO TO 100
103: UGM=AA(JJJ)*AREA0/(FLUX*FSAT)
104: PPMEUGM/WEIGHT
105: ATOMT=6.02E17*UGM*DENS/(PMOL(JJJ)*WEIGHT)
106: GO TO 151
107: 100 IF(STAND(6,JJJ).NE.BLANK) GO TO 99
108: PPMEALANK
109: GO TO 101
110: 99 PPME(1./STAND(6,JJJ))*(AREA0/WEIGHT)
111: C
112: 101 H1=TL
113: IF(KKK.EQ.1) LARGE=IC1-TL
114: IF(KKK.EQ.2) LARGE=IL-TC2
115: IF(KKK.EQ.1) TWR=6
116: IF(KKK.EQ.2) TWR=7
117: CALL PRINT(TWR,TPIG)
118: 1 CONTINUE
119: RETURN
120: END

```

TN 363 IBANK 99 DBANK 13922 COMMON  
 SPECTRA SENSI

R1 \*06/16/82-22:13(2,)

```

1. SUBROUTINE SENSI(RAD)
2. INTEGER H1,H2
3. REAL*8 EL1,ELEM
4. COMMON EL1(10),EN1(10),ICAN(10),INT(10)
5. COMMON ELEM(50),EN(50),FWT(50),XLAM(50),AA(50)
6. COMMON COUNT(4096),SPSM(4096),PER(4096)
7. COMMON ISTAR,IEND,INDEX,JMAX,EMEDIO
8. COMMON AREA(50),ERR(50),FWHM(50)
9. COMMON LS(50),CENTR(50),LD(50),PMOL(50)
10. COMMON DECAY(10),VALA(10),PESO(10)
11. COMMON TDEC1,TIRR,TCON,ALFA,BETA,FLUX,WEIGHT
12. COMMON/ET2/PPM,ATOMI,PFRC,AKEV,CPM,AREA0,UGM,LARG,H1,H2,J1
13. C
14. SP=0.
15. CAPPA=4./1.66
16. DO 1 J=H1,H2
17. 1 SP=SP+COUNT(J)
18. 1 RADCAPPA=(1.+SP)*SORT(1.+2.*SP))
19. RETURN
20. END

```

TN 34 IBANK 16 DBANK 13041 COMMON

SPECTRA PRINT

R1 \*06/16/82-22:13(2,)

```

1. C
2. C **** TN QUESTA ROUTINE SI FANNO TUTTE LE STAMPE ****
3. C
4. REAL*8 EL1,ELEM,EL2D
5. INTEGER H1,H2
6. C
7. COMMON EL1(10),EN1(10),ICAN(10),INT(10)
8. COMMON ELEM(50),EN(50),FWT(50),XLAM(50),AA(50)
9. COMMON COUNT(4096),SPSM(4096),PER(4096)
10. COMMON ISTAR,IEND,INDEX,JMAX,EMEDIO
11. COMMON AREA(50),ERR(50),FWHM(50)
12. COMMON LS(50),CENTR(50),LD(50),PMOL(50)
13. COMMON DECAY(10),VALA(10),PESO(10)
14. COMMON TDEC1,TIRR,TCON,ALFA,BETA,FLUX,WEIGHT
15. COMMON STAND(6,50),NFLST,IREL
16. COMMON/ET1/NTRR(10)(5),MO(5),ANOME(5),ASAMPL(3)
17. COMMON/ET2/PPM,ATOMI,PFRC,AKEV,CPM,AREA0,UGM,LARG,H1,H2,J1
18. COMMON/ET3/ENERG(50)
19. COMMON/ET7/C1,C2,JDOUR,KKK,IND2
20. COMMON/ET9/EL2D(50),VCD(50),P1D(50),V1D(50),CL1D(50),TPICD

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- GPF1371
- GPF1372
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GPF1432

```

21.      C      DATA BLANK/, /
22.      C      JJJ=J1
23.      C      TF(IRIG-53) 20,21,21
24.      21      WRITE(6,906)
25.      C      IRIGEO
26.      C      WRITE(6,902)
27.      C      WRITE(6,900)
28.      C      WRITE(6,901)
29.      C      WRITE(6,900)
30.      C      WRITE(6,902)
31.      C      IRIG=IRIG+5
32.      C      20 GO TO(1,2,3,4,5,6,7,8,9,10),TWP
33.      C      1 CONTINUE
34.      C      WRITE(6,1008) NIRR,TIRR,(TO(K),K=1,5),FLUX
35.      C      WRITE(6,1009) TCON,(MO(K),K=1,5),TDEC1
36.      C      WRITE(6,1012) (ASAMPL(K),K=1,3),(ANOMF(K),K=1,5)
37.      C      WRITE(6,1011)
38.      C      GO TO 100
39.      C      2 CONTINUE
40.      C      WRITE(6,1008) NIRR,TIRR,(TO(K),K=1,5),FLUX
41.      C      WRITE(6,1009) TCON,(MO(K),K=1,5),TDEC1
42.      C      WRITE(6,1010) (ASAMPL(K),K=1,3),WFIGHT,ALFA,BETA,(ANOMF(K),K=1,5)
43.      C      WRITE(6,1011)
44.      C      GO TO 100
45.      C      3 IRIGEO
46.      C      WRITE(6,902)
47.      C      WRITE(6,900)
48.      C      WRITE(6,901)
49.      C      WRITE(6,900)
50.      C      WRITE(6,902)
51.      C      IRIG=IRIG+5
52.      C      GO TO 100
53.      C      4 CONTINUE
54.      C      WRITE(6,900)
55.      C      IF(IREL.EQ.1) GO TO 200
56.      C      WRITE(6,904) ELEM(J),EN(J)
57.      C      GO TO 201
58.      200     WRITE(6,1904) STAND(1,J),EN(J)
59.      201     IRIG=IRIG+2
60.      C      GO TO 100
61.      C      5 CONTINUE
62.      C      WRITE(6,900)
63.      C      IF(IREL.EQ.1) GO TO 202
64.      C      WRITE(6,905) ELEM(J),PPM,AA(J),EN(J),ATOMT
65.      C      GO TO 203
66.      202     IF(PPM.NE.BLANK) GO TO 300
67.      C      WRITE(6,900)
68.      C      WRITE(6,3000) STAND(1,J),EN(J)
69.      C      GO TO 203
70.      300     WRITE(6,1905) STAND(1,J),PPM,EN(J)
71.      203     IRIG=IRIG+2
72.      C      GO TO 100
73.      C      6 CONTINUE
74.      C      WRITE(6,900)
75.      C      IF(IREL.EQ.1) GO TO 204
76.      C      WRITE(6,909) ELEM(JJJ),PPM,PERC,AA(JJJ),EN(JJJ),ENERG(JMAX-1),H1,L
77.      C      1ARG,CPM,ENERG(JMAX-1),FNERG(JMAX),ATOMT
78.      C      GO TO 205
79.      204     IF(PPM.NE.BLANK) GO TO 301
80.      C      WRITE(6,900)
81.      C      WRITE(6,3000) STAND(1,JJJ),EN(JJJ)
82.      C      GO TO 205
83.      301     WRITE(6,1909) STAND(1,JJJ),PPM,PERC,EN(JJJ),ENERG(JMAX-1),H1,LARG,
84.      C      1CPM,ENERG(JMAX-1),EMERG(JMAX)
85.      205     IRIG=IRIG+2
86.      C      GO TO 100
87.      C      7 CONTINUE
88.      C      WRITE(6,900)
89.      C      IF(IREL.EQ.1) GO TO 206
90.      C      WRITE(6,910) ELEM(JJJ),PPM,PERC,AA(JJJ),EN(JJJ),ENERG(JMAX),H1,LAP
91.      C      1G,CPM,ENERG(JMAX-1),ENERG(JMAX),ATOMI
92.      C      GO TO 207
93.      C      21      DATA BLANK/, /
94.      C      JJJ=J1
95.      C      TF(IRIG-53) 20,21,21
96.      C      WRITE(6,906)
97.      C      IRIGEO
98.      C      WRITE(6,902)
99.      C      WRITE(6,900)
100.      C      WRITE(6,901)
101.      C      WRITE(6,900)
102.      C      IRIG=IRIG+5

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• GPF1512  
• GPF1513  
• GPF1514



185: 1907 1FORMAT(1H,'T',10X,A4,I4,X,11X,F11X,T,11X,F11X,T)  
186: 1F7.2,,I,,F7.2,,I,,2I4,,I,,1PF9.3,,I,,E9.3,,I,,9X,,I,,9 : GPF1597  
187: 1908 2FORMAT(1H,,I,,A4,4X,,I,,1PF9.3,,I,,0PF6.2,,I,,9X,,I,,9 : GPF1598  
188: 1F7.2,,I,,F7.2,,I,,2I4,,I,,1PF9.3,,I,,E9.3,,I,,9X,,I,,9 : GPF1599  
189: 1909 2FORMAT(1H,,I,,A4,4X,,I,,1PF9.3,,I,,0PF6.2,,I,,9X,,I,,9 : GPF1600  
190: 1F7.2,,I,,F7.2,,I,,2I4,,I,,1PF9.3,,I,,PRIMO(,,0PF7.2,1X,F7 : GPF1601  
191: 1910 2FORMAT(1H,,I,,A4,4X,,I,,1PF9.3,,I,,0PF6.2,,I,,9X,,I,,9 : GPF1602  
192: 1F7.2,,I,,F7.2,,I,,2I4,,I,,1PF9.3,,I,,SECOND(,,0PF7.2,1X,F7 : GPF1603  
193: 1911 2FORMAT(1H,,I,,A4,4X,,I,,1PF9.3,,I,,0PF6.2,,I,,9X,,I,,9 : GPF1604  
194: 1F7.2,,I,,F7.2,,I,,2I4,,I,,1PF9.3,,I,,SECOND(,,0PF7.2,1X,F7 : GPF1605  
195: 1912 3000 FORMAT(1H+,2X,A4,43X,F7.2) : GPF1606  
196: C 100 RETURN : GPF1607  
197: END : GPF1608  
198: : GPF1609  
199: : GPF1610

N 255 TBANK 1217 DBANK 13768 COMMON

SPECTRA  
28R1 F35 S74T11 06/16/82 22:13:21  
EP. GRETHEL\*SPECTRA(1) 16 REL 18 ENTRY PT(S) 1 DUP(S)  
N SPECTRA.MAIN  
R1 S74T11 06/16/82 22:13:22

AP. ERRORS: 0 TIME: 34.292 STORAGE: 19328/6/037777/077777  
SPECTRA.MAIN

-132-

APPENDIX J

LISTING OF THE INPUT DATA FOR  
SAMPLE PROBLEM



APPENDIX K

LISTING OF THE OUTPUT OF SAMPLE  
PROBLEM



1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100

118 3 27 100 8 21 8 000 8 00 8 47 7 1 000 1 12 47 47 8 000 1 1 16 68 1 17 54 87 15

የዚህ የፍትሬ ሰነድ የሰውን በፊርማ እና የመሆኑን የሰውን በፊርማ እና

የኢትዮጵያውያንድ የሰውን ስም አይደለም ተስፋል ይችላል

15061506450671506771507345150771507815079150821508415085150861508715088150891509015091150921509315094150951509615097150981509915100151011510215103151041510515106151071510815109151101511115112151131511415115151161511715118151191512015121151221512315124151251512615127151281512915130151311513215133151341513515136151371513815139151401514115142151431514415145151461514715148151491515015151151521515315154151551515615157151581515915160151611516215163151641516515166151671516815169151701517115172151731517415175151761517715178151791518015181151821518315184151851518615187151881518915190151911519215193151941519515196151971519815199152001520115202152031520415205152061520715208152091521015211152121521315214152151521615217152181521915220152211522215223152241522515226152271522815229152210

- TRAGGIMENTO - 91  
 - MITSURA - TEMPO CONTEGGIO 2400.000 MINUTI  
 - CAMPIONE - CALIBR 13.333 MINUTI

FLUSSO .0000  
DECANTATO .2310.000 MINUTI  
PROBLEMA ALFALEA

n.	ELEM	E.N	PESO (g)	CENTR	C.P.M	AREA ZER	A SPFR	A TFR	FATT CORR
1	EU1	345.88	.0000228000	246.51	3.122+002	3.133+002	.000	1.286+006	.000
2	EU2	775.48	.0000228000	780.01	1.726+002	1.732+002	.000	1.286+006	.000
3	EU3	963.50	.0000228000	964.96	1.519+002	1.524+002	.000	1.286+006	.000
4	EU4	1332.40	.0000228000	1333.83	1.341+003	1.351+003	.000	1.761+006	.000
5	EU5	1408.00	.0000228000	1409.44	1.473+002	1.479+002	.000	1.286+006	.000

VALORE MEDIO NEL FATTORE CORRETTIVO SU 6 PICCHI

.000

CALIBRAZIONE Y= 1.000\*x+ -1.712





၁၃၈၂ ခုနှစ်၊ မြန်မာနိုင်ငံ၊ ရန်ကုန်မြို့၊ ရန်ကုန်မြို့၏ အနောက် ၁၇၅၀ ပါတီ၊ မြန်မာနိုင်ငံ၏ အနောက် ၁၇၅၀ ပါတီ၊

१८५२-१८५३ वर्षात् यहां आया था।

ଶ୍ରୀମତୀ କଣ୍ଠମାତ୍ର ପାଦମାତ୍ର ପାଦମାତ୍ର ପାଦମାତ୍ର ପାଦମାତ୍ର ପାଦମାତ୍ର

କେବେଳମାତ୍ରାକୁ ନିର୍ଦ୍ଦିଷ୍ଟ କାହାର ପାଇଁ କାହାର ପାଇଁ କାହାର ପାଇଁ

ପ୍ରକାଶିତ ମହାନାଳୀଙ୍କ ପଦାର୍ଥକାଣ୍ଡର ଯେତେବେଳେ ଏହାର ଅଧିକାରୀ ହେଲାମାତ୍ର ଏହାର ପଦାର୍ଥକାଣ୍ଡର ହେଲାମାତ୍ର

ଫୁଲଟିମାତ୍ର କଥା କଥା କଥା କଥା କଥା କଥା କଥା କଥା କଥା କଥା କଥା

ରେଣ୍ଡିନ୍ ମାତ୍ରାମାତ୍ରା ଦେଖିବାକୁ ପାଇଁ ଏହାର ଅଧିକ ଗତିଶୀଳ ହେଲାଯାଇଥାଏ

159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204
160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	

- IRRAGGIAMENTO = 91  
 - MTSURA = TEMPO CONTEGGIO 165.667 MINUTI  
 - CAMPIONE = STANG2 PE50 \*001a89006 CALIP. Y= 1.000\*X+ -1.712

ELEM	P.P.M.	ERR.0/0	VALORE A	KEV (T)	KVF (S)	LS	NT	CDM	APFA ZERO	U/GM	AT/CC
CF	4.900+000	4.22		145.40							
C0	9.000+000	60.03	*	1332.48	1333.16	1330	10	7.309+000	7.457+000		
CR				320.08	320.53	320	5	1.362+000	2.502+000		
CS				795.80							
EJ	1.500+000	7.57		1408.11	1408.61	1404	13	4.275+000	4.291+000		
HF	7.500+000	5.99		482.60	482.71	479	11	2.431+001	3.540+001		
HG				279.20							
IN				1300.00							
NT				810.31							
RB	2.340+002	19.85		1076.60	1077.16	1074	11	4.284+000	4.377+001		
SB				1691.00							
SC	3.990+000	1.35		889.25	889.65	886	11	1.083+002	1.323+002		
TA				1221.60							
TB				870.33							
TH	2.520+001	2.65		311.90	312.75	309	13	8.126+001	8.519+002		
YB	1.000+000	14.88	*	197.80	193.26	192	7	9.813+000	1.663+001		
YB	1.000+000	51.39	*	197.30	198.91	198	6	2.424+000	4.108+000		
ZN	7.490+001	9.37		1115.51	1115.75	1109	8	1.247+001	1.115.75 1120.00		
ZN	7.400+001	1.29		1115.51	1120.98	1118	10	8.305+001	8.995+001		
ZR	3.160+002	37.47		765.80	766.41	764	8	2.478+000	3.215+000		
BA	1.950+003	26.80		216.00	216.91	214	10	7.002+000	8.051+001		
FR	1.868+004	2.73		1099.27	1099.71	1094	15	4.296+001	6.236+001		

LIBRERIA METODO RELATIVO  
 ELEM EN(KEV) RES(KEV) DEC(MIN) UGM CPM0/UIGM

ELEM	EN(KEV)	RES(KEV)	DEC(MIN)	UGM	CPM0/UIGM
CE	145.40	3.000	1.502-005	3.136-001	
CO	1332.48	3.200	2.496-007	9.256-003	8.0056+002
CR	320.00	3.070	1.730-005	1.700-002	1.472+002
CS	795.30	3.120	5.980-007	2.834-003	
EU	1408.11	3.220	1.055-007	2.834-003	1.514+003
HF	482.60	3.100	1.069-005	1.417-002	2.498+003
H6	279.20	3.000	1.035-005	8.312-005	
IN	1390.00	3.200	9.820-006	7.367-005	
NI	810.81	3.100	6.750-005	1.209-002	
RB	1076.60	3.150	3.320-005	4.420-001	3.114+001
SB	1691.00	3.250	8.030-006	1.001-004	
SC	889.25	3.120	5.675-006	7.367-003	1.755+004
TA	1221.60	3.200	4.185-006	1.719-003	
TB	879.33	3.100	6.592-006	2.823-004	
TH	311.90	3.050	1.780-005	4.760-002	3.192+003
YB	197.80	3.000	1.500-005	1.889-003	2.174+003
ZN	1115.51	3.170	1.964-006	1.415-001	6.358+002
ZR	765.89	3.100	7.494-006	5.969-001	5.396+000
RA	216.00	3.000	4.150-005	3.684+000	8.283+000
FE	1099.27	3.170	1.060-005	3.566+001	1.749+000





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				1	24	7	30		
1	8030.	276.	114.	114567.	153.	123.	2921.	7.	1179.
2	7533.	2.	136.	10220.	5627.	190.	12823.	6.	2035.
3		3.	136.	10220.	5627.	190.	1051.	5.	1118.
4		4.	136.	10220.	5627.	190.	10657.	8.	780.
5		5.	136.	10220.	5627.	190.	10657.	9.	420.
6		6.	136.	10220.	5627.	190.	10657.	10.	459.
7		7.	136.	10220.	5627.	190.	10657.	11.	564.
8		8.	136.	10220.	5627.	190.	10657.	12.	11014.
9		9.	136.	10220.	5627.	190.	10657.	13.	12548.
10		10.	136.	10220.	5627.	190.	10657.	14.	77140.
11		11.	136.	10220.	5627.	190.	10657.	15.	67046.
12		12.	136.	10220.	5627.	190.	10657.	16.	67706.
13		13.	136.	10220.	5627.	190.	10657.	17.	67051.
14		14.	136.	10220.	5627.	190.	10657.	18.	53107.
15		15.	136.	10220.	5627.	190.	10657.	19.	48900.
16		16.	136.	10220.	5627.	190.	10657.	20.	58162.
17		17.	136.	10220.	5627.	190.	10657.	21.	49326.
18		18.	136.	10220.	5627.	190.	10657.	22.	46394.
19		19.	136.	10220.	5627.	190.	10657.	23.	45797.
20		20.	136.	10220.	5627.	190.	10657.	24.	46394.
21		21.	136.	10220.	5627.	190.	10657.	25.	43046.
22		22.	136.	10220.	5627.	190.	10657.	26.	42486.
23		23.	136.	10220.	5627.	190.	10657.	27.	42754.
24		24.	136.	10220.	5627.	190.	10657.	28.	22724.
25		25.	136.	10220.	5627.	190.	10657.	29.	22118.
26		26.	136.	10220.	5627.	190.	10657.	30.	21209.
27		27.	136.	10220.	5627.	190.	10657.	31.	21209.
28		28.	136.	10220.	5627.	190.	10657.	32.	22064.
29		29.	136.	10220.	5627.	190.	10657.	33.	27718.
30		30.	136.	10220.	5627.	190.	10657.	34.	25448.
31		31.	136.	10220.	5627.	190.	10657.	35.	25448.
32		32.	136.	10220.	5627.	190.	10657.	36.	25448.
33		33.	136.	10220.	5627.	190.	10657.	37.	25448.
34		34.	136.	10220.	5627.	190.	10657.	38.	25448.
35		35.	136.	10220.	5627.	190.	10657.	39.	25448.
36		36.	136.	10220.	5627.	190.	10657.	40.	25448.
37		37.	136.	10220.	5627.	190.	10657.	41.	25448.
38		38.	136.	10220.	5627.	190.	10657.	42.	25448.
39		39.	136.	10220.	5627.	190.	10657.	43.	25448.
40		40.	136.	10220.	5627.	190.	10657.	44.	25448.
41		41.	136.	10220.	5627.	190.	10657.	45.	25448.
42		42.	136.	10220.	5627.	190.	10657.	46.	25448.
43		43.	136.	10220.	5627.	190.	10657.	47.	25448.
44		44.	136.	10220.	5627.	190.	10657.	48.	25448.
45		45.	136.	10220.	5627.	190.	10657.	49.	25448.
46		46.	136.	10220.	5627.	190.	10657.	50.	25448.
47		47.	136.	10220.	5627.	190.	10657.	51.	25448.
48		48.	136.	10220.	5627.	190.	10657.	52.	25448.
49		49.	136.	10220.	5627.	190.	10657.	53.	25448.
50		50.	136.	10220.	5627.	190.	10657.	54.	25448.
51		51.	136.	10220.	5627.	190.	10657.	55.	25448.
52		52.	136.	10220.	5627.	190.	10657.	56.	25448.
53		53.	136.	10220.	5627.	190.	10657.	57.	25448.
54		54.	136.	10220.	5627.	190.	10657.	58.	25448.
55		55.	136.	10220.	5627.	190.	10657.	59.	25448.
56		56.	136.	10220.	5627.	190.	10657.	60.	25448.
57		57.	136.	10220.	5627.	190.	10657.	61.	25448.
58		58.	136.	10220.	5627.	190.	10657.	62.	25448.
59		59.	136.	10220.	5627.	190.	10657.	63.	25448.
60		60.	136.	10220.	5627.	190.	10657.	64.	25448.
61		61.	136.	10220.	5627.	190.	10657.	65.	25448.
62		62.	136.	10220.	5627.	190.	10657.	66.	25448.
63		63.	136.	10220.	5627.	190.	10657.	67.	25448.
64		64.	136.	10220.	5627.	190.	10657.	68.	25448.
65		65.	136.	10220.	5627.	190.	10657.	69.	25448.
66		66.	136.	10220.	5627.	190.	10657.	70.	25448.
67		67.	136.	10220.	5627.	190.	10657.	71.	25448.
68		68.	136.	10220.	5627.	190.	10657.	72.	25448.
69		69.	136.	10220.	5627.	190.	10657.	73.	25448.
70		70.	136.	10220.	5627.	190.	10657.	74.	25448.
71		71.	136.	10220.	5627.	190.	10657.	75.	25448.
72		72.	136.	10220.	5627.	190.	10657.	76.	25448.
73		73.	136.	10220.	5627.	190.	10657.	77.	25448.
74		74.	136.	10220.	5627.	190.	10657.	78.	25448.
75		75.	136.	10220.	5627.	190.	10657.	79.	25448.
76		76.	136.	10220.	5627.	190.	10657.	80.	25448.
77		77.	136.	10220.	5627.	190.	10657.	81.	25448.
78		78.	136.	10220.	5627.	190.	10657.	82.	25448.
79		79.	136.	10220.	5627.	190.	10657.	83.	25448.
80		80.	136.	10220.	5627.	190.	10657.	84.	25448.
81		81.	136.	10220.	5627.	190.	10657.	85.	25448.
82		82.	136.	10220.	5627.	190.	10657.	86.	25448.
83		83.	136.	10220.	5627.	190.	10657.	87.	25448.
84		84.	136.	10220.	5627.	190.	10657.	88.	25448.
85		85.	136.	10220.	5627.	190.	10657.	89.	25448.
86		86.	136.	10220.	5627.	190.	10657.	90.	25448.
87		87.	136.	10220.	5627.	190.	10657.	91.	25448.
88		88.	136.	10220.	5627.	190.	10657.	92.	25448.
89		89.	136.	10220.	5627.	190.	10657.	93.	25448.
90		90.	136.	10220.	5627.	190.	10657.	94.	25448.
91		91.	136.	10220.	5627.	190.	10657.	95.	25448.
92		92.	136.	10220.	5627.	190.	10657.	96.	25448.
93		93.	136.	10220.	5627.	190.	10657.	97.	25448.
94		94.	136.	10220.	5627.	190.	10657.	98.	25448.
95		95.	136.	10220.	5627.	190.	10657.	99.	25448.
96		96.	136.	10220.	5627.	190.	10657.	100.	25448.
97		97.	136.	10220.	5627.	190.	10657.	101.	25448.
98		98.	136.	10220.	5627.	190.	10657.	102.	25448.
99		99.	136.	10220.	5627.	190.	10657.	103.	25448.
100		100.	136.	10220.	5627.	190.	10657.	104.	25448.
101		101.	136.	10220.	5627.	190.	10657.	105.	25448.
102		102.	136.	10220.	5627.	190.	10657.	106.	25448.
103		103.	136.	10220.	5627.	190.	10657.	107.	25448.
104		104.	136.	10220.	5627.	190.	10657.	108.	25448.
105		105.	136.	10220.	5627.	190.	10657.	109.	25448.
106		106.	136.	10220.	5627.	190.	10657.	110.	25448.
107		107.	136.	10220.	5627.	190.	10657.	111.	25448.
108		108.	136.	10220.	5627.	190.	10657.	112.	25448.
109		109.	136.	10220.	5627.	190.	10657.	113.	25448.
110		110.	136.	10220.	5627.	190.	10657.	114.	25448.
111		111.	136.	10220.	5627.	190.	10657.	115.	25448.
112		112.	136.	10220.	5627.	190.	10657.	116.	25448.
113		113.	136.	10220.	5627.	190.	10657.	117.	25448.
114		114.	136.	10220.	5627.	190.	10657.	118.	25448.
115		115.	136.	10220.	5627.	190.	10657.	119.	25448.
116		116.	136.	10220.	5627.	190.	10657.	120.	25448.
117		117.	136.	10220.	5627.	190.	10657.	121.	25448.
118		118.	136.	10220.	5627.	190.	10657.	122.	25448.
119		119.	136.	10220.	5627.	190.	10657.	123.	25448.
120		120.	136.	10220.	5627.	190.	10657.	124.	25448.
121		121.	136.	10220.	5627.	190.	10657.	125.	25448.
122		122.	136.	10220.	5627.	190.	10657.	126.	25448.
123		123.	136.	10220.	5627.	190.	10657.	127.	25448.
124		124.	136.	10220.	5627.	190.	10657.	128.	25448.
125		125.	136.	10220.	5627.	190.	10657.	129.	25448.
126		126.	136.	10220.	5627.	190.	10657.	130.	25448.
127		127.	136.	10220.	5627.	190.	10657.	131.	25448.
128		128.	136.	10220.	5627.	190.	10657.	132.	25448.
129		129.	136.	10220.	5627.	190.	10657.	133.	25448.
130		130.	136.	10220.	5627.	190.	10657.	134.	25448.
131		131.	136.	10220.	5627.	190.	10657.	135.	25448.
132		132.	136.	10220.	5627.	190.	10657.	136.	25448.
133		133.	136.	10220.	5627.	190.	10657.	137.	25448.
134		134.	136.	10220.	5627.	190.	10657.	138.	25448.
135		135.	136.	10220.	5627.	190.	10		





- IRRAGGIAMENTO = 91  
- MISURA = TEMPO CONTEGGIO  
- CAMPIONE = ALFA 19

ELEM.	P.P.M.	R2R. 0/0	VALORF A	KRFV (S)	KRFV (T)	DATA 1974	DATA 1975	MINUTI 12	MINUTI 1	FLUSSO 24	FLUSSO 0
										DECADIMENTO	MISURA
CF						145.40					
CO	(7.026-002)			1332.48							
CR	(3.844+000)			320.08							
CS				795.80							
EU	(1.930-002)			1408.11							
HF	(1.262-001)			432.50							
HG				279.20							
IN				1300.00							
NT				810.81							
RR	2.572+002	6.25		1070.52		1067		11		3.837+002	
RI	6.991+001	19.13		1076.60	1079.98	1077	0	1		1.043+002	
S <sub>3</sub>				1691.00							
SP				1691.00							
SC	(1.466-002)			889.25							
TA				1221.60							
TR				879.33							
TH	1.560+001	*93		311.90	314.15	311	11			8.709+002	
YR	(2.615-001)			197.80							
ZN	7.102+001	*36		1115.51	1114.22	1106	21			2.163+003	
ZR	(3.820-001)			765.80							
RA	(2.981-002)			216.00							
FC	(1.212+002)			1099.27							

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CE	7.922+000	•85		145.40							
CO	3.754+002	1.10		1332.48	1328.86	1324	13	3.598+002	3.639+002		
CR				320.08	316.56	313	11	1.162+003	3.149+003		
CS				795.80							
EJ	5.778-001	3.59		1409.11	1404.41	1401	11	4.057+001	4.087+001		
HF	3.655+000	3.18		482.60	478.35	476	9	2.911+002	5.205+002		
HG				270.20							
IM				1300.00							
NT				810.81							
RJ	4.441+002	6.06		1076.60	1072.94	1068	13	1.164+002	7.884+002		
SB				1691.00							
SC	5.306+000	•38		889.25	885.28	879	17	3.915+003	5.430+003		
TA				1221.60							
TR				870.33							
TH	3.596+000	4.60		311.90	308.42	306	9	2.345+002	6.542+002		
YB	2.394+000	12.22		197.80	194.54	201	5	1.250+002	SFCOMN( 199.06	194.54)	
YB	2.956+000	3.54		197.80	189.06	187	9	1.543+002	3.664+002		
ZH	1.214+002	•29		1115.51	1116.70	1108	21	3.930+003	4.401+003		
ZR	2.975+002	16.55		765.90	761.75	758	12	5.961+001	6.134+001		
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225.3	2006
224.7	2000
224.1	216.
224.3	165.
224.0	177.
227.6	172.
229.2	150.
228.2	155.
220.1	152.
220.5	150.
216.0	123.
216.5	125.
216.7	117.
217.2	102.
217.5	95.
217.7	115.
217.8	103.
218.1	87.
218.5	75.
218.6	80.
218.7	77.
218.8	77.
218.9	74.
219.1	72.
219.3	64.
219.5	100.

2185	2553	2554	2453	2615	3715	2173	2119	2016	1907	1915	1618	1612	1426	1197	1167	1102	1083	7240	6535	85	88	81	76	67	67	4788	2229	4665
2186	2555	2556	2454	2616	3716	2174	2120	2017	1908	1916	1619	1613	1427	1198	1168	1103	1084	7241	6536	86	89	82	77	68	68	4789	2230	4666
2187	2557	2558	2455	2617	3717	2175	2121	2018	1909	1917	1620	1614	1428	1199	1169	1104	1085	7242	6537	87	90	83	78	69	69	4790	2231	4667
2188	2559	2560	2456	2618	3718	2176	2122	2019	1910	1918	1621	1615	1429	1200	1170	1105	1086	7243	6538	88	91	84	79	70	70	4791	2232	4668
2189	2561	2562	2457	2619	3719	2177	2123	2020	1911	1919	1622	1616	1430	1201	1171	1106	1087	7244	6539	89	92	85	79	71	71	4792	2233	4669

165 74 178 192 195 200 205 210 215 220 225 230 235 240 245 250 255 260 265 270 275 280 285 290 295 300 305 310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440 445 450 455 460 465 470 475 480 485 490 495 500 505 510 515 520 525 530 535 540 545 550 555 560 565 570 575 580 585 590 595 600 605 610 615 620 625 630 635 640 645 650 655 660 665 670 675 680 685 690 695 700 705 710 715 720 725 730 735 740 745 750 755 760 765 770 775 780 785 790 795 800 805 810 815 820 825 830 835 840 845 850 855 860 865 870 875 880 885 890 895 900

50	123	456	789	0
500	1234	567	890	0
5000	12345	678	90	0
50000	123456	789	0	0
500000	1234567	89	0	0
5000000	12345678	9	0	0
50000000	123456789	0	0	0

- IRRAGGIAMENTO - 91  
 - MISURA - TEMPO CONTEGGIO 108.983 MINUTI  
 - CAMPTONE - ALFA 515 PESO •06230000 6 CALIBR. Y= 1.000\*x+ -1.712 PROBLEMA ALFALEA

FLEM	P.P.M.	FPR. 0/0	VALORE A	KFV (T)	KFV (S)	I.S	WT	C.P.M.	ALFA ZERO	U.CM	AT/CC
CF	7.156+000	•83		145.40							
CO	3.788+002	•99		1330.48	1328.74	1324	13	3.540+002	3.500+002		
CR				320.08	316.44	313	11	1.250+003	3.474+003		
CS				795.80							
EII	7.119-001	3.13		1408.11	1404.31	1400	13	6.675+001	6.716+001		
Hf	3.651+000	3.82		680.60	678.23	674	13	3.200+002	5.004+002		
HG				279.20							
IN				1300.00							
NT				810.81							
RH	4.027+002	5.46		1076.60	1072.75	1069	11	1.115+002	7.914+002		
SA				1691.00							
SC	1.791-002	37.39		890.25	893.30	892	3	1.436+001	PPITMO ( 893.30 ) 890.12 )		
SC	5.857-001	5.41		889.25	898.12	919	20	4.606+002	SFCOND ( 893.30 ) 890.12 )		
SC	5.666+000	•30		880.25	885.15	880	15	4.543+003	6.337+003		
TA				1221.60							
TH	4.186+000	3.69		879.33							
TH	2.884+000	15.08		311.90	308.29	306	9	2.930+002	8.324+002		
Y13	3.409+000	5.29		197.80	194.42	205	9	1.621+002	SFCOND ( 190.02 ) 194.42 )		
Y13	2.758+001	1.26		197.80	189.02	189	7	1.914+002	6.618+002		
ZB	8.355+001	•33		1115.51	1111.02	1102	11	0.737+002	PPITMO ( 1111.02 ) 1116.57 )		
ZI	2.627+002	14.61		1115.51	1116.57	1114	9	2.040+003	3.300+003		
ZI	( 3.993+002 )			765.80	761.69	759	10	5.700+001	8.914+001		
BA	1.532+004	•96		216.00							
FF				1090.27	1095.24	1090	15	8.062+002	1.660+003		



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159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204
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TRAGGIAMENTO -		91	2400.000	MINUTI	DATA	1974	12	15	24	0	FLUSSO .0000
- MISURA - TEMPO CONTEGGIO			1'41.783	MINUTI	DATA	1975	1	27	4	30	DECADIMENTO 60750.000 MINUTI
- CAMPIONE - ALFA 274		PESO	.05500000 G	CALIB.	Y=	1.000*Y+	-1.712				PROBLEMA ALFA/LEA
ELEM	P.P.M.	FRR.0/0	VALORE A	KFV (T)	KFV (S)	LS	WT	C P M	APPAZ FFRN	BRN	ATT/CC
CF				145.40							
CA	(6.233-002)			1332.48							
CP	(3.649+000)			320.08							
CS				795.80							
EU	(2.006-002)			1408.11							
HF	(1.242-001)			482.60							
HG				279.20							
IN				1300.00							
NT				810.81							
RR	1.741+002	10.04		1076.60	1076.50						
Si				1691.00							
SC	(1.339-002)			880.25							
TA				1221.60							
TR				879.33							
TH	1.309+001	1.10		311.90	313.84	310	11	7.793+002	2.200+003		
YB	(2.513-001)			197.80							
ZN	7.916+001	*33		1115.51	1113.99	1103	25	2.457+003	2.760+003		
ZP	(3.772+001)			765.80							
RA	(3.211+002)			216.00							
FF	(1.164+002)			1090.27							

SPESSO N.	CANALI	TCON	139.083 MINUTI	DATA	1975	1	2	3	4	5	6	7	8	9	10	DECAD	63210.000	
						11	12	13	14	15	16	17	18	19	20	21	22	23
1	8345	4929	17631	19748	19750	19751	19752	19753	19754	19755	19756	19757	19758	19759	19760	19761	19762	19763
2	76215	4929	19750	19751	19752	19753	19754	19755	19756	19757	19758	19759	19760	19761	19762	19763	19764	19765
3	4929	4929	19751	19752	19753	19754	19755	19756	19757	19758	19759	19760	19761	19762	19763	19764	19765	19766
4	34867	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153
5	1724	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153
6	1093	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153
7	637	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153
8	538	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153
9	710	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153
10	354	17137	17138	17139	17140	17141	17142	17143	17144	17145	17146	17147	17148	17149	17150	17151	17152	17153

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