

FOR REFERENCE

COMPUTER AIDED NEUTRON ACTIVATION ANALYSIS TAKEN FROM THIS ROOM

by

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ABSTRACT

Neutron Activation Analysis (NAA) has become a widely used and important analytical technique in the determination of the minor constituents of many samples. The composition of these samples may range from macro-quantities (greater than 1%) down to micro-quantities (parts per million). The micro qualitative and quantitative analyses can be performed by NAA. For this purpose the basic concepts and the theory of NAA is introduced. The detection methods and various types of detectors are discussed. The auxiliary electronic equipments and the statistical methods used in the evaluation of the results are also given. A pre-developed computer code, namely CORGAM, is presented in order to unfold the gamma-ray spectra obtained from the activation analysis of mixtures of materials. The code which was previously programmed for the IBM 360/50 computer is updated for use in the BOĞAZİÇİ University computer UNIVAC-1106. The data from a sample problem are used as input to run the program in B.U. computer. The output obtained from this run is observed to fit exactly to the results previously obtained. Finally the program and the input library are recorded onto a magnetic tape, and the necessary information required to run the program is given.

ÖZET

Günümüzde Nötron Aktivasyon Analizi (NAA) yolu ile, çeşitli malzeme kompozisyonlarında, malzemeyi teşkil eden elementlerin cins ve miktarlarının tayini oldukça önem kazanmıştır. Bu çalışmada, NAA'nın dayandığı prensipler, genel teorisi, analiz sırasında kullanılan detektör sistemleri incelenmiş ve neticelerin istatistikî değerlendirilmesi için kullanılan teknikler tanıtılmıştır. Diğer analitik yöntemlere oranla daha hassas sonuç verme üstünlüğüne sahip olan nötron aktivasyon analizinde sonuçların değerlendirilmesi sırasında karşılaşılan uzun zaman alan hesaplamalar, bilgisayarların hızlı hesaplama yeteneğinden yararlanılarak yapılmaya çalışılmıştır. Bu amaçla, daha önce hazırlanmış olan bir bilgisayar programından yararlanılmış ve bu program (CORGAM) üzerinde gerekli değişiklikler yapılarak sadece tasarlandığı üzere IBM 360/50 tipi bilgisayarlarda değil UNIVAC-1106 tipi bilgisayarlarda da kullanılabilmesi sağlanmıştır. Program değiştirilmiş hali ile manyetik bir banda kaydedilmiş ve gelecekteki uygulamalar için gerekli bilgiler ayrıca sunulmuştur.

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TABLE OF CONTENTS

	Page
ABSTRACT	1
ÖZET	11
ACKNOWLEDGMENT	111
LIST OF TABLES	v
LIST OF FIGURES	vi
1. INTRODUCTION	
1.1 GENERAL	1
1.2 NEUTRON ACTIVATION ANALYSIS	3
1.3 BASIC PRINCIPLES OF GAMMA-RAY SPECTROMETRY	5
1.4 OUTLINE OF THE THESIS	7
2. GENERAL PRINCIPLES	
2.1 FORMATION OF RADIOACTIVE NUCLEI THROUGH THE INTERACTION OF NEUTRONS WITH MATTER	8
2.2 INTERACTION OF GAMMA-RAYS WITH MATTER AND GAMMA-RAY SPECTRUM	12
2.3 SCINTILLATION DETECTORS	21
2.4 AUXILIARY ELECTRONIC EQUIPMENT	28
2.5 STATISTICAL INTERPRETATION OF THE RESULTS	30
2.6 USE OF COMPUTERS IN NEUTRON ACTIVATION ANALYSIS	35
3. CORGAM	
3.1 A COMPUTER CODE FOR NEUTRON ACTIVATION ANALYSIS	37
3.2 THEORY OF CORGAM	39
3.3 EXPERIMENTAL PROCEDURE OF CORGAM	46
4. DISCUSSION AND CONCLUSION	
REFERENCES	52
APPENDICES	
A. PROPERTIES OF ESTIMATORS	55
B. THE LEAST SQUARES METHOD	57
C. CURVE FITTING METHODS	59
D. LAGRANGIAN INTERPOLATION	62
E. DETERMINANT EVALUATION BY CHIO'S METHOD	64
F. DESCRIPTION OF THE PROGRAMS	65

G.	LISTING OF THE INPUT DATA AND INPUT OPTIONS	77
H.	LISTING OF THE UNIVAC VERSION OF THE CODE (CORCAM) ...	84
J.	FLOW DIAGRAM OF THE CODE	101
K.	LISTING OF THE INPUT DATA FOR SAMPLE PROBLEM	104
L.	LISTING OF THE OUTPUT OF THE SAMPLE PROBLEM	115
M.	LISTING OF THE UPDATING PROGRAMS	148
N.	COMPUTER CODES LISTING	152

LIST OF TABLES

Table	Page
2.1a Calibration sources for gamma-ray spectrometry.....	19
2.1b Energies and relative intensities in the decay of 1200 y $^{166}\text{Ho}^m$	20
2.2 Properties of some commonly used phosphors	22
2.3 Characteristics of a few commercial photomultipliers .	26
2.4 Probability levels	31
3.1 Compilation of nuclear properties of several isotopes.	40
3.2 Neutron flux levels for KSU TRIGA Mark II reactor.....	47
3.3 Reference spectra information	48

LIST OF FIGURES

Figure	Page
1.1 Comparison of a theoretical and actual response of a scintillation spectrometer.....	6
2.1 Decay scheme of ^{60}Co	9
2.2 Decay scheme of ^{137}Ce	10
2.3 Photoelectric cross section as a function of photon energy for lead	13
2.4 Schematic diagram of Compton scattering	14
2.5 Absorption coefficient for NaI(Tl) as a function of gamma-ray energy	17
2.6 Gamma spectrum of ^{24}Na measured with a NaI(Tl)	18
2.7 PM tube (Venetian-blind dynode structure)	24
2.8 PM tube (Box type dynode structure)	24
2.9 PM tube (Circularly focussed dynode structure)	25
2.10 Pulse-height spectrum of ^{137}Cs	25
2.11 Spectrometer system	29
2.12 Pulse-height to time conversion	29
2.13 The normal distribution function	32
2.14 Signal detection and critical level	33
3.1 Outline of correlation algorithm	45
3.2 Shielded counting cavity dimensions	49
3.3 Block diagram of the NAA instrumentation system	47

1. INTRODUCTION

1.1- GENERAL

The nuclei of atoms are stable only when they contain a certain number of neutrons and protons. The number of neutrons in the nucleus of an atom determines whether that atom is radioactive or stable. (There are exceptions. For a few elements there are no stable nuclei. In some cases, there are other differences that make certain nuclei radioactive.) Thus, while all sodium atoms contain 11 protons, only those sodium atoms that contain 12 neutrons are stable. For other elements there may be more than one number of neutrons that results in stability; for instance there are 10 stable atoms (isotopes) of tin; each containing a different number of neutrons in their nuclei.

The fact that nuclei can absorb additional neutrons, which, in many cases, results in the conversion of a stable nucleus to a radioactive one, makes Neutron Activation Analysis (NAA) possible. Because radioactive nuclei decay in unique ways and yield radiations that are often distinct, and can be measured even in very small amounts, measurements of these radiations can determine the kind and the number of radioactive atoms that are present.

In order to perform NAA, the first condition is that the element of interest gives by some nuclear reaction a radioactive isotope. The probability of the reaction (cross-section), the isotopic abundance of the target nucleus, and the half-life of the formed isotope should be large enough to allow measurements of the emitted radiation. The type and the energy of this radiation is also of interest, mainly in overcoming nuclear interferences induced by the matrix and the other impurities.

Through its nuclear character, the neutron activation technique allows the analysis of a wide variety of elements in widely differing matrices, making it 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 has been used to determine traces in ultra pure elements, in biological materials and minerals, in analysis where only small samples are available, in identification of industrial products by trace characterization, in industrial analysis of steel, in geochemistry for the determination of isotopic abundancies, etc. (Al-61, Ch-60, Pi-62)

Although NAA was proposed by von Hevesey and Levi (He-36) followed in 1938 by charged particle activation analysis applied by Seaborg et al. (Se-38) the method was considered as rather a curiosity until mid-forties. Micro constituents analysis by NAA, however became possible only after the development of high flux reactors, accelerators and reliable scintillation spectrometers. Basic principles of NAA are discussed in detail by many authors (So-69, Ba-64, Ev-55, Pr-64, OK-72). In addition some application of digital computers to NAA were presented at a symposium in 1962 (OK-62).

1.2- NEUTRON ACTIVATION ANALYSIS

The irradiation of most atomic nuclei by thermal neutrons causes these nuclei to become radioactive. The subsequent emission of beta or gamma radiations from these nuclei is characteristic of the particular isotope. If the energy of emission of the radiations are known, the isotope can be identified. The magnitude of the radioactivity is directly related to the amount of the isotope present in the specimen. The detection of radioactivity requires sensitive techniques. However neutron activation analysis permits the accurate appraisal of very small amounts of an element. Neutrons are able to pass through a considerable thickness of most substances. It is possible, therefore to analyze materials in solid, liquid or gaseous phases (Wa-63).

Besides the high sensitivity of thermal neutron 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, etc. In principle this means that in most cases only neutron capture reactions have to be considered and that consequently there is no change in the nature of the irradiated elements.

Unfortunately thermal NAA can not solve a number of important trace analysis problems, as for instance those of light elements, e.g. carbon, nitrogen and oxygen. These problems can sometimes be solved by applying an other method of activating particles: photons or charged particles such as protons, deuterons, helions, etc. If neutron analysis is possible for 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 NAA is in many cases the selectivity or even specificity of its nature. It should be remembered that the activation is a reaction of the nucleus, and thus independent of the chemical state of the considered element (So-69).

By applying gamma scintillation spectrometry to activation analysis it becomes possible to analyze simultaneously a number of different elements. A careful statistical treatment can demonstrate that NAA can be as precise and even better than other analytical methods.

The procedure can be 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 element of interest. If one takes activation in a thermal reactor, one should remember among many other parameters that 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. 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, irreproducible geometry, absorption of radiation, instability of the instrumentation, non-linearity in detector response, etc. From this short list of errors it can be concluded that NAA is a complex analytical technique and that experience is required to obtain satisfactory results.

1.3- BASIC PRINCIPLES OF GAMMA-RAY SPECTROMETRY

The basic principle of NAA is the determination of the activity of the product nuclei Y from the activation of the parent nuclei X by means of neutrons. The nuclear reaction of this type can be represented in short notation, as follows



where n refers to neutron and k to the emitted particles or radiation during the reaction. If the activation process of nuclei X, is assumed to be carried out in constant neutron flux, and if the initial number of atoms of the parent nuclei is also assumed to be constant, then the well known differential equation governing the rate of formation of Y will have the following solution, as given in detail in section 3.2.

$$A_y \equiv N_y \lambda_y = \sigma \phi_0 N_x (1 - e^{-\lambda_y t}) \quad (1.2)$$

where, A_y is the activity of Y, atoms/sec.,

N_y is the number of atoms of Y,

N_x is the number of atoms of X,

λ_y is the decay constant for product Y, sec.⁻¹

ϕ_0 is the neutron flux, neutrons/cm² sec,

σ is the activation cross-section for production of Y from X, cm²,

t is the time of irradiation, sec.

When a sample is removed from the neutron flux, the activity begins to decrease exponentially. Then the equation 1.2 becomes,

$$A_y \equiv N_y \lambda_y = \sigma \phi_0 N_x (1 - e^{-\lambda_y t}) e^{-\lambda_y t^0} \quad (1.3)$$

where, t^0 is the corrected decay time to account for decay of the sample during a finite counting time, and is given by;

$$t^0 = t_r - \frac{t_{1/2}}{0.693} \left[\frac{t_{1/2} (1 - \exp(-0.693 t_s / t_{1/2}))}{0.693 t_s} \right] \quad (1.4)$$

where, t_r is the time from removal from neutron flux to the beginning of the count, t_s is the counting time, $t_{1/2}$ is the half-life of the radioactive product.

The activated atoms will decay to lower energy levels, in order to reach more stable states. If during this decay process, the emitted excess energy is in the form of gamma-rays, both qualitative and quantitative analysis are possible.

The interaction principle of gamma-rays with matter can be used in NAA to identify the gamma emitting isotope and its quantity in the decaying material. In this work main reference is made to scintillating crystals as interacting matter with gamma-rays.

A scintillation detector converts the incoming gamma-rays into scintillations, and into electrical signals through a photomultiplier (PM) tube. These electrical signals are then amplified, measured and registered. The measurements are performed by the use of multi-channel analyzers (MCA). A MCA is an electronic equipment which stores the electrical signals in different locations (channels) according to their amplitudes. Since the amplitude of the signal is proportional to the incident gamma-ray energy a pulse height versus energy distribution can be obtained. Figure 1.1 is a plot of the expected theoretical response of a monoenergetic gamma emitter of energy E_0 and the actual spectrometer response, i.e., gamma-ray spectrum (He-64).

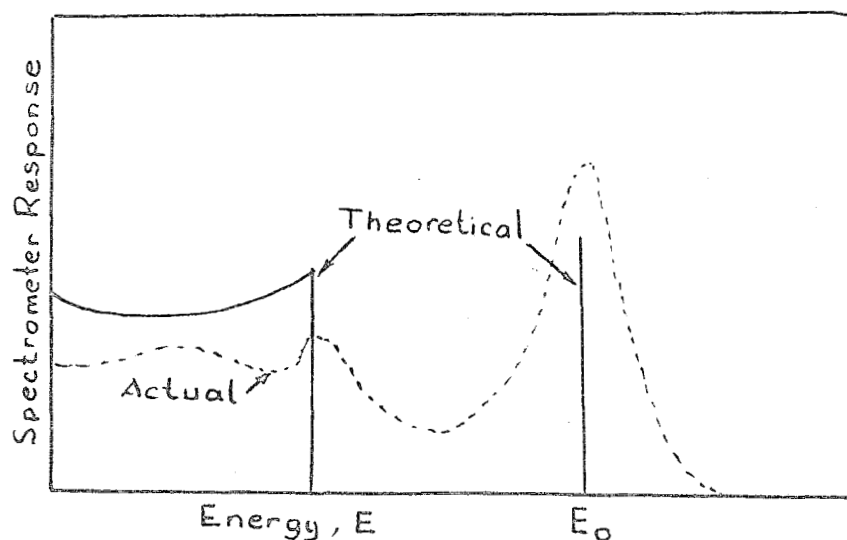


Figure 1.1- Comparison of a theoretical and actual response of a scintillation spectrometer to a monoenergetic gamma emitter of energy E_0 (He-64).

1.4- OUTLINE OF THE THESIS

The NAA technique is defined, its use and a brief history is given in section 1. The theory of NAA is briefly stated in the subsection 1.2. Before going into a more detailed study of the general principles of NAA, a short summary of the principles behind NAA are stated and the gamma-ray spectrometry is introduced in the same section. Section 2. is a more detailed discussion of the general principles of NAA. In this section, the interaction of neutrons with matter, formation of radioactive nuclei, their decay schemes are studied. The following subsection defines the types of interaction of gamma radiation with matter. The formation of gamma spectrum is also introduced in more detail in this subsection. The detectors used in common NAA work, their principle of operation, the scintillation process and scintillation detectors are studied in subsection 2.3. Information on the electronic equipment used in NAA and the statistics of radiation can be found in subsections 2.4 and 2.5 respectively. The use of computers in NAA being an important event, some predeveloped computer codes are named in the last subsection of the second section. Among the computer codes which were available in NEA Computer Library (NEA-CPL), CORGAM is analyzed in detail. It is in section 3 that CORGAM is introduced and the theory used in in this computer program is given in some detail in subsection 3.2. One can find the experimental procedures considered in this code in subsection 3.3. In this computer program, there exist some special techniques. These techniques are given in the appendices A, B, C, D and E. Finally a listing of the program, its flow diagram, the input data and the input options, the updating programs and a sample problem run are given in the appendices F, G, H, J, K, L and M.

2. GENERAL PRINCIPLES

2.1- FORMATION OF RADIOACTIVE NUCLEI THROUGH THE INTERACTION OF NEUTRONS WITH MATTER

If a moving particle collides with another one, kinetic energy is exchanged between them in agreement with the laws of conservation of energy and momentum. If the potential energy of the system remains unchanged, kinetic energy being conserved during the collision, the phenomenon is called elastic scattering. The scattering is inelastic if one of the particles is left in an excited state after collision. The symbols (n,n) and (n,n') are often used to denote these processes in neutron elastic and inelastic scattering. Neutrons may disappear in an interaction as the result of absorption reactions, the most important of which, is the (n,γ) reaction. This process is also known as radiative capture, since one of the products of the reaction is instantaneous gamma radiation. Neutrons also disappear in charged-particle reactions such as (n,p) or (n,α) reactions. Sometimes, two or more neutrons are emitted when a nucleus is struck by a high energy neutron. The process here are of the $(n,2n)$ or $(n,3n)$ type. A closely related process is the (n,pn) reaction, which also occurs with highly energetic incident neutrons. Finally, when a neutron collides with certain heavy nuclei, the nucleus splits into two large fragments with the release of considerable energy. This is the fission process. Detailed discussion of these interactions are given in many text books (Ev-55, La-72, Pi-64, Fr-67).

In neutron activation analysis the most important reaction is of the (n,γ) type. This type of reaction is the most common of all reactions, since thermal neutrons induce this reaction in nearly all nuclei. It also occurs with a very high probability for a number of nuclei at particular energies in the epithermal range. This latter phenomenon is known as resonance capture. The gamma-rays which are emitted in the (n,γ) reaction usually have energies of several MeV.

The emission of this gamma radiation is due to the release of excess energy of the excited nucleus. The energy of this gamma-ray is equal to the difference in 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. These gamma-rays are usually emitted within 10^{-13} sec. after the beta-particle, electron capture or alpha-particle decay occurs. Sometimes, this excited state has a characteristic half-life of its own.

Whenever this 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 atom. And the subsequent decay of this isomer by the emission of a gamma-ray is called an isomeric transition (Ga-67). The usual case is illustrated by ^{60}Co (Figure: 2.1).

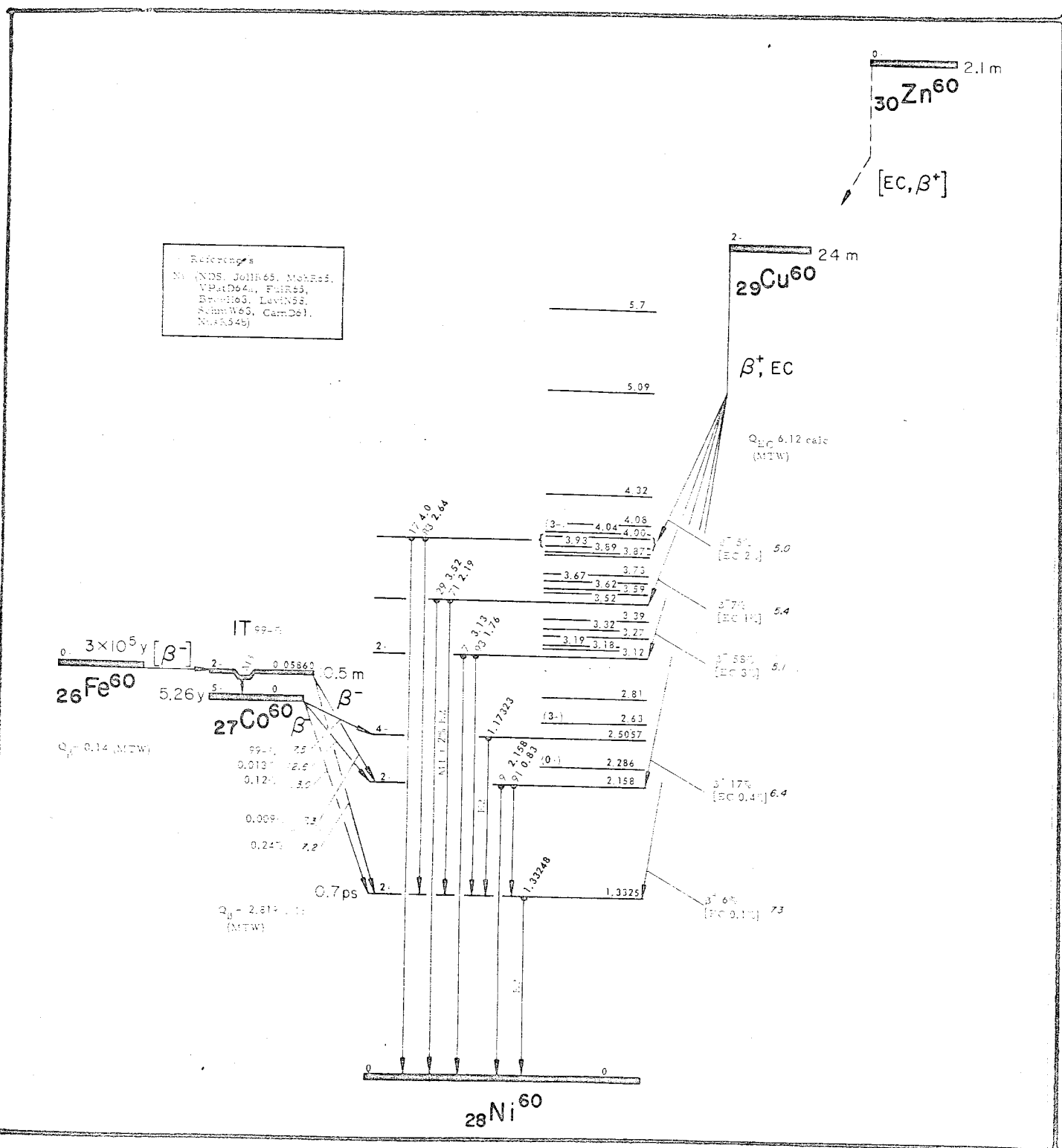


Figure: 2.1- Decay scheme of ^{60}Co (Le-68).

The ^{60}Ni nucleus formed by the β^- decay is rapidly converted from ^{60}Co with emission of 2.50 Mev energy gamma-ray. This conversion takes place by the emission of a photon of 1.17 Mev energy and immediately thereafter a photon with 1.33 Mev. A meta-stable state is found e.g. $^{60\text{m}}\text{Co}$ (half-life: 10 minutes) which is converted to ^{60}Co by emission of a gamma-ray, which decays as shown in Figure 2.1.

In some cases alternative ways for the conversion exist, resulting in a more complicated decay scheme. In Figure 2.2 the decay scheme of ^{137}Ce is illustrated.

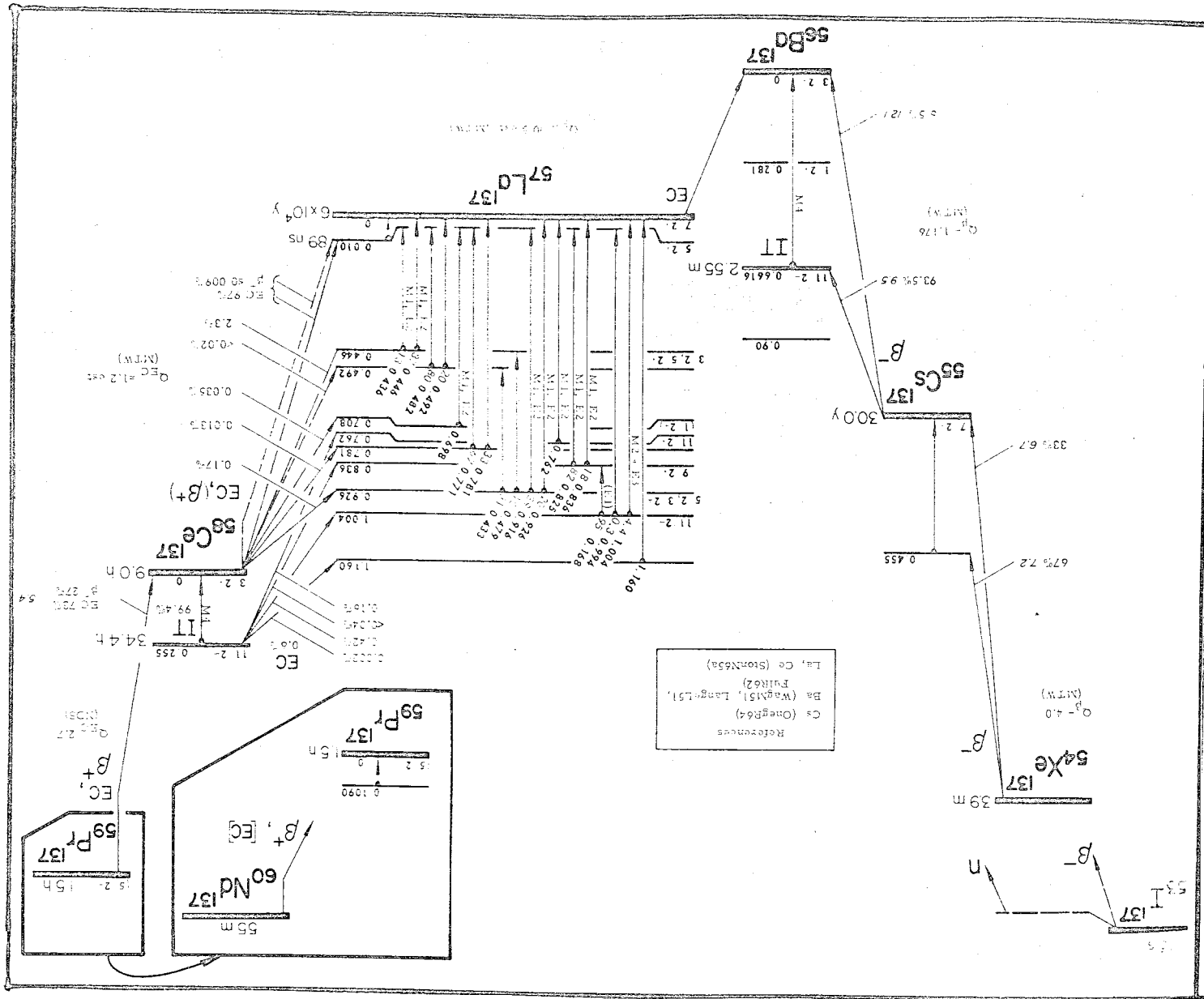


Figure: 2.2- Decay scheme of ^{137}Ce (Te-68).

The detection of these gamma radiations by suitable detectors, and the analysis of the spectrum formed by these radiations, may be used to identify the radiating nuclide, its amount, etc. The spectrum formed by these gamma-rays, due to the reasons discussed in the following subsections is unique. That is a given radionuclide has its own spectrum. Once the gamma spectrum is obtained from an unknown nuclide, qualitative and quantitative analysis is possible by using special techniques. These techniques are studied in detail in many text books (So-69, He-64, Cu-68). A brief description of these methods can be found in the following subsections, and a computer application of a specially developed method, namely the correlation algorithm is presented in section 3 (Ec-68).

2.2- INTERACTIONS OF GAMMA-RAYS WITH MATTER AND GAMMA-RAY SPECTRUM

Gamma-rays, like other electromagnetic radiation, have the properties of both waves and of discrete particles, or quanta. At the relatively high energies of isotopic gamma radiation, the quantum characteristics are the most important. Thus, for the purposes of considering their interaction with matter, gamma photons may be regarded as particles having a given energy. There are four kinds of interaction of photons with matter. Fano (Fa-53) in his article states that these are:

- 1- Basic interaction with atomic electrons
- 2- Basic interaction with nuclear particles (nucleons)
- 3- Interaction with electric field surrounding charged particles (nuclei and electrons)
- 4- Interaction with meson field surrounding nucleons.

And there are three effects that the interaction may have upon a photon,

- A- Outright absorption
- B- Elastic (coherent) scattering
- C- Inelastic (incoherent) scattering.

Different types of processes may arise from each kind of interaction (1,2,3,4) leading to each of the end results (A,B,C). Thus there are twelve types of processes in all. Many of these processes are quite infrequent, some have not yet been observed. The following three processes are the most important ones. These are;

- a) Photoelectric effects, which is the basic interaction with atomic electrons leading to an outright absorption,
- b) Compton scattering, which is the basic interaction with atomic electrons leading to inelastic (incoherent) scattering,
- c) Pair production, which is the interaction with electric field surrounding charged particles (nuclei and electrons) leading to an outright absorption.

PHOTOELECTRIC EFFECT is most important for photons of low energy. In this process, an incident gamma photon impinges on a bound orbital electron and transfers all of its energy to the electron, ejecting it from the atom. If E_b is the binding energy of the electron and the recoil energy of the atom is neglected, then $E = h\nu - E_b$, where $h\nu$ is the energy of the electromagnetic quantum and E is the kinetic energy imparted to the electron. The quantum of radiation is possible only because the remainder of the atom can receive some momentum. The photoelectric effect is frequently used to

determine gamma-ray energies. This may be accomplished by measurement of the total ionization due to the photoelectrons in a proportional or scintillator counter.

The photoelectric effect has its highest probability for electrons that are more tightly bound. The incident photon energy must exceed the binding energy of the electron, of course, before this reaction can occur. For incident photon energies above the K-shell binding energy, experiments show that 80 % of the photoelectric effect interactions occur with K-shell electrons. The probability for this interactions, increases rapidly with decreasing photon energies. Figure 2.3 shows how the photoelectric effect probability varies with incident photon energy.

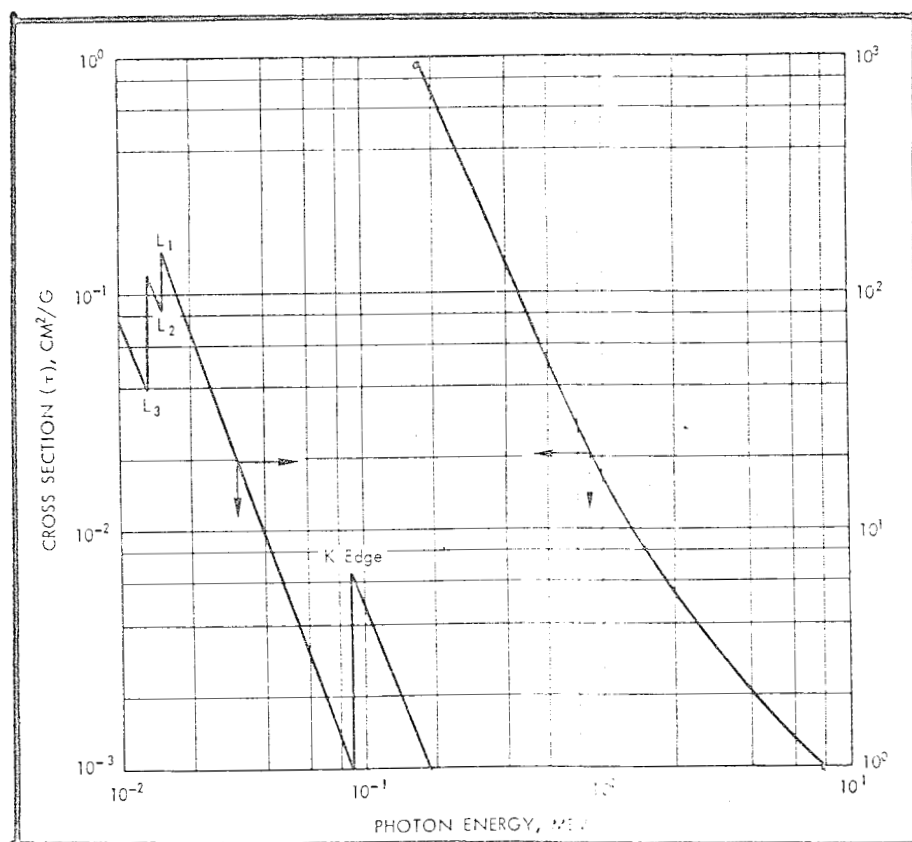


Figure: 2.3- Photoelectric cross-section as a function of photon energy for lead (Ga-67).

The discontinuities occurring at the K and L shell binding energies are called the K and L absorption edges. The probability of photoelectric interaction is approximately proportional to $Z^{4.4}$ of the absorber and to $E^{-3.5}$ of the interacting photon (Ga-67). Thus the photoelectric effect occurs with high Z absorbers and low photon energies.

Instead of giving up its entire energy to a bound electron, a photon may transfer only a part of its energy to an electron, which in this case may be either bound or free; the photon is not only degraded in energy but also deflected from its original path. This process is called the Compton effect or COMPTON SCATTERING named after A.H. Compton who first reported it in 1922 (Ko-61). This effect is shown schematically in figure 2.4.

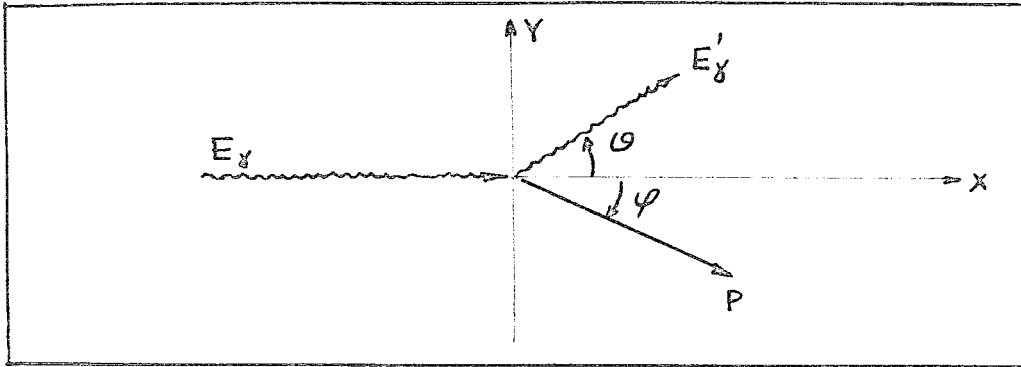


Figure: 2.4- Schematic diagram of Compton scattering of a gamma-ray by an electron (Fr-67).

Consider the expression which relates the total energy of a particle E to its momentum p .

$$E = (E_0^2 + c^2 p^2)^{1/2} \quad (2.1)$$

The quantity E_0 is the total energy of the particle when it is at rest and is given by $m_0 c^2$ where m_0 is the rest mass of the particle. It must also be recalled that the rest mass of a photon is zero.

If E_γ is the energy of the initial gamma-ray, E'_γ is the energy of the gamma-ray after being scattered by an angle θ , E_0 is the rest energy of the electron (0.511 MeV), p and φ are the momentum of the electron and the scattering angle of the electron respectively. Then the conservation of total energy requires that;

$$E_\gamma + E_0 = E'_\gamma + (E_0^2 + c^2 p^2)^{1/2} \quad (2.2)$$

The conservation of momentum along the X direction and Y direction are

$$\frac{E_\gamma}{c} = \frac{E'_\gamma}{c} \cos \theta + p \cos \varphi \quad \text{X-direction} \quad (2.3)$$

$$\frac{E'_\gamma}{c} \sin \theta = p \sin \varphi \quad \text{Y-direction} \quad (2.4)$$

Combining equations 2.3 and 2.4 the following equations are obtained.

$$E_{\gamma}^2 - 2E_{\gamma}E'_{\gamma} \cos \theta + E'^2_{\gamma} = c^2 p^2 \quad (2.5)$$

$$\frac{1}{E'_{\gamma}} - \frac{1}{E_{\gamma}} = \frac{1 - \cos \theta}{E_0} \quad (2.6)$$

Since $E = \frac{hc}{\lambda}$ where c is the velocity of light, equation 2.6 becomes;

$$\lambda' - \lambda = \frac{h}{m_e c} (1 - \cos \theta) \quad (2.7)$$

where m_e is the rest mass of the electron. The quantity $\frac{h}{m_e c} = 2.426 \times 10^{-10} \text{ cm}$ is the well known Compton wavelength of the electron. Equation 2.7 shows that for a given incident energy there is a minimum energy (maximum wavelength) for the scattered gamma-ray and that this occurs for scattering in the backward direction ($\cos \theta = -1$).

$$(E'_{\gamma})_{\min} = \frac{E_0}{2} \frac{1}{1 + E_0/2E_{\gamma}} \quad (2.8)$$

For large incident gamma-ray energies ($E_{\gamma} \gg \frac{1}{2} E_0$) the minimum energy of the scattered gamma-rays approaches $\frac{1}{2} E_0 = 250 \text{ KeV}$. For this reason scintillation spectra of high-energy gamma-rays always show a "back-scattering" peak at $\leq 250 \text{ KeV}$ which is caused by Compton scattering and a valley between photopeak and Compton continuum whose width corresponds to the minimum energy ($\leq 250 \text{ KeV}$) carried off by gamma-rays Compton scattered in the crystal (Fr-67).

The Compton effect is important for photons in the energy range of 0.6 to 2.5 MeV. The probability of Compton interaction increases with increasing Z of the absorber and with decreasing energy of the gamma-ray.

The third mechanism by which electromagnetic radiation can be absorbed is the PAIR PRODUCTION process. The process is so termed because it results in the production of a pair of particles of opposite sign, the electron and the positron. As has been pointed out above, the positron is a particle having the mass and dimensions of an electron, but a positive rather than a negative charge. Pair production is possible only for a photon having an energy of at least 1.02 MeV. When such an energetic photon traverses a powerful electric field, such as that surrounding a nucleus, the photon can be annihilated with the production of a pair of particles of equal and opposite charge. In this way, the electrical neutrality of the original photon is conserved.

The energy equivalent of the mass of each particle is 0.51 MeV and the sum of these masses, 1.02 MeV, is the minimum photon energy required for production of particles. If the photon has an energy in excess of 1.02 MeV, that excess energy is dissipated as the kinetic energy of the electron and positron created. As in the case of photoelectric effect, the incident photon disappears in this process. The positron so formed is then annihilated by collision with orbital electrons, both positron and electron being destroyed in the collision. The energy resulting from the annihilation process is emitted as electromagnetic or gamma radiation. It can be seen that positron annihilation is the reverse of pair production, in that the positron is destroyed with the consequent production of two 0.51 MeV gamma photons. The absorption of a gamma photon by matter through pair production is always associated with the emission of this relatively low energy gamma-radiation.

From the figure 2.5 it can be seen that the photoelectric process is the most important process below about 1 MeV. The Compton process is fairly important over the range from 0.1 to 10 MeV, and pair production can take place only above 1.02 MeV. Because a gamma-ray can interact with a detector by these three principal processes, a fairly complex response, Figure 2.6 is obtained from the spectrometer system. The photoelectric process which results in the total deposition of the gamma-ray's energy in the scintillation crystal is characterized by the Gaussian-shaped full energy-peak. Compton scattering is characterized by the nearly flat continuum below the four small peaks. The backscatter peak corresponds to the photoelectric process for a source gamma-ray whose initial direction of travel was 180° away from the scintillator but was backscattered into the crystal. The energy of the source gamma-ray in excess of the rest mass energy of the electron-positron pair (1.02 MeV) is transferred to the electron-positron pair as kinetic energy. Therefore, a small peak, called the two photon escape peak (or double escape), will occur at a point equal to the source gamma-ray energy minus 1.02 MeV. If one of the 0.51 MeV annihilation gamma-rays interact in the crystal by the photoelectric process and the other escapes interaction, there will be a small peak, called the one photon escape peak (or single escape), located at a point equal to the source gamma-ray energy minus 0.51 MeV. The third peak, called the annihilation peak, is a result of photoelectric interaction of 0.51 MeV gamma-rays produced by the pair production process occurring in materials outside the scintillator detector. Because of these interactions, a gamma-ray interacting in a particular scintillation crystal produces a unique gamma-ray spectrum.

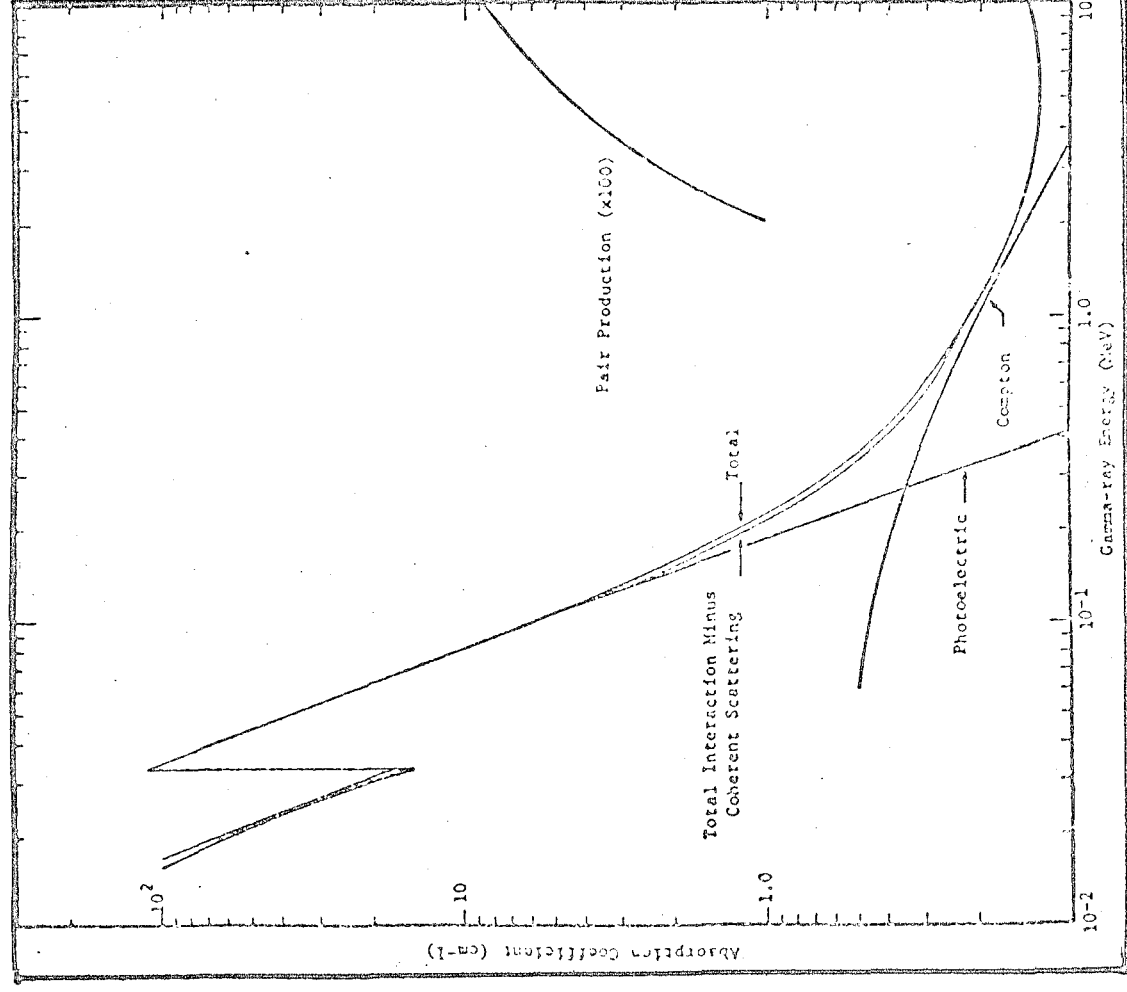


Figure: 2.5- Absorption coefficient for NaI(Tl) as a function of gamma-ray energy (Ec-68).

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 energy of the incident gamma-ray energy, spectrometry is possible. According to the size and the absorbing properties of the detector and to the energy of the measured gamma-ray, total or partial absorption can occur. Figure 2.6 shows the gamma spectra ^{24}Na (E_1 2.76 MeV, E_2 1.38 MeV) obtained with a "X2" NaI(Tl) detector. In this figure (a), (b), (c) represents the total absorption while (d), (e), (f) denote partial absorption. All processes giving rise to total absorption contribute to the formation of the peak at the highest energy side of the spectrum: the so called photo-peak. The coincidence of two or more gamma-rays in the detector, gives rise

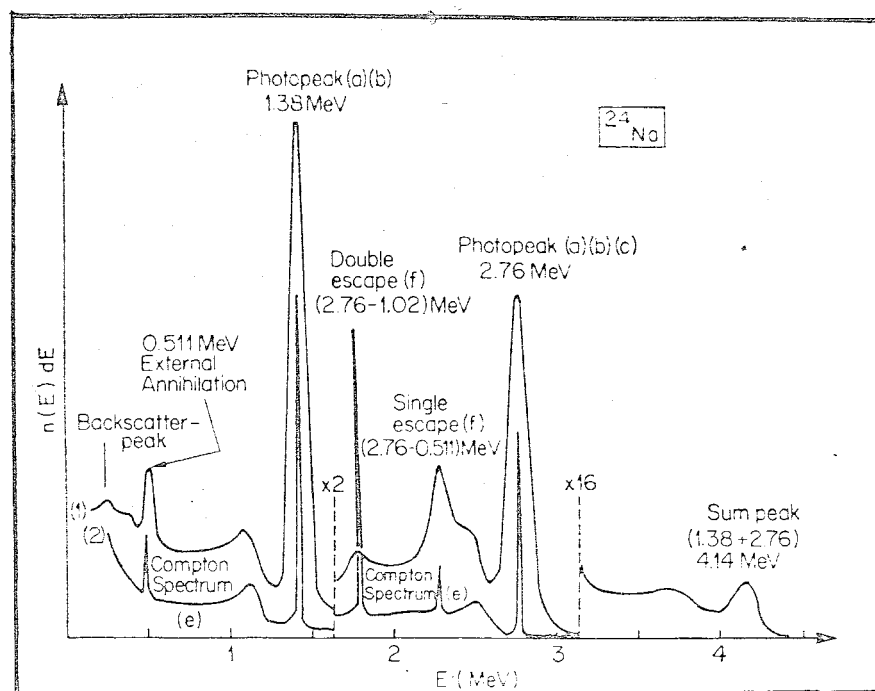


Figure: 2.6- Gamma spectrum of ^{24}Na measured with a NaI(Tl) (1) and with a Ge(Li) (2) detector (So-69).

to a sumpeak. The relative intensity of the sumpeak to the single peak is a function of the source detector geometry.

The energy of the unknown gamma-ray can be determined from the pulse-height of the photopeak maximum. The calibration of the spectrometer can be performed by means of isotopes emitting gamma-rays of known energies. catalogues of gamma-ray spectra measured with NaI(Tl) and Ge(Li) detectors are also available for the identification of gamma spectra (Cr-64, He-64, Le-68). In table 2.1a and 2.1b some calibration sources and respective energies are given.

Quantitative data of the gamma-ray intensity can be obtained from the area or the height of the photopeak. Since radiation is a statistical phenomenon, the photopeak can be described as a Gaussian error curve. The qualitative and quantitative of complex spectra, can be simplified by computer techniques. The qualitative analysis of the sample by comparison with the standards (reference spectra) can be performed by means of a least squares method, which also allows the calculation of the statistical error. The use of computers can be appreciated in activation analysis not only when dealing with a large number of routine analysis, but also for various tasks, e.g. gamma spectrum analysis, decay curve analysis, statistical treatment of data

optimizing, decay and counting conditions, etc. In section 3 a computer code "CORGAM" for complex gamma-ray analysis, is presented in detail. The method used in this code is given in the subsections of the same section, together with a complete listing of the program and a sample problem, in the appendices H, K and L.

Isotope	Energy (keV)	Isotope	Energy (keV)
^{241}Am	59.568 ± 0.017	^{95}Nb	765.83 ± 0.07
^{131}I	80.166 ± 0.009	^{54}Mn	834.84 ± 0.07
^{153}Gd	97.43 ± 0.02	^{88}Y	898.01 ± 0.07
^{153}Gd	103.18 ± 0.02	^{207}Bi	1063.82 ± 0.28
^{177}Lu	112.97	^{60}Co	1173.13 ± 0.04
^{141}Ce	145.44 ± 0.05	^{60}Co	1332.39 ± 0.05
^{139}Ce	165.84 ± 0.03	^{24}Na	1368.40 ± 0.04
		$^{60}\text{Co (D.E.)}$	1576.9 ± 0.32
^{177}Lu	208.36	$^{208}\text{Tl (ThC'') (D.E.)}$	1592.3 ± 0.13
^{203}Hg	279.12 ± 0.05	$^{24}\text{Na (D.E.)}$	1731.6 ± 0.16
^{131}I	364.47 ± 0.005	^{88}Y	1836.1 ± 0.07
		^{60}Co	2035.2 ± 0.50
		$^{60}\text{Co (D.E.)}$	2232.2 ± 0.67
^{198}Au	411.776 ± 0.01	$^{24}\text{Na (S.E.)}$	2242.6 ± 0.14
Annihilation	511.006 ± 0.02	^{60}Co	2598.9 ± 0.30
^{207}Bi	569.65 ± 0.10	$^{208}\text{Tl (ThC'')}$	2614.3 ± 0.09
^{137}Cs	661.59 ± 0.07	^{24}Na	2753.6 ± 0.12
		^{60}Co	3202.4 ± 0.65
		^{60}Co	3254.2 ± 0.65
		^{60}Co	3273.6 ± 0.4
		^{60}Co	3452.5 ± 0.75

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

Table: 2.1a- Calibration sources for gamma-ray spectrometry (So-69).

Energies (keV)	Relative energies			
	This work	Ref. 5	Ref. 4	Ref. 2
80.57 ± 0.20	14.48 ± 0.48	14.55 ± 0.45	13.33	14.50 ± 2.9
94.55 ± 0.15	0.3			0.16 ± 0.03
121.60 ± 0.15	0.78 ± 0.18			0.7 ± 0.50
160.70 ± 0.20	0.36 ± 0.15			0.35 ± 0.1
184.50 ± 0.25	100	100 ± 1	100	100
215.60 ± 0.25	3.94 ± 0.09	4.15 ± 0.06	4.44	3.8 ± 0.4
231.20 ± 0.30	0.36 ± 0.03	0.32 ± 0.05		0.3 ± 0.2
260.15 ± 0.30	1.77 ± 0.12	1.42 ± 0.10	1.11	1.8 ± 0.5
280.30 ± 0.30	38.61 ± 0.46	43.6 ± 0.4	33.33	39.5 ± 2.8
300.45 ± 0.40	4.77 ± 0.09	5.45 ± 0.05	4.44	4.8 ± 0.4
365.80 ± 0.30	2.93 ± 0.06	3.72 ± 0.07	2.22	2.9 ± 3
410.95 ± 0.30	15.50 ± 0.19	16.8 ± 0.2	13.33	15.8 ± 1.2
451.55 ± 0.25	3.48 ± 0.07	4.30 ± 0.08	3.32	3.5 ± 0.7
464.90 ± 0.25	2.00 ± 0.07	1.66 ± 0.08	2.22	2 ± 0.4
529.95 ± 0.30	10.16 ± 0.32	13 ± 0.40	13.33	10.3 ± 1
570.50 ± 0.30	6.77 ± 0.14	7.08 ± 0.14	7.77	6.8 ± 0.7
594.90 ± 0.20	1.28 ± 0.18	0.74 ± 0.10		1.2 ± 0.4
610.95 ± 0.15	1.48 ± 0.27	1.59 ± 0.32		1.4 ± 1.0
670.48 ± 0.2	7.01 ± 0.25	7.35 ± 0.29	6.66	7 ± 0.7
691.15 ± 0.15	1.85 ± 0.09	1.62 ± 0.08	1.11	1.9 ± 0.4
711.70 ± 0.20	71.65 ± 0.68	71.5 ± 0.7	64.44	72.5 ± 6
725.50 ± 0.2	0.2			0.19 ± 0.1
736.70 ± 0.20	0.46 ± 0.04	0.50 ± 0.05		0.45 ± 0.15
752.50 ± 0.25	16.06 ± 0.40	15.2 ± 0.30	15.55	16.1 ± 1.2
779.20 ± 0.45	3.72 ± 0.07	3.88 ± 0.06	4.44	3.8 ± 0.3
793.10 ± 0.20	0.2			0.17 ± 0.1
810.80 ± 0.40	76.38 ± 0.82	76.4 ± 0.80	66.66	76 ± 8
830.80 ± 0.30	12.07 ± 0.25	12.9 ± 0.30	12.22	12.5 ± 1.5
875.90 ± 0.20	1.14 ± 0.07	0.91 ± 0.04	0.88	1.15 ± 0.15
889.20 ± 0.15	0.7 ± 0.15			0.73
896.50 ± 0.10	0.7 ± 0.15			0.73
951.50 ± 0.20	3.5 ± 0.14	3.16 ± 0.12	3.66	3.6 ± 0.6
995.35 ± 0.25	0.68 ± 0.18			0.73 ± 0.24
1118.10 ± 0.20	0.30	0.26 ± 0.02	0.33	
1147.20 ± 0.20	0.38 ± 0.05	0.26 ± 0.02	0.22	0.38 ± 0.06
1241.80 ± 0.30	1.22 ± 0.05	1.06 ± 0.04	1.11	1.25 ± 0.25
1275.00 ± 0.25	0.75 ± 0.20			0.8 ± 0.15
1283.10 ± 0.20	0.38 ± 0.04	0.22 ± 0.02	0.33	0.8 ± 0.15
1401.30 ± 0.15	0.86 ± 0.05	0.72 ± 0.02	0.77	0.93 ± 0.09
1427.50 ± 0.20	0.65 ± 0.03	0.69 ± 0.02	0.66	0.69 ± 0.07

^a The intensity 184.50 keV is taken as 100 units.

Table: 2.1b- Energies and relative intensities^a in the decay of 1200 y ¹⁶⁶Ho^m. The errors quoted are one standard deviation.

2.3- SCINTILLATION DETECTORS

One of the oldest methods of nuclear-radiation detection makes use of light scintillations. It is well known that Rutherford and his collaborators used this technique for detecting alpha particles in the famous alpha-scattering experiments (Pr-64). The principle of these detectors is the classical one, long used in the spinthariscopes also (Pi-62). The same principle is applied in the detectors of radioactivity which are called scintillation counters; these consist of two parts, a scintillator in which the luminous effects are produced, and a photomultiplier (PM) to convert the light pulses into high amplitude electrical signals. The chief advantages of scintillation counters are that they provide pulses proportional to the energy of the particles, and they have high efficiency for gamma radiation as well as having large sensitive areas. Before discussing the scintillation detection mechanism, it is necessary to discuss the scintillation phenomenon itself. Many materials are excited by radiation and subsequently lose part of this excitation energy by the emission of low energy photons of radiation. However very few materials emit radiation of a wavelength that easily interacts with photomultiplier phosphor material and yet easily penetrate common glasses. Even fewer are transparent to their own emitted radiation (Ga-67). Luminescence is the general term describing the absorption of energy of any type by a substance and the reemission of some fraction of it as photons of visible or near visible light. Radiation energy is but one type of energy that can excite materials to initiate luminescence. Two types of luminescent emission can occur. By absorption of energy, electrons can be raised to higher excited states and can return to the ground state either directly or via a metastable state. This deexcitation which occurs in a time shorter than 10^{-8} s is called fluorescence (immediate emission). The energy of the emitted light is less than that of the absorbed one to reach the excited state. The electron occupying a metastable state, can be raised to a higher excited state and subsequently return to the ground state by emission of a photon. This process called phosphorescence, occurs after a time interval of about 10^{-8} sec after excitation (delayed emission). Scintillation theory is discussed in more detail by many authors (Bi-53, Cu-53).

The following groups of materials are known to possess desired properties as scintillators:

1. Crystalline inorganic substances
2. Crystalline organic substances

3. Solid organic solutions (plastics)

4. Liquid organic solutions

5. Rare gases

Among the desirable properties for good scintillators are high yield of fluorescent light, transparency for this emitted light, rapid light-emission in combination with the lowest possible phosphorescence and finally, a spectral distribution of the light suitable with regard to the sensitivity of existing photomultipliers. The demands in other respects, (density, size, geometrical shape, etc.) depend on the special situation in which the detector is to be used. A survey of the characteristics of the most commonly used phosphors is given in table 2.2.

Materials	Group	Density gm/cm ³	Wavelength of maximum emission Å°	Relative pulse height %	Alpha beta ratio %	ev/photon	Decay time nsec
Anthracene crystal	Single cryst. organic	1.25	4470	100	9	65	30
Trans-stilbene crystal	Single cryst. organic	1.15	4110	60	9	100	5
Liquid phosphors	Organic solution	0.86	~4000	40-60	9	150	5
Plastic phosphors	Organic solution	1.06	~4000	28-48	9	150	4
NaI(Tl)	Single cryst. inorganic	3.67	4130	210	44	30	250
ZnS(Ag)	Single cryst. inorganic	4.10	4500	200-300	100		200
LiI(Eu)	Single cryst. inorganic	4.06	4700	70	95		1200

Table: 2.2- Properties of some commonly used phosphors (Pr-64, So-69).

The inorganic scintillators are crystals of inorganic salts, primarily the alkali-halides, containing small amounts of impurities as activators for the luminescent process. The yield of fluorescent light is connected with the existence of luminescent centers in the crystal lattice. For these, the transition from the excited state, to the ground level is accompanied by the emission of a photon. Luminescent centers are created by the addition of certain activating substances. Sodium Iodide, activated by the addition of thallium, is the most widely used scintillator for gamma-ray spectrometry.

The important properties, and the theory of various other scintillators are given in many text books (Pr-64, Bi-53, Cu-53, So-69).

Radiation can be measured by the fluorescence phenomenon if a means of measuring the amount of light produced is available. The photomultiplier tube serves this purpose. A PM tube is a phototube in which the currents of photo-electrons from the tubes cathode is multiplied many times through the process of electron multiplication. The principle elements in each of these tubes are the photocathode for releasing the photoelectrons, the dynodes for producing the electron multiplication, and the anode for collecting the current pulse. An incident photon interacts with the photocathode material (usually a mixture of Antimony and Cesium) deposited on the inside of the glass cylinder and produces a photo-electron. A positive voltage applied to the first dynode with respect to the photocathode draws this photo-electron to the dynode. The photo-electron is accelerated sufficiently to cause electron multiplication upon its interception by the first dynode. Several electrons are typically emitted in the interaction of the photo-electron with the first dynode. These, in turn, are drawn to the second dynode which is maintained at a positive potential higher than the first one. The electron multiplication continues in this fashion at each dynode until all the electrons so produced are collected at the anode, which is located at the end of the dynode chain. The amount of electron multiplication at each dynode is a strong function of the voltage between dynodes. An approximate relation for the multiplication factor, M , at each stage is,

$$M = KV^7 \quad (2.9)$$

where V is the voltage in volts and K is a constant, and the total multiplication is given as :

$$A = M^n \quad (2.10)$$

where M is the multiplication at each stage and n is the number of stages. A more detailed discussion on PM tubes is given by Price (Pr-64). Figures 2.7, 2.8 and 2.9 are the schematic diagrams of three type of dynode arrangement for PM tubes.

Two important properties of PM tubes are the relative constancy of the electron multiplication factor M and of the transit time of the electrons through the multiplier structure. The former property effects the pulse-height resolution of the scintillation detector and the latter the resolving time. The resolution of a detector system is a measure of the extent

to which monoenergetic particles produce pulse heights of a single value. In gamma-ray spectrometry, the spread in the total-energy peak is a measure of the resolution, which is normally defined as,

$$R = \frac{W_n}{E_n} (100) \quad (2.11)$$

where R is the resolution in %, W_n is the full width at half maximum (MeV), E_n is the gamma-photon energy (MeV).

^{137}Cs generally is used as a comparison standard for resolution of a crystal. Literature values for typical resolutions range from 5-13 % (Pr-64).

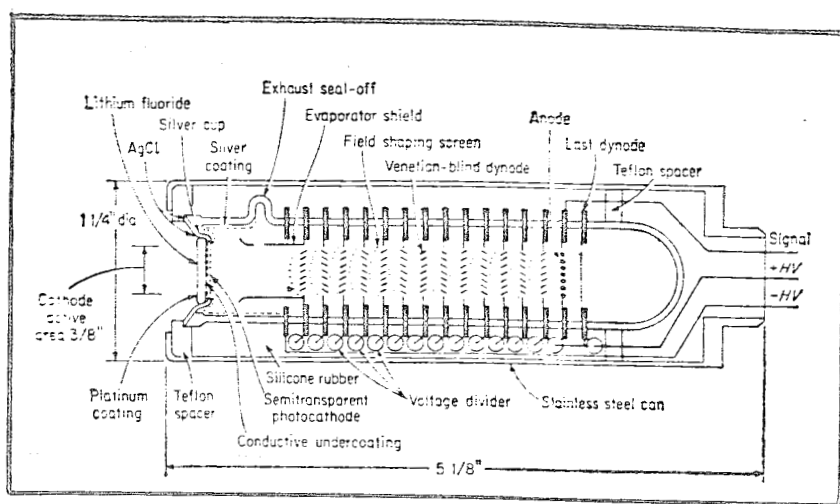


Figure: 2.7- ASCOP photomultiplier tube with Venetian-blind dynode structure. (Pr-64)

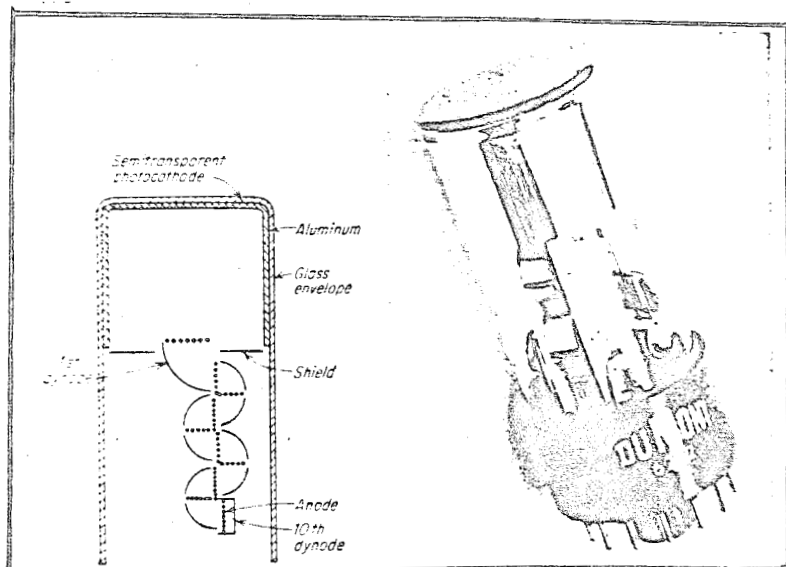


Figure: 2.8- Du Mont 6292 photomultiplier tube; diagram and photograph Box type dynode structure. (Pr-64)

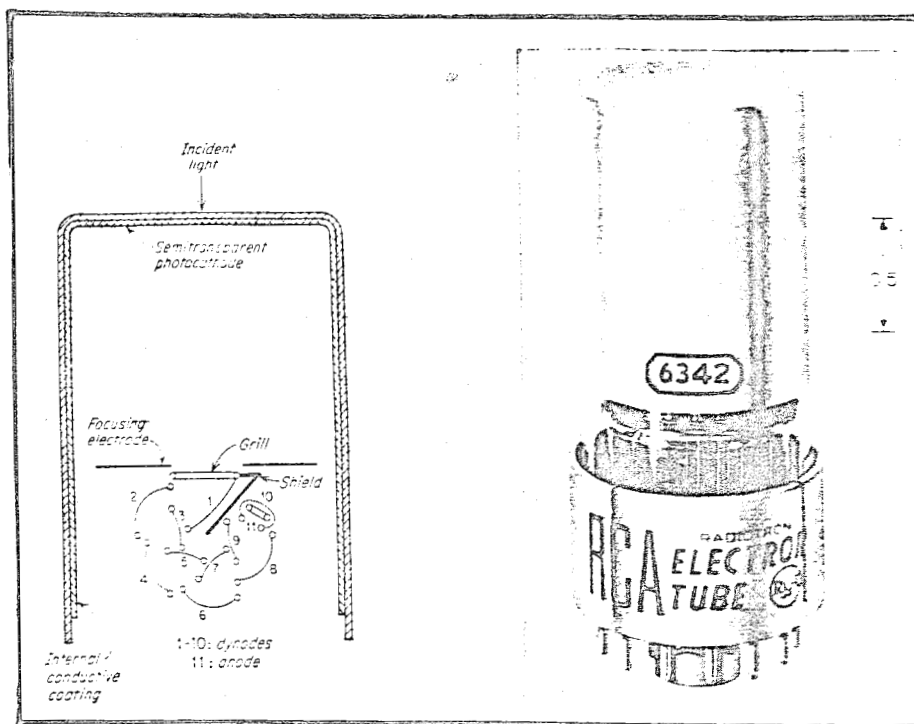


Figure: 2.9- RCA 6342 photomultiplier tube; diagram and photograph circularly focussed dynode structure. (Pr-64)

Figure 2.10 is the pulse-height spectrum obtained with a NaI(Tl) counter for a ^{137}Cs source.

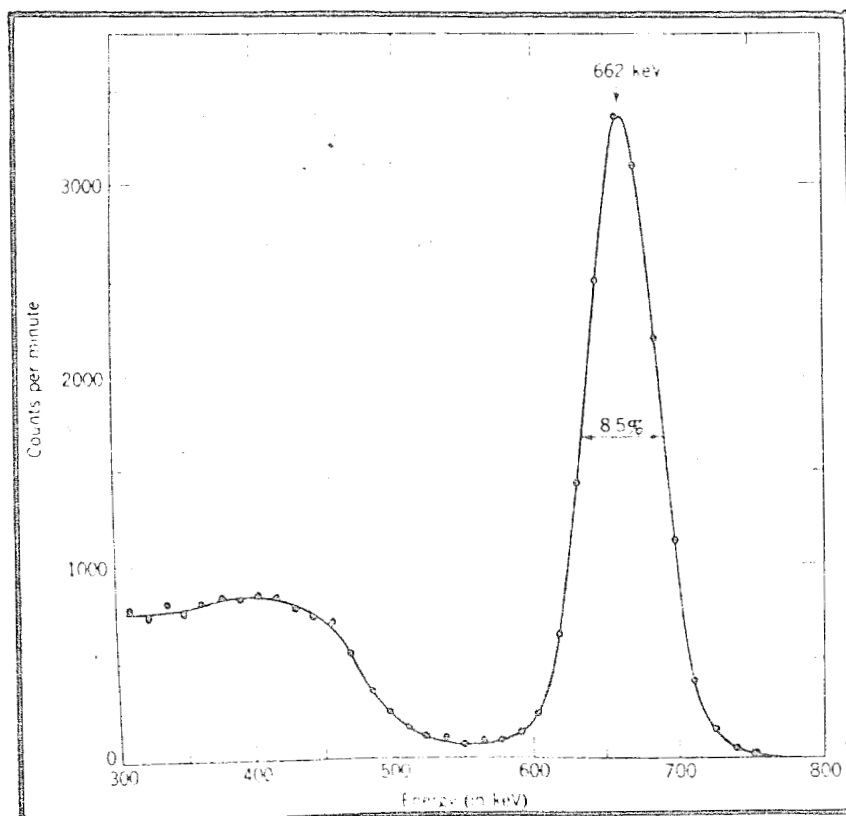


Figure: 2.10- Pulse-height spectrum obtained with a NaI(Tl) scintillation counter for a ^{137}Cs source. (P1-62)

The resolving time for counting measurements is the minimum time which must exist between successive events if they are to be counted as two events. Table 2.3 is a compilation of the important properties of various PM tubes.

Type	Maximum outside dimensions, in.		Cathode			Dynode system				Over-all voltage, volts
	Diam.	Length	Area, cm ²	Response	Av. sensitivity, $\mu\text{a/lumen}$	No. of dynodes	Type	Material	Gain	
RCA:										
5819	2 $\frac{1}{4}$	5 $\frac{13}{16}$	14.2	S-11	50	10	Circ. focused	Cs ₃ Sb	2.3×10^5	1,250
6342	2 $\frac{1}{4}$	5 $\frac{13}{16}$	14.2	S-11	60	10	Circ. focused	AgMg	0.55×10^6	1,500
6655	2 $\frac{1}{4}$	5 $\frac{13}{16}$	14.2	S-11	50	10	Circ. focused	Cs ₃ Sb	2.3×10^5	1,250
6199	1 $\frac{3}{16}$	4 $\frac{9}{16}$	7.75	S-11	45	10	Circ. focused	Cs ₃ Sb	2.8×10^5	1,250
6372	2 $\frac{9}{16}$	7 $\frac{3}{4}$	80	S-11	33	10	Circ. focused	Cs ₃ Sb	2.5×10^5	1,200
1P28	1 $\frac{5}{16}$	3 $\frac{11}{16}$	1.9	S-5	40	9	Circ. focused	Cs ₃ Sb	5.3×10^5	1,250
6819A	2 $\frac{1}{4}$	5 $\frac{13}{16}$	14.2	S-11	...	14	Circ. focused	AgMg	12.5×10^5	2,000
8055	5 $\frac{1}{2}$	6 $\frac{3}{4}$	97	S-11	75	10	Venetian blind	CuBe	1.5×10^5	2,000
Du Mont:										
6291	1 $\frac{1}{2}$	4 $\frac{1}{4}$	6.4	S-11	60	10	Box	AgMg	2×10^5	2,100
6292	2 $\frac{1}{16}$	5 $\frac{5}{8}$	13.4	S-11	60	10	Box	AgMg	2×10^5	2,100
6363	...	6 $\frac{1}{8}$	31.4	S-11	60	10	Box	AgMg	2×10^5	1,800
6364	5 $\frac{1}{4}$	7 $\frac{1}{2}$	88.8	S-11	60	10	Box	AgMg	2×10^5	1,800
6365	3 $\frac{1}{4}$	2 $\frac{3}{4}$	1.26	S-11	50	6	Box	AgMg	3×10^3	1,200
EMI-US:										
9536B	2	4 $\frac{3}{4}$	14.6	S-11	70	10	Venetian blind	Cs ₃ Sb	3×10^5	1,700
9545B	12 $\frac{1}{5}$	14 $\frac{1}{8}$	470	S-11	50	11	Venetian blind	Cs ₃ Sb	4×10^5	2,000
CBS:										
CL1012	1 $\frac{1}{2}$	4 $\frac{3}{4}$	8	S-11	60	10	Venetian blind	AgMg	2×10^5	1,750
ASCOP:										
541A	1 $\frac{1}{4}$	4 $\frac{1}{4}$	5.1	(Depends on window)	70	11	Venetian blind	AgMg	10^5	2,100
543A	2	7 $\frac{1}{2}$	11.6	S-11	60	11	Venetian blind	AgMg	10^5	2,100

Table: 2.3- Characteristics of a few commercial photomultipliers. (

Besides scintillation counters a wide variety of detectors are used for radiation detection purposes. A detailed study of these detectors may be found in references (Pr-64, Cr-64, Bi-53, Cu-53, Ko-61, Ga-67, Ev-55).

Gas filled detectors:

Three of the oldest but still very useful nuclear radiation detector types are the ionization chambers, the proportional counter, and the Geiger-Müller (GM) tubes. The difference in the three systems can be seen through the pulse-height versus applied-voltage curves of figure 2.11. The system consists of a gas-filled chamber with a central electrode well insulated from the chamber walls. These detectors use the principle of electrical conductivity of the gas resulting from the ionization produced by the nuclear radiation.

Semiconductor radiation detectors:

In this detector, an electric field is set up across a semiconducting medium of low electrical conductivity. When a charged particle passes through the medium, electron hole pairs are produced in it. The charges are separated by the field and collected at electrodes, producing an electrical signal which can be amplified, recorded and used to give information about the particles detected.

Several other types of detectors are in use and are quite important for specialized detection problems. These detectors are Cloud Chambers, Nuclear Track Plates, Spark Chambers, Cherenkov Counters, Chemical Detectors, Calorimetric Methods, and various types of Neutron Detectors. (Pr-64).

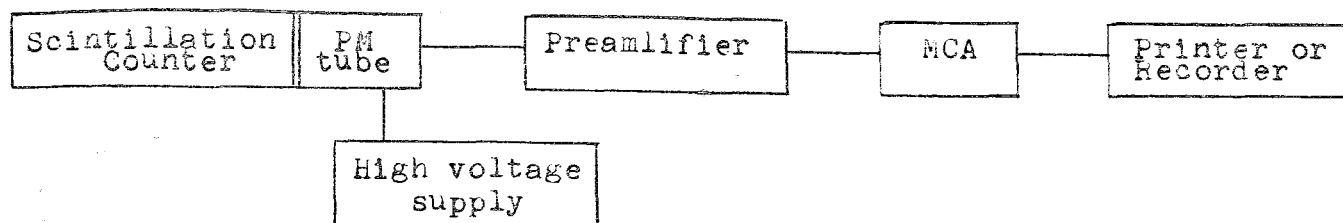
2.4- AUXILIARY ELECTRONIC EQUIPMENT

As it is discussed in the previous subsections the output of a scintillation detector is an electrical signal. In order to analyse this signal some auxiliary equipment is needed. A complete instrument for the measurement of nuclear radiation consists of a combination of a detector one or more electronic units which perform the functions required. The main functions of these electronic devices are supplying the necessary voltage to the detector amplifying the detector output signal to a suitable level; registering, presenting and analysing the amplified signal (Er-64).

Like all others, scintillation detectors also, need a very well stabilized high voltage supply, which is used to create a potential difference between the successive dynodes of the PM tube. Preamplifiers are used where signals are so small that a normal amplifier is not able to amplify them sufficiently or where some amplification or impedance matching is required to offset cable losses. Finally there exists a large variety of electronic equipment which is used as the analysing apparatus (Pr-64).

One of the important properties of a scintillation detector is its ability to give an indication of the energy of the incident radiation. Because of this property, the pulse-height distribution curves from a scintillation detector can be used to determine the energy spectrum of incident radiation. The object in pulse-height analysis is to determine the total number of pulses whose heights fall in selected intervals or channels. If this analysis is made by sampling one channel at a time, the device is referred to as a single-channel pulse-height analyzer (SCA). However, in many applications it is essential to accumulate data without any loss, so multi-channel analyzers (MCA) are used for this purpose. These instruments all consist of some or all of the following elements: 1) a section that associates each input signal with a specific amplitude channel, 2) a memory, or data storage device that contains the information on this number of pulses in each channel until this information is recorded otherwise, 3) a data display device, 4) auxiliary readout devices such as curve plotters, paper-tape or card-punches, magnetic tape, typewriters, etc.

Below is a block diagram of an electronic arrangement used in pulse-height spectrometry. An over all discussion of the techniques of MCA's as well as other methods for pulse-height-to-digital conversion is given by Chase (Ch-61).



The most widely used method employs pulse-height-to-time converters. Figure 2.12 illustrates this process. First the signal pulse "a" is converted to a flat-topped one "b" by means of a pulse-stretching circuit. At the start of the pulse, a linearly rising signal "c" is switched on, and a series of equally spaced pulses "d" is started. When "c" reaches "b", the pulse train "d" is stopped. In this manner the pulse heights are converted into trains of clock pulses, and different channels now correspond to trains with different numbers of clock pulses. These trains of pulses can be sorted, stored, displayed and read out by various techniques that have been developed for digital computers (Ch=61).

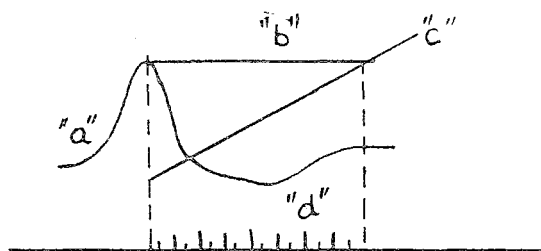


Figure: 2.12- Schematic representation of pulse-height-to-time conversion.

The MCA's are a logical extension of SCA's. By employing n differential discriminators set at successive window levels and each having its own counting system, an n -channel analysis is obtained. The principle advantage of this approach is that its time resolution can be made less than 1 μ sec. However there are two serious disadvantages. First, this arrangement, having n separate channels consequently n circuits, is costly to construct and maintain. Second, it is a difficult design to maintain equal window widths. In general the MCA's are very sophisticated instruments, with good accuracy and versatility.

2.5- STATISTICAL INTERPRETATION OF THE RESULTS

The measurement of nuclear radiation by the detection systems introduced in previous subsections, involve phenomena which are statistical in nature. By the use of statistical analysis, estimates can be made of the accuracy of the measurements, and procedures can be devised which will minimize errors due to random nature of the process. Obviously, the statistical analysis cannot obviate the need for sound analytical techniques, but unnecessary loss of operator time in the laboratory can be eliminated and the reliability of the results increased by the use of statistical methods.

Two kinds of error can be met in radiation detection; 1) systematic errors, which determine the accuracy of a result, 2) random errors, which determine the reproducibility or precision. By systematic errors the experimental results deviate from the true value, because of a bias. Statistics, on the other hand, deal with random errors. It makes no sense to define an error as the deviation of a measurement from the true value, as the latter is usually unknown. Thus "error" can only be defined after evaluation of the most probable value of the quantity measured. For a number "n" of observations $x_1, x_2, \dots, x_n$, made under the same conditions and all equally reliable, the arithmetic mean ($\bar{x}$) is the best value for this set of observations.

$$\bar{x} = \sum_{i=1}^n x_i / n \quad (2.12)$$

If all observations are not equally reliable a statistical weight w_i can be introduced. The most probable value is then the "weighted mean", sometimes called "general or probable mean" (Gr-74):

$$\bar{x} = \frac{\sum_{i=1}^n w_i x_i}{\sum_{i=1}^n w_i} \quad (2.13)$$

The choice on w_i , the weighing parameters, depends upon the experimental conditions and the scatter of data. The reproducibility of an analytical method is usually expressed by the standard deviation $\sigma(x)$ on a single determination. The standard deviation is defined as the square root of the average value of the square of the individual deviations from the most probable value (mean), taken for a large number of observations. Thus,

$$\sigma^2 = \frac{1}{n-1} \sum_{i=1}^n (\bar{x} - x_i)^2 \quad (2.14)$$

where $n-1$ indicates the degrees of freedom of the observation set.

As the arithmetic mean for an infinite number of observations is usually not accessible, it is only possible to calculate the probability that this value is contained within the limits $\bar{x} \pm \Delta x$. The number Δx can be chosen arbitrarily small. It is common practice to express Δx in terms of the standard deviation, e.g. $\pm \Delta x = \pm t \sigma$, where t depends on the probability level and on the number of degrees of freedom. If the latter is large, t is replaced by u . Where " u " is the number of standard deviations for large degrees of freedom. The degree of confidence increases, as the "confidence interval" increases (see table 2.4).

Constant u	Probability P	P'	Error
0.6745	0.500	0.500	"Probable error"
1.000	0.683	0.317	"Standard deviation" (σ) (rms error)
1.177	0.761	0.239	
1.645	0.900	0.100	"nine-tenths error" or "reliable error"
1.960	0.950	0.050	"ninety-five hundredths error"
2.576	0.990	0.010	"ninety-nine hundredths error"
2.807	0.995	0.005	
3.000	0.9973	0.0027	3σ
3.291	0.999	0.001	
4.000	0.99994	0.00006	4σ

Table: 2.4- Probability levels (So-69).

The radioactive decay has a statistical character. If a radionuclide is counted several times in identical experimental conditions, different counting rates (number of counts per unit time) will be observed, even for very long lived species. It can be shown that the probability $P(n)$ of obtaining n disintegrations in a time Δt from N_0 original radioactive atoms is given by the Binomial distribution (Fr-67).

$$P(n) = \frac{N_0!}{(N_0 - n)! n!} (1 - e^{-\lambda \Delta t})^n (e^{-\lambda \Delta t})^{N_0 - n} \quad (2.15)$$

where $(1 - e^{-\lambda \Delta t})$ is the probability of an atom disintegrating in a time Δt and $e^{-\lambda \Delta t}$ the probability of surviving through the time Δt . The Binomial distribution may be replaced by the simpler Poisson distribution (Fr-67), the probability $P(n)$ of finding n disintegration is then given by equation 2.16, where m is the average to be expected

$$P(n) = \frac{m^n e^{-m}}{n!} \quad (2.16)$$

on condition that $\lambda \Delta t < 0.01$ and $N_0 \geq 100$.

For small disintegration rates, the distribution is not symmetrical around $n=m$. For m (or n) > 100 and $m \approx n$ the Poisson distribution can be replaced by the normal or Gaussian distribution:

$$P(n) = \frac{(2\pi)^{-1/2}}{\sigma} \exp \left(-\frac{(m-n)^2}{2\sigma^2} \right) \quad (2.17)$$

where, σ and m designate the standard deviation and the true mean, respectively. Figure 2.13 illustrates the form of the distribution along with its most important properties.

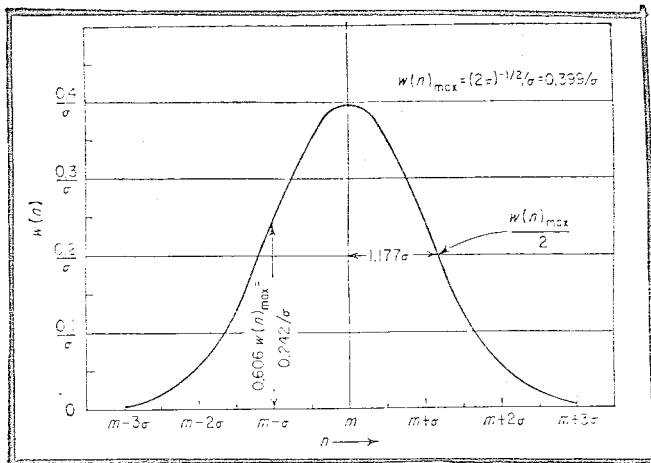


Figure: 2.13- Illustration the normal distribution function (Pr-64).

It will be noticed that this distribution is symmetrical about $n=m$. For the Poisson and Gaussian distributions one may derive $\sigma = \sqrt{m}$, or for large n , $\sigma \approx \sqrt{n}$.

An important concept of statistical interpretation of radioactive disintegration is the confidence intervals, discussed in detail by Curie (Cu-68). If the observed number of counts from a sample + background and from the background alone, for an equal time of measurement Δt , are respectively C_{s+b} and C_b , then the count difference $C_s = C_{s+b} - C_b$ is a measure of the net activity of the sample. However, owing to the statistical fluctuations, this count difference at the averages of the background $\bar{C}_b$ and the sample $\bar{C}_s$ may obtain various values. At a relatively small value of C_s , the presence of the activity in the sample becomes doubtful. Therefore a so-called "critical value" L_c is introduced, that is often called "decision limit" (Cu-68). For $C_s > L_c$ one assumes that the signal is present, for $C_s < L_c$ the signal will not be detected. Due to this assumption, two kinds of errors may occur:

1-The measured value $C_s > L_c$, one concludes that the activity > 0 when in fact it is equal to zero (type 1 error).

2-The measured value $C_S < L_C$, one concludes that the activity is equal to zero when in fact the activity > 0 (type 2 error).

As appears from figure 2.14, the critical level is mathematically given by:

$$L_C = u_1 \sigma(0) \quad (2.18)$$

The parameter u_1 is a multiple of the standard deviation, determining the probability of making the type 1 error. Usual values for u_1 are 1.645, 1.960, 3.000. Contrary to table 2.4, this does not correspond to a confidence level of 90, 95 and 99.73 % respectively but to a confidence level of 95, 97.5 and 99.865 % respectively. Indeed the probability of making the type 1 error is respectively 5, 2.5, 0.135 % only (one side of the Gauss curve). For that reason, the symbol u has been replaced by u_1 .

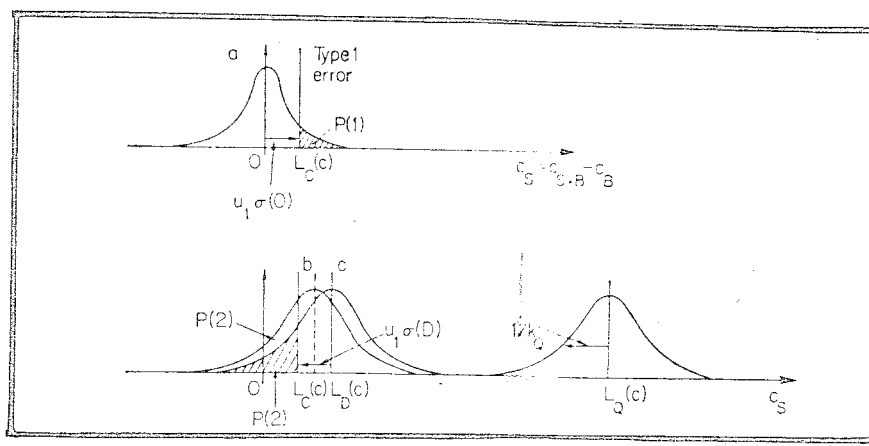


Figure: 2.14- Signal detection. Definition of critical level L_C (So-69).

A number of tests have been devised to answer the question as to whether or not a given set of data fits a certain distribution function. The concept of Poisson's index of dispersion is particularly useful in this regard. To make this test, the quantity χ^2 , defined as

$$\chi^2 = \frac{\sum_{i=1}^n (\bar{x} - x_i)^2}{\bar{x}} \quad (2.19)$$

is calculated. Here n is the number of times that a given counting determination is made, x_i is the value obtained in the i^{th} measurement, and $\bar{x}$ is the

average value. If the value of χ^2 is sufficiently large so that there is only a small probability of occurrence of a value this high, it is an indication of trouble in the experiment. Likewise if χ^2 is small, the corresponding data should be questioned because the spread in it is so small. Thus it is seen that the Poisson index-of-dispersion test can be helpful in determining whether or not the counting equipment is functioning satisfactorily.

Chauvenet's criterion is frequently used for the rejection of outlying data. The criterion states that any one in a series of n readings may be rejected when its deviation from the mean of the series is such that the probability of occurrence of all deviations from the mean as large or larger is less than $n/2$ (So-69, Gr-74).

An overall application of statistical methods briefly mentioned here can be found in the computer code CORGAM, which is introduced in section 3.

2.6- USE OF COMPUTERS IN NEUTRON ACTIVATION ANALYSIS

When experimental data resulting from an activity counting and thus subject to statistical fluctuations, have to be treated, a smoothing routine can be desirable. This is the case when dealing with gamma spectra or decay curves, which have to be analyzed by means of a computer. The simplest smoothing routine is the graphical smoothing, but it can be applied only when data are graphically evaluated.

Mathematical data convolution techniques largely correct for statistical scatter. The simplest convolution sets the convolution integer equal to one, giving rise to a "rectangular" convolution, i.e., a normal moving average. One also can use a symmetrical triangular convolution, one-sided exponential or symmetrical exponential convolution. But a more exact procedure can be achieved by using a least squares method. In this technique one tries to fit the best curve through the set of points under consideration. In this way it is possible to obtain a set of equations of the n^{th} order with $2n+1$ coefficients as unknowns. It is obvious that the calculations needed for one smoothed point are time consuming.

After data smoothing, the analysis of the gamma spectra can be performed in several ways. With the development of high resolution detectors, using a large number of channels per spectrum, the computer becomes practically unavoidable for analysis purposes.

The location of the photo-peak in a gamma spectrum, and the calculation of the corresponding area is of extreme importance in NAA. This can be done by a computer program, and qualitative and quantitative analysis can be made possible in this way. The technique employed in photo-peak positioning is the use of the first derivative of the smoothed spectrum. The exact location of the peak can be found by means of the second derivative. Both, first and second derivative can be calculated according to the least squares method.

Once the photo-peaks have been located, the activity under the peaks can be determined by subtracting the detector background. As the net photo-peak activities are obtained, one could conceive a complete activation analysis program. By treating the spectra of standards and samples in the same way, and correcting for irradiation time, decay time, and counting time, the results of the analysis can be computed. When the components or constituents of a complex gamma spectrum are qualitatively known, as is often the case in NAA, the only problem is to determine "how much" of each is present

in the sample. From a complex spectrum and from the spectra of composing standards one can compute the best value for the ratios of each component to its respective standard and also the standard deviation (So-69).

A great number of computer programs are available, for the analysis of complex gamma-ray spectra (NEA-CPL). Among them the ones recently prepared are given in the appendix N.

3. C O R G A M

3.1- CORGAM-A COMPUTER CODE FOR NEUTRON ACTIVATION ANALYSIS

The importance of computers in NAA was mentioned in previous sections, and a list of computer programs developed for the analysis of gamma-ray spectra is also given in appendix N.

Each of these codes have their own techniques in unfolding complex gamma-ray spectra. All these codes are prepared in order to estimate the intensity coefficients of the general linear hypothesis, which will be discussed in the subsection 3.2. There are many methods for estimating these coefficients. These methods, stripping, least squares, incremental, iterative, vector analysis, and stepwise regression, have been used for estimating these coefficients. All of these procedures may use either least squares or approximate least squares techniques. "Regression analysis" has been used to describe 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. Because a model is used in which only significant variables are retained in the final solution, a more appropriate description for this work is "Correlation Analysis". (NEA-CPL, Ec-68).

Among the codes available by NEA-CPL in the experimental data processing field, "CORGAM" (A Correlation Algorithm for Gamma-Ray Spectra) is the one which uses correlation analysis in unfolding gamma-ray spectra.

In the present section of the thesis, a detailed description of CORGAM will be given. The listing of the program, flow diagram, input data for sample problem, instruction for users and the output of a sample problem are given in the appendices.

In CORGAM, a correlation algorithm is coded to allow the unfolding of complex gamma-ray spectra, typically collected in a NAA procedure.

CORGAM,

- a) Compensates for electronic shifts in the data,
- b) Corrects for the background,
- c) Normalizes the data to a fixed neutron flux level,
- d) Allows a choice of weighting factors,
- e) Allows a choice of methods for calculation of standard deviations.

The code requires a matrix of reference gamma-ray spectra. These spectra

can be in a raw data form. All of the modifications available to the complex gamma-ray spectra are also available to the reference gamma-ray spectra. In addition, a decay correction is available for the reference gamma-ray spectra. Only the reference gamma-ray spectra that have intensity coefficients which have significance at a prescribed level of significance are retained in the final solution. The intermediate ones, i.e., those solutions that contain reference gamma-ray spectra which have nonsignificant intensity coefficients at the prescribed level, are printed out. Therefore, several solutions are imbedded in the final solution.

A backward elimination least squares method is employed. The elimination is one in which the student's t value of each intensity is compared to a t value at a prescribed level of significance (Gr-74). The calculation of the standard deviation for each intensity coefficients accounts for randomness in both the complex and reference gamma-ray spectra.

Currently the program is restricted to a problem of 400 channels and 15 reference spectra. There would be no difficulty in expanding this to as many as 4096 channels. However, the number of reference spectra is limited by the accuracy desired in the inversion procedure. The inversion program currently being used would suffer (from the accuracy standpoint) if the number of reference spectra were greater than 25.

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. The intermediate results can be printed, and the level of significance of each of the intensity coefficients can be observed.

A typical analysis, involving 256 channels and 14 reference spectra and using reference spectra which were suitably aligned, requires less than 1 minute of execution time on IBM 360/50.

CORGAM was coded for IBM 360/50 using Fortran IV, level G. An intermediate disk storage is required. The source deck contains 1303 cards. The code is updated by the author for UNIVAC-1106 using Fortran IV and Cobol. The updated form of the code is recorded onto a magnetic tape for further use in BU-NE Department.

The tape contains in the,

1. File: IBM 360/50 version of CORGAM sample data,
2. File: UNIVAC-1106 version of CORGAM,
3. File: Sample problem input data,
4. File: Sample problem output data.

3.2- THEORY OF CORGAM

If a nuclear reaction, such that

$$X (n, \gamma) Y, \quad (3.1)$$

is forced to proceed, the radioactivity of the product nuclei Y, is directly proportional to the number of the atoms of the parent nuclei X. The equation governing the rate of formation of Y is given by the well known differential equation.

$$\frac{dN}{dt} = \dot{N} = \sigma N_0 \phi - \lambda N \quad (3.2)$$

where,

- N is the time dependent nuclide (Y) concentration,
- $\dot{N}$ is the derivative with respect to time,
- N_0 is the time dependent parent nuclide (X) concentration,
- σ is the microscopic activation cross-section,
- ϕ is the time dependent neutron flux.

The parent nuclide concentration can be given in terms of N and the initial parent nuclide concentration, N_0^0 , as

$$N_0 = N_0^0 - N \quad (3.3)$$

Therefore equation 3.2 can be written as,

$$\frac{dN}{dt} = \dot{N} = \sigma \phi N_0^0 - (\lambda + \sigma \phi) N \quad (3.4)$$

If the neutron flux is a constant $\phi = \phi_0$ then equation 3.4 has the following solution,

$$N = \frac{\sigma \phi_0 N_0^0}{(\lambda + \sigma \phi_0)} (1 - e^{-(\lambda + \sigma \phi_0)t}) \quad (3.5)$$

It can be seen from equation 3.5 that the time dependency of N_0 can be ignored if $\sigma \phi_0 \ll \lambda$ or $\sigma \phi_0 / \lambda \ll 1.0$.

The following table is a compilation of λ , σ and $\sigma \phi_0$ values for many of the elements used in common NAA work. The value for ϕ_0 used in this table

of the Nuclides" by D.T.Goldman 1965.

isotope	$t_{1/2}$ $\text{sec} \times 10^{-3}$	λ $\text{sec}^{-1} \times 10^4$	$\sigma \phi_0$ $\text{sec}^{-1} \times 10^{11}$	$\sigma \phi_0 / \lambda$
Na ²⁴	54.00	0.128	0.13	1.01×10^{-7}
Mg ²⁷	0.57	12.160	0.03	2.47×10^{-10}
Al ²⁸	0.14	50.220	0.23	4.55×10^{-10}
S ³⁷	0.31	22.650	0.14	6.16×10^{-10}
Cl ³⁸	2.24	3.097	0.43	1.39×10^{-8}
K ⁴²	44.64	0.155	1.10	7.09×10^{-7}
Ca ⁴⁹	0.53	13.120	1.10	8.38×10^{-9}
Ti ⁵¹	0.35	19.910	0.14	7.03×10^{-10}
V ⁵²	0.23	30.640	4.90	1.60×10^{-8}
Mn ⁵⁶	9.29	0.746	13.30	1.76×10^{-6}
Cu ⁶⁴	46.44	0.144	4.50	3.12×10^{-7}
Br ⁸⁰	1.08	6.416	11.40	1.78×10^{-7}
Br ⁸²	127.08	0.055	3.20	5.87×10^{-6}
I ¹²⁸	1.50	4.620	6.40	1.39×10^{-7}

Table: 3.1- Compilation of nuclear properties of several isotopes (Ec-68).

The values for $\sigma \phi_0 / \lambda$ given in table 3.1 been much less than unity, the time dependency of the equation 3.5 can be ignored. With these assumptions equation 3.2 can be solved to obtain A, an expression for activity,

$$A \equiv \lambda N = \sigma N_0 \phi_0 (1 - e^{-\lambda t}) e^{-\lambda t} \quad (3.6)$$

where t is the time of neutron flux exposure, t' is the time after removal from the neutron flux, ϕ_0 is the neutron flux, a constant.

When the activity is predominantly gamma radiation, both a qualitative and quantitative analysis can be performed through the use of a gamma-ray spectrometer system and the proper data analysis procedure.

The gamma-ray spectrum of a complex sample containing several isotopes (m in number) may be represented by:

$$y_i = \sum_{j=1}^m B_{ij} \quad , \quad i=1,2,3,\dots,n \quad (3.7)$$

where, y_i is the counts registered in channel i of a MCA,

B_{ij} is the counts registered in channel i from j^{th} constituent isotope

Reference gamma-ray spectra are collected for each of the m constituent isotopes using known quantities of radioisotopes. The reference gamma-ray spectra of each of the m constituent isotopes are related to the complex gamma-ray spectrum by,

$$y_i = \sum_{j=1}^m x_{ij} B_j + e_i \quad , \quad i=1,2,3,\dots,m \quad (3.8)$$

where, B_j is the intensity coefficient for isotope j , i.e., a coefficient proportional to the quantity of isotope j in the complex sample,

x_{ij} is the counts registered in channel i from the j^{th} isotope of known quantity,

e_i is the deviation at point i of the estimated value of y_i , $\sum_{j=1}^m x_{ij} B_j$, from the observed value, y_i ,

Since negative quantities of radioactivity are physically impossible, the following restriction is necessary:

$$B_j \geq 0 \quad , \quad j=1,2,3,\dots,m \quad (3.9)$$

Equation 3.8 and inequality 3.9 form a constrained general linear hypothesis. Therefore, the problem is to estimate the intensity coefficients. The minimization of the sum of the squared error, i.e., least squares, generally yield estimators for the intensity coefficients with desirable statistical properties, e.g., least squares estimators are unbiased if the data are free of systematic errors (Ec-68).

The linear hypothesis, in matrix form, is

$$\underline{Y} = \underline{XB} + \underline{e} \quad (3.10)$$

where,

Y: (nx1) vector of dependent variable values,
 X: (nxm) matrix of independent variable values,
 B: (mx1) vector of solution values,
 e: (nx1) vector of errors (deviation values),
 n: number of data points (channels),
 m: number of reference isotopes.

The sum of the squared errors is given by:

$$e'e = (Y - XB)'(Y - XB) , \quad (3.11)$$

which reduces to,

$$e'e = Y'Y - 2B'X'Y + B'X'XB \quad (3.12)$$

The estimator, b for B results from minimizing $e'e$. If the elements of B are linearly independent, $e'e$ is differentiated with respect to each element of B, term by term, the result is equated to zero, and arranged in matrix form after B is replaced by its estimator, $\hat{B}$. This results in;

$$(X'X) b = X'Y \quad (3.13)$$

The estimate, b, is obtained by solving equation 3.13 for b:

$$b = (X'X)^{-1}(X'Y) \quad (3.14)$$

Irrespective of the error probability distribution function, the estimates, b, for the true parameters, B, calculated from equation 3.14 minimize the sum of the squared error. Rewriting equations 3.13 and 3.14 and including the error variance-covariance matrix, the following equations are obtained (Gr-74)

$$(X'V^{-1}X) b = (X'V^{-1}Y) \quad (3.15)$$

$$\text{and} \quad b = (X'V^{-1}X)^{-1}(X'V^{-1}Y) \quad (3.16)$$

where V^{-1} is the inverse of the error variance-covariance matrix and is often denoted as a weighting matrix, W.

$$W \equiv V^{-1} \quad (3.17)$$

If the errors are assumed to be statistically independent, the covariance terms for e will be zero and estimate for the variance of e_1 , $\sigma^2(e_1)$, can be obtained from,

$$\sigma^2(e_i) = \sigma^2(y_i) + \sum_{j=1}^m [B_j^2 \sigma^2(x_{ij}) + x_{ij}^2 \sigma^2(B_j)] \quad (3.18)$$

where $\sigma^2(x_{ij})$: the variance of the counts in channel i from isotope j
 $\sigma^2(B_j)$: variance of the estimator for the j^{th} isotope.

An iterative approach is used to solve for b , as follows:

1. Estimate $\sigma^2(e_1)$, given in equation 3.18 using only $\sigma^2(y_1)$,
2. Calculate the first estimate, b_1 , of b given in equation 3.16 using the estimated $\sigma^2(e_1)$ from step 1.,
3. Estimate $\sigma^2(e_1)$ by using b_1 for B and $\sigma^2(b_1)$ for $\sigma^2(b)$ in equation 3.18,
4. Calculate b_2 using the estimated $\sigma^2(e_1)$
5. Continue this procedure until a termination criterion is met.

This iterative procedure can be mathematically stated as,

$$b_n = (X^0 W_n X)^{-1} (X^0 W_n Y) , \quad (3.19)$$

$$W_{in} = [\sigma_n^2(e_i)]^{-1} = \left\{ \sigma^2(y_i) + \sum_{j=1}^m [b_{j,n-1}^2 \sigma^2(x_{ij}) + x_{ij}^2 \sigma_{n-1}^2(b_j)] \right\} \quad (3.20)$$

$$b_{j_0} = \sigma_0^2(b_j) = 0 \quad (3.21)$$

The termination criterion used is:

$$\chi^2/DF \leq 1 + U_p \sqrt{(2/DF)} \quad (3.22)$$

where, χ^2 : Chi squared, i.e., $\sum_{i=1}^n \frac{[y_i - \sum_{j=1}^m x_{ij} b_j]^2}{\sigma^2(e_i)}$

U_p : Confidence interval factor,

DF: Degrees of freedom, i.e., $n-m-1$,

/DF; is called the quality of fit number.

U_p factor corresponds to a desired level of significance. Since the numerator of χ^2 is the minimization criterion used in this method, it is not reasonable to assume that the iteration procedure will increase χ^2/DF . Therefore, only a one-sided region is included in equation 3.22 (Ec-68). The mathematical model of this approach can be found in some detail in

The least squares is a logical method to determine the intensity coefficients for NAA problem. (Ak-77). However, one of the difficulties in applying least squares technique to the resolution of gamma spectra is that the calculated intensity coefficients can be negative or it may be difficult to determine the reference spectra that comprise the complex spectrum. For example, the least squares technique may yield positive intensity coefficients for all the reference spectra, but some may not be significant. To overcome those difficulties, the t value for the null hypothesis is calculated for each intensity coefficient (Gr-74). The t values then are used in the correlation algorithm to eliminate reference spectra for which the calculated intensity coefficients are negative or not significant. An outline of the correlation algorithm used in the code is given in figure 3.1. Some of the statistical techniques used in CORGAM, namely, properties of estimators, least squares technique, curve fitting method, interpolation and determinant evaluation methods are given in the appendices. And a more detailed logic diagram is also given in the appendix J. If needed a complete description of the methods used in CORGAM can be found in its manual.

This code, CORGAM has been used to analyze many gamma-ray spectra from several cereal and feed grain samples (Ec-68). Each sample was irradiated in the rotary specimen rack of a KSU TRIGA Mark II nuclear reactor at 100 kW power for 15 minutes. A small (0.02 gm) copper powder sample was irradiated with each grain sample. The area of the 0.511 MeV photopeak from ^{64}Cu was used for neutron fluence normalization. Each sample was transferred to a nonirradiated container and was counted at 10 cm from 3" x 3" NaI(Tl) scintillation crystal, which was interfaced to a TMC-4096 multiparameter system. The reference spectra required by CORGAM had been collected in an identical manner (Ec-68).

Due to the special purpose of cereal analysis problems, the reference spectra contained in the library of the code is formed from those spectra of the elements contained in agricultural samples. These reference isotopes are: ^{24}Na , ^{42}K , ^{56}Mn , ^{38}Cl , ^{80}Br , ^{82}Br , ^{49}Ca , ^{28}Al , ^{27}Mg , ^{64}Cu , ^{128}I , and ^{37}S . But it is possible to replace the reference spectra by the ones needed for the analysis of other mixtures. It should be remembered that the reference data collection and that of the complex one should be done in identical conditions.

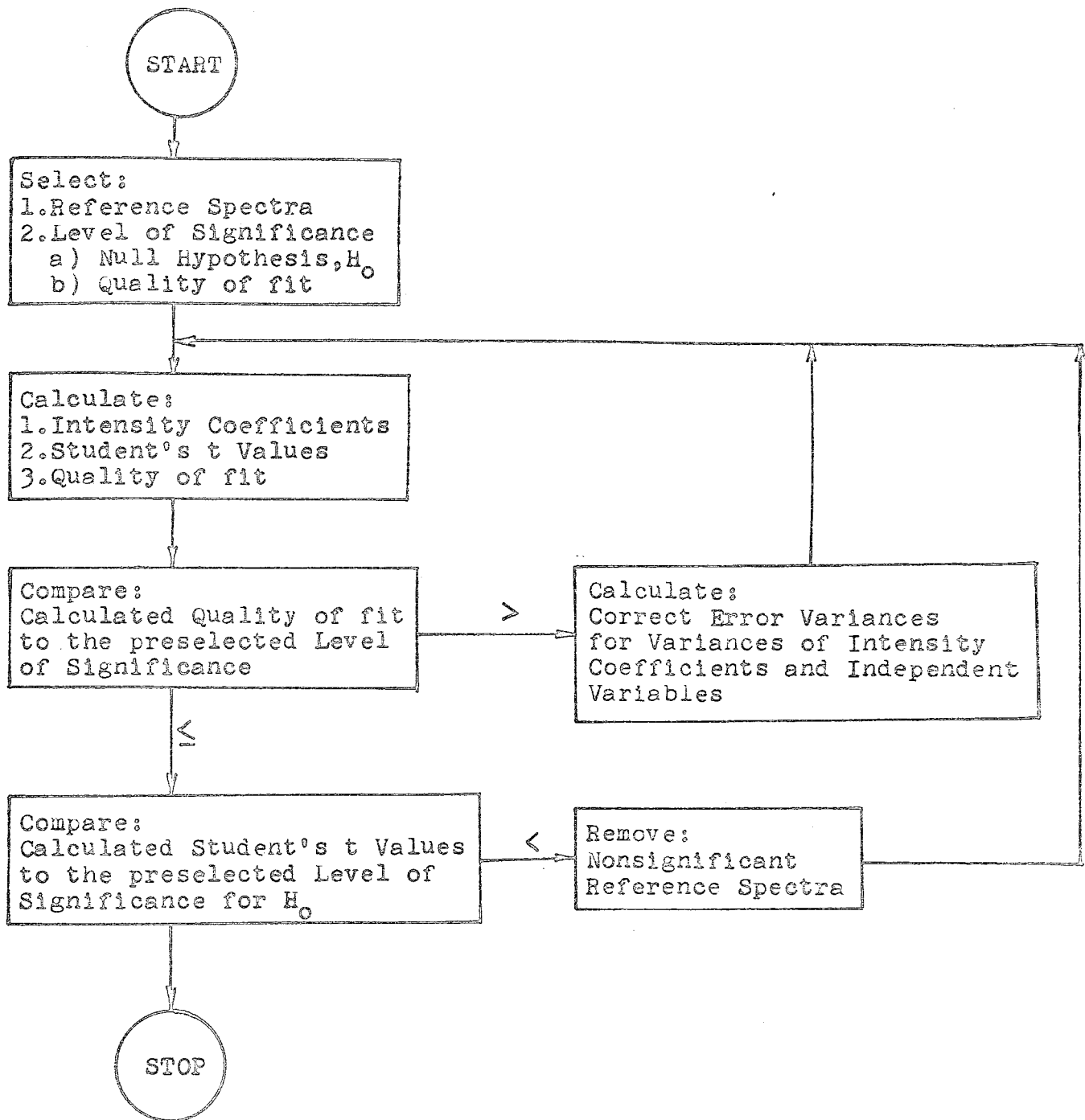


Figure: 3.1- Outline of correlation algorithm for resolution of gamma spectra.

3.3- EXPERIMENTAL PROCEDURE OF CORGAM

Previous use of CORGAM was for the routine analysis of agricultural samples. In order to perform this analysis, the experimental procedure used is given in this section (Ec-68). The input data of the same experiment is used to run the program. The listing of the input data and that of the output obtained from the sample problem run are given in the appendix L. During the data collection of the sample problem the following equipment were used.

1. Shielded counting arrangement: A lead shielded counting cavity with interior dimensions of 24" x 24" x 30" was constructed of 2" x 4" x 8" lead bricks, with exterior walls 4" thick, and top and bottom 2" thick. The interior of the cavity was lined with 0.025" thick cadmium sheet followed by 0.025" thick copper sheet. Shielded counting cavity and wall construction details are illustrated in figure 3.2. By using this cavity background is reduced by a factor of 20 %.
2. Detector assembly: The scintillation crystal used is Harshaw 3"x3" NaI(Tl), solid type crystal, Model 12512, serial CC362 integral line. It uses an RCA 8054 photomultiplier tube, the resolution of the crystal is 8.07 %.
3. Preamplifiers: Two main purposes of a preamplifier are to serve an impedance matching and an amplification function. The preamplifier used in this experiment was TMC model DS-13 with a gain of approximately 2.0.
4. Multichannel analyzer: The multichannel analyzer is used to sort and store voltage pulses according to their respective heights. The pulses are sorted into differential pulse height units, i.e., from V_0 to $V_0 + V$. That function is carried out by converting the pulse height to time and measuring the elapsed time from pulse base to pulse height. The analyzer used in this experiment was the TMC 4096 multiparameter system.
5. Neutron source: KSU TRIGA Mark II nuclear reactor was used as a source of thermal neutrons. A typical irradiation for neutron activation analysis is made in either the pneumatic transfer unit or in the rotary specimen rack. In table 3.2 the approximate neutron flux values per watt of power at those two locations are compared.

The block diagram of the NAA instrumentation system is shown in figure

3.3.

6. Reference spectra: Spectroscopically pure compounds were irradiated to collect the reference spectra used in this experiment. Table 3.3 is a compilation of information about each of these compounds.

Neutron Energy	Pneumatic transfer unit $\text{n/cm}^2\text{-sec-watt}$	Rotary specimen rack $\text{n/cm}^2\text{-sec-watt}$
Thermal	1.7×10^7	7.2×10^6
Fast	1.4×10^7	6.0×10^6

Table: 3.2- Neutron flux levels for KSU TRIGA Mark II nuclear reactor (EG-68)

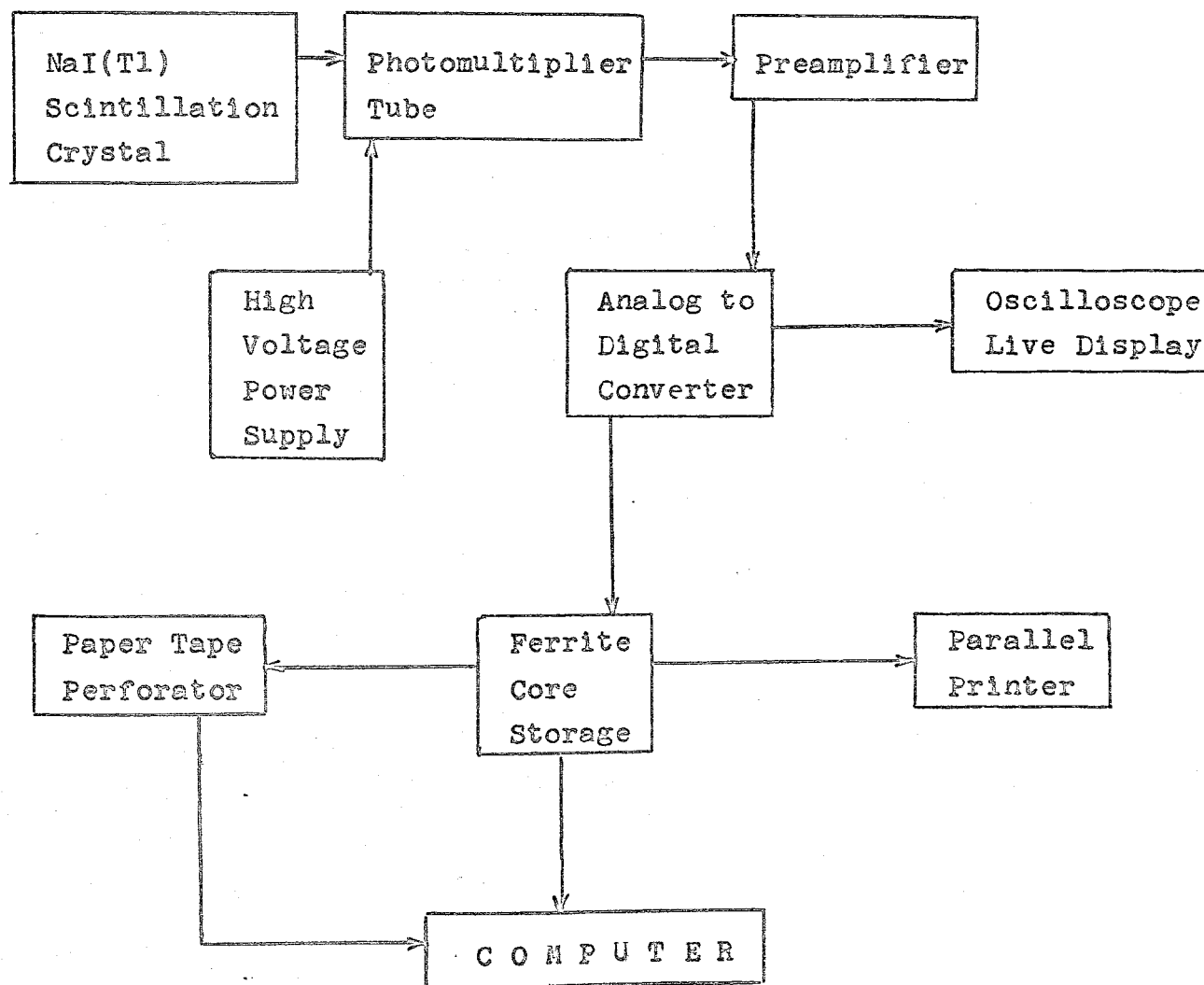


Figure: 3.3- Block Diagram of the NAA instrumentation system.

Table: 3.3- Reference spectra information.(Ec-68)

Element	Chemical Form	%H ₂ O Hydration	Reference isotope	Half Life (min)	Irradiation Policy "	Weight (gm)
Na	Na ₂ CO ₃	6.8	Na ²⁴	900.0	1-4-2-10	0.229
K	K ₂ CO ₃	5.1	K ⁴²	744.0	4-4-5-10	0.299
Mn	metal	0.0	Mn ⁵⁶	154.8	2-4-2-0.1	0.0806
Cl	NH ₄ Cl	0.0	Cl ³⁸	37.3	2-5-2-50	0.0130
Br	NH ₄ Br	0.0	Br ⁸⁰	18.0	2-65-2-90	0.0304
			Br ⁸²	2118.0	2-1707-10	
Ca	CaCO ₃	1.4	Ca ⁴⁹	8.8	2-5-2-10	0.194
Al	Al ₂ O ₃	3.9	Al ²⁸	2.3	1-12-2-10	0.0628
Mg	MgO	5.5	Mg ²⁷	9.5	2-5-2-10	0.0788
Cu	powder	0.0	Cu ⁶⁴	774.0	1-112-3-10	0.0321
I	KI	0.3	I ¹²⁸	25.0	2-5-2-50	0.0252
S	powder	0.0	S ³⁷	5.1	2-5-2-50	0.2064

" The first number is the irradiation time in minutes.The second number is the decay time in minutes.The third number is the counting time in minutes.The fourth number is the reactor power level in kilowatts.

The reference spectra were collected using the following procedure: A small amount (≤ 1.0 gram) of each spectroscopically pure reference compound, and a small amount of copper powder were irradiated in the rotary specimen rack (RSR) of the KSU TRIGA Mark II nuclear reactor for the times given in table 3.3.After the respective times had elapsed,the reference spectra were collected for the counting time given in table 3.3,using the solid " x3" NaI(Tl) scintillation crystal.

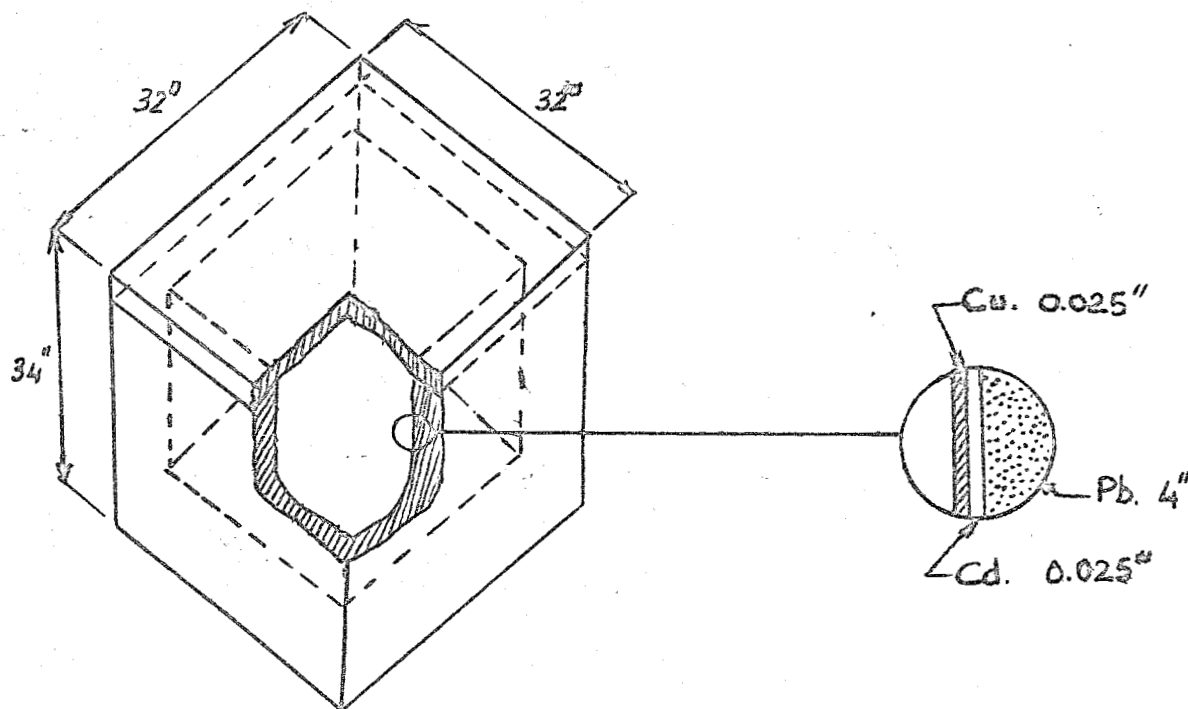


Figure: 3.2- Shielded counting cavity dimensions and details (Ec-68).

Instabilities in the spectrometer system used to collect the gamma-ray spectra can cause shifts to occur in these spectra. To compensate for these inconsistencies, the gamma-ray photopeaks of the spectra were fit to a Gaussian function using a linearized least squares method. The mid-point corresponding to the gamma-ray energy was calculated from the relation, $X_0 = E/G$ where E is the gamma-ray energy in MeV. If a reference spectrum contains more than one gamma-ray photopeak, these mid-channel values were used to calculate the slope and intercept of the relation, $E = a_0 + GX_0$, where E is the gamma-ray energy in MeV and X_0 is the mid-channel value of the photopeak. However, if the reference spectrum contains only one photopeak, the intercept was assumed to be zero. Using these parameters, each spectrum was shifted to a slope and intercept of 14.5 keV/ch and zero, respectively. Each of the gamma-ray photopeaks in the shifted spectra was fitted to a Gaussian function (Ec-68).

A more detailed description of the procedure and various applications performed by using CORGAM can be found in the reference Ec-68.

4. DISCUSSION AND CONCLUSION

The importance of neutron activation analysis was mentioned in the previous subsections. It is also mentioned that the determination of the micro constituents of a complex sample was possible down to the ppm (parts per million) level. In the study of the principles of NAA, it is noticed that the interaction of gamma radiation with the detector material was very important. The gamma-rays resulting from the decay of activated nuclei, interact with the detector. If the material of the detector is a phosphor, scintillations are produced in the phosphor resulting from the interaction of the incoming photons with the detector material. These scintillations are transformed into electrical signals by the photomultiplier tube. The signals are then amplified, measured and recorded by the use of proper electronic equipments. The most widely used electronic equipment is a multichannel analyzer, which gives a distribution of the incoming photons with respect to their energies. This amplitude versus energy distribution of the photons is called the gamma-ray spectrum of the activated nuclei. Due to the character of the interactions of gamma-rays with a particular scintillation crystal, produces a unique gamma-ray spectrum. The analysis of this spectrum by the methods described in this work, gives the necessary information about the nature and the concentration of the constituents of the complex sample. Among the methods used in common NAA work, the correlation algorithm is found to be the best method for the resolution of gamma-ray spectra.

A predesigned computer code which uses the correlation algorithm in the unfolding procedure of a complex gamma-ray spectrum is also analyzed. In this analysis it is observed that the program is restricted to a problem of 400 channels and 15 reference spectra. There would be no difficulty in expanding this to as many as 4096 channels. However due to the accuracy desired in the inversion procedure, the number of reference isotopes is limited. CORGAM is a novel method of unfolding complex gamma-ray spectra because only reference spectra that have intensity coefficients which are significant at a preselected level are retained in the output and the variance calculations include contributions from both the reference and complex spectra. The large computing time required by the NAA can be eliminated by the use of a computer program. A typical analysis, involving 256 channels and 14 reference spectra, requires less than 1 minute of execution time on an IBM 360/50. Although the computer memory requirements are large for the correlation

algorithm as it was programmed for the IBM 360/50, it is possible to segment the program for adaptation to a smaller computer. In order to use this program in NAA, changes should be made on the reference spectra and on the flux reference spectra according to the laboratory conditions. The choice of the spectrometr system affects the results in various ways. When a NaI(Tl) crystal is used the interferences of the various reference spectra became significant. Use of a Ge(Li) semiconductor detector eliminates these interferences to a desired level.

Presently the code contains eleven reference spectra in its library, if needed these spectra can be changed by the ones required for a specific analysis. Since the number of reference spectra is limited by 15 isotopes, at each special problem, need may arise to change the reference library. It is concluded that this procedure was very time consuming when the spectrometer system is not branched to the computer where the program will be run.

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APPENDICES

APPENDIX A

-PROPERTIES OF ESTIMATORS

The estimate of the intensity coefficients (concentrations) of the equation 3.14 have the following properties;

- a) Unbiased (Gr-61): An estimator, a , for the parameter α is defined as an unbiased estimator of α if

$$E(a) = \alpha \quad (A-1)$$

where E represents the mathematical expectation. The mathematical expectation is defined by the following theorem (Ho-63).

Theorem: Let $\underline{x}$ be a random variable with density $f(x)$. The expected value of a function u of the random variable $\underline{x}$ is,

$$E(u(x)) = \sum_x u(x_1) f(x_1) \quad (A-2)$$

if $\underline{x}$ is discrete, and

$$E(u(\underline{x})) = \int_{-\infty}^{\infty} u(x) f(x) dx \quad (A-3)$$

if $\underline{x}$ is continuous.

Therefore, the mathematical expectation is just the mean value of the function u of the random variable $\underline{x}$.

- b) Minimum variance (Gr-61): An estimator, a , is defined to be the minimum variance estimator of the parameter α if

$$E((a - E(a))^2) \leq E((a' - E(a'))^2) \quad (A-4)$$

The term $E((a - E(a))^2)$ is defined to be the variance of the parameter α .

- c) Sufficiency (Ho-63): Let $f(\underline{x}, \alpha)$ be a joint frequency function involving the parameter α and the random variable $\underline{x}$, n in number. Let $a_1, h_1(\underline{x}), a_2, h_2(\underline{x}), \dots, a_k, h_k(\underline{x})$ be a set of statistics and $a'_1, h'_1(\underline{x}), a'_2, h'_2(\underline{x}), \dots, a'_k, h'_k(\underline{x})$ be any other set of estimators which are not functions of a_1, a_2, a_k . If $g(\underline{a}'/\underline{a})$, the conditional density function of $\underline{a}'$ given $\underline{a}$, does not involve α , the set $\underline{a}$ is called a set of sufficient statistics. This means that "all the information" contained in the n values of $\underline{x}$ is given

by the k parameters $\underline{a}$ where $k \leq n$.

- d) Consistency (Mo-63): If $\underline{a}$ is a sequence of estimators of α , they are simple consistent estimators, if for every $\epsilon > 0$

$$\lim_{n \rightarrow \infty} P(|\bar{a}_n - \alpha| \leq \epsilon) = 1 \quad (\text{A-5})$$

Further, the estimators, $\underline{a}$, are squared error consistent estimators of α , if

$$\lim_{n \rightarrow \infty} \left\{ E((\bar{a}_n - \alpha)^2) - \frac{1}{n} \sum_i (a_i - \alpha)^2 \right\} = 0 \quad (\text{A-6})$$

where

$$\bar{a}_n = \frac{1}{n} \sum_i a_i$$

Squared error consistency implies that both the bias and variance of $\underline{a}$ approach zero as the number of sample points increase.

- e) Efficiency (Br-65): efficiency of an estimator is defined to be the ratio of the variance of the minimum variance estimators to the variance of the estimator in question. Thus, minimum variance estimators are said to be efficient estimators.

APPENDIX B-THE LEAST SQUARES METHOD

The method is used to determine the intensity coefficients for the NAA problem. To illustrate the method, consider a set of n points, (x, y) . The points are assumed to be related by the linear hypothesis (Gr-74):

$$y_i = B_0 + B_1 x_i + e_i, \quad i = 1, 2, 3, \dots, n \quad (B-1)$$

where e_i is the deviation at point i of the estimated value, from its observed value, y_i . B_0, B_1 are the true values of the intercept and slope, respectively. The estimators, b_0 and b_1 , for B_0 and B_1 can be obtained by minimizing the sum of the squared errors;

$$S = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - (B_0 + B_1 x_i))^2 \quad (B-2)$$

S is minimized by differentiating with respect to B_0 , and B_1 and equating the results to zero. Also, b_0 and b_1 , the estimators, are substituted for B_0 and B_1 . The resulting equations are;

$$\sum_{i=1}^n (y_i - (b_0 + b_1 x_i)) = 0 \quad (B-3)$$

$$\sum_{i=1}^n \{x_i (y_i - (b_0 + b_1 x_i))\} = 0 \quad (B-4)$$

Equations B-3 and B-4 can be rearranged into a form called the normal equations.

$$b_0 n + b_1 \sum_{i=1}^n x_i = \sum_{i=1}^n y_i \quad (B-5)$$

$$b_0 \sum_{i=1}^n x_i + b_1 \sum_{i=1}^n x_i^2 = \sum_{i=1}^n y_i x_i \quad (B-6)$$

Solving equations B-5 and B-6 for b_0 and b_1 , results in

$$b_1 = \frac{\sum_{i=1}^n x_i y_i - ((\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i))/n}{\sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2/n} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (B-7)$$

$$b_0 = \bar{y} - b_1 \bar{x} \quad (B-8)$$

where,

$$\bar{y} = (\sum_{i=1}^n y_i)/n, \quad \bar{x} = (\sum_{i=1}^n x_i)/n.$$

Equation B-1 can be rewritten in terms of the estimator, b_1 , and the mean value $\bar{x}$ and $\bar{y}$, through the use of equation B-8.

$$y_i = \bar{y} + b_1(x_i - \bar{x}), \quad i=1,2,3,\dots,n \quad (B-9)$$

Equation B-9 can be rewritten in matrix form as,

$$\underline{Y} = \underline{X}b_1, \quad (B-10)$$

where $\underline{Y} = (y - \bar{y}) = (n \times 1)$ vector of the dependent values

$\underline{X} = (x - \bar{x}) = (n \times m)$ matrix of the independent variables.

In matrix form, the linear hypothesis model, equation B-1, is more appropriately written as,

$$\underline{Y} = \underline{B}'\underline{X}' + \underline{e} \quad (B-11)$$

where $\underline{X}'$ is the transpose of the $(n \times m)$ matrix $\underline{X}$

$\underline{B}'$ is the transpose of the $(m \times 1)$ solution vector $\underline{B}$

$\underline{e}$ is the $(n \times 1)$ vector of deviations.

More often equation B-11 is written in the following form:

$$\underline{Y} = \underline{X}\underline{B} + \underline{e} \quad (B-12)$$

APPENDIX C

-CURVE FITTING METHODS

The following method was used to fit the photopeaks to a Gaussian function (Ec-68).

First the photopeaks were assumed to be pure Gaussian, i.e.,

$$y_1 = y_0 \exp(-(x_1 - x_0)^2 / b_0) , \quad (C-1)$$

y_1 is the counts in channel 1 of a photopeak,

y_0 is the count corresponding to channel x_0 ,

x_0 is the mean channel of the Gaussian function

x_1 is the channel number

$$b_0 = 2\sigma^2,$$

σ^2 is the variance of the Gaussian function.

Equation C-1 is non linear and must be linearized to apply the principle of least squares. The logarithm of equation C-1 yields a linear form.

$$\ln y_1 = \ln y_0 - \frac{x_0^2}{b_0} + \frac{2x_0}{b_0} x_1 - \frac{1}{b_0} x_1^2 \quad (C-2)$$

Equation C-2 can be rewritten in terms of new variables,

$$z_1 = a_1 + a_2 x_1 + a_3 x_1^2 \quad (C-3)$$

where,

$$z_1 \equiv \ln y_1 ,$$

$$a_1 \equiv \ln y_0 - \frac{x_0^2}{b_0} , \quad a_2 = \frac{2x_0}{b_0} ,$$

$$a_3 = -\frac{1}{b_0}$$

The principle of least squares applied to equation C-3 yields the following matrix equation

$$a = (X^0 W X)^{-1} (X^0 W Z) , \quad (C-4)$$

where a is a (3×1) vector of the coefficients a_1, a_2 and a_3 ,

X is a $(n \times 3)$ matrix whose first column is composed of all unity values; the second column is composed of the x_i values, and the third column is

composed of the x_2 values

X' is the transpose of X ,

Z is a $(n \times 1)$ vector of the z_1 values,

W is a $(n \times n)$ diagonal weighting matrix whose elements are the inverse of the variances of the z_1 values,

n is the number of data points.

The variance of z_1 can be obtained by

$$\sigma^2(z_i) = \frac{1}{y_i^2} \quad \sigma^2(y_i) = \frac{1}{y_i} \quad (C-5)$$

It should be noted that by applying the principle of least squares to equation C-3 instead of to equation C-1 the minimum total squared deviation is,

$$S_D = \sum_{i=1}^n \left\{ y_i - y_0 \exp \left[- (x_i - x_0)^2 / b_0 \right] \right\}^2 \quad (C-6)$$

The desired minimum total deviation is,

$$S_L = \sum_{i=1}^n \left[\ln y_i - \left(\ln y_0 - \frac{x_0^2}{b_0} + \frac{2x_0}{b_0} x_i - \frac{1}{b_0} x_i^2 \right) \right]^2 \quad (C-7)$$

Minimizing S_L does not guarantee a minimum for S_D . To minimize S_D requires an iterative technique which employs a Taylor's series expansion and can result in unstable solutions for cases with variations in the data. In addition this method requires a significantly longer amount of computation time.

Variance values of y_0 , x_0 , and b_0 , could be obtained by

$$\sigma^2(y_0) = \left[C_{4,4} + \frac{a_2^2}{4a_3^2} (C_{2,2} + \frac{a_2^2}{4a_3^2} C_{3,3}) \right] \exp \left[2(a_1 - \frac{a_2^2}{4a_3}) \right] \quad (C-8)$$

$$\sigma^2(x_0) = \frac{1}{4a_3^2} \left[C_{2,2} + \left(\frac{a_2}{a_3} \right)^2 C_{3,3} \right] \quad (C-9)$$

$$\sigma^2(b_0) = C_{3,3} / a_3^4, \quad (C-10)$$

where,

a_1, a_2, a_3 , are the elements of the vector a , and $C_{4,4}, C_{2,2}, C_{3,3}$ are the diagonal elements of the $(X'WX)^{-1}$ matrix. Since the y_0 value is just a normalization term, it could also be calculated by minimizing S_D after x_0 and b_0 were obtained by minimizing S_L . This method yielded lower variance values for y_0 (Gr-74). Hence, y_0 and (y_0) were calculated from,

$$y_0 = \sum_{i=1}^n w_i y_i k_i / \sum_{i=1}^n w_i k_i^2, \quad (C-11)$$

$$\sigma^2(y_0) = \left[\sum_{i=1}^n w_i k_i^2 \right]^{-1} \quad (C-12)$$

where

n is the number of data points used in the fit,

$$k_i = \exp(-(x_i - x_0)^2 / b_0)$$

In deriving equation C-12 it was assumed that $w_i = \frac{1}{y_i}$.

APPENDIX D-LAGRANGIAN INTERPOLATION

This interpolation method is used in the subprogram REFIN, to interpolate between the decay spectra of a reference isotope.

The method is based on polynomial interpolating functions (Ak-77). Assume that a function $y = f(x)$ is given at $(n-1)$ points, say $x_0, x_1, x_2, \dots, x_n$, and determine a polynomial $F(x)$ of degree n or less such that

$$F(x_i) = f(x_i) \quad i = 0, 1, 2, \dots, n \quad (D-1)$$

It may be proved that the polynomial exists and it is unique. For this purpose two alternative proofs will be given.

Proof 1:

Let $F(x)$ function is written as

$$F(x) = L_0 y_0 + L_1 y_1 + \dots + L_n y_n \quad (D-2)$$

where

$$y_0 = f(x_0), \quad y_1 = f(x_1), \quad \dots, \quad y_n = f(x_n) \quad (D-3)$$

and

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \left(\frac{x - x_j}{x_i - x_j} \right) \quad i = 0, 1, 2, \dots, n \quad (D-4)$$

It is clear that each $L_i(x)$ term is a polynomial of degree n or less and rewriting it explicitly as

$$L_i(x) = \frac{(x-x_0)(x-x_1)(x-x_2)\dots(x-x_{i-1})(x-x_{i+1})\dots(x-x_n)}{(x_i-x_0)(x_i-x_1)(x_i-x_2)\dots(x_i-x_{i-1})(x_i-x_{i+1})\dots(x_i-x_n)} \quad (D-5)$$

it is obvious that $f(x_j) = F(x_j)$ because for $j \neq i$, where $j = 0, 1, \dots, n$, all $L_i(x_j)$ terms are zero. For $j = i$ case $L_i(x_j) = 1$ and therefore,

$$F(x_j) = L_0(x_j)y_0 + L_1(x_j)y_1 + L_2(x_j)y_2 + \dots + L_n(x_j)y_n \quad (D-6)$$

$$\text{becomes} \quad F(x_j) = y_i \quad \text{where} \quad y_i = f(x_i) \quad (D-7)$$

Proof 2:

An alternative method to determine the interpolating polynomial will be given using the method of undetermined coefficients.

(a) being any convenient value, then

$$F(x_1) = C_0(x-a)^n + C_1(x-a)^{n-1} + \dots + C_n \quad (D-8)$$

The coefficients $C_0, C_1, \dots, C_n$ will be such that

$$F(x_i) = f(x_i) \quad \text{or} \quad F(x_i) = y_i \quad (D-9)$$

is satisfied. Obviously, C_k coefficients must satisfy the following system of linear algebraic equations,

$$\begin{array}{rcl} C_0(x_0-a)^n + C_1(x_0-a)^{n-1} + \dots + C_n & = & y_0 \\ C_0(x_1-a)^n + C_1(x_1-a)^{n-1} + \dots + C_n & = & y_1 \\ \vdots & & \vdots \\ C_0(x_n-a)^n + C_1(x_n-a)^{n-1} + \dots + C_n & = & y_n \end{array} \quad (D-10)$$

This system of $n+1$ equations in terms of $n+1$ unknowns will have a solution if the coefficient matrix is nonsingular. The determinant of the coefficient matrix, which is known as Vandermonde determinant, is written as

$$\Delta = \begin{vmatrix} (x_0-a)^n & (x_0-a)^{n-1} & \dots & (x_0-a) & 1 \\ (x_1-a)^n & (x_1-a)^{n-1} & \dots & (x_1-a) & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ (x_n-a)^n & (x_n-a)^{n-1} & \dots & (x_n-a) & 1 \end{vmatrix} \quad (D-11)$$

and its value is given as

$$\Delta = \prod_{\substack{i,j=0 \\ i < j}}^n (x_i - x_j) \quad (D-12)$$

Since x_i are distinct, it follows that $\Delta \neq 0$ and C_k can be uniquely determined. Quite often in computations $a=0$ is taken (Jo-74).

APPENDIX E-DETERMINANT EVALUATION BY CHIO'S METHOD (PIVOTAL CONDENSATION)

This method is used in the subprogram DET in order to evaluate the determinant of the (X^0WX) matrix.

This method continuously reduces the order of the determinant by one, using a series of subtractions (Ak-77). For the explanation of the method suppose a $(4,4)$ matrix A is given.

$$|A| = a_{11} \begin{vmatrix} 1 & a'_{12} & a'_{13} & a'_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix} = a_{11} \begin{vmatrix} 1 & 0 & 0 & 0 \\ a_{21} & a''_{22} & a''_{23} & a''_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix}$$

1 2 3

where

$$a'_{12} = \frac{a_{12}}{a_{11}}, \quad a'_{13} = \frac{a_{13}}{a_{11}}, \quad a'_{14} = \frac{a_{14}}{a_{11}}$$

in the second step, performing the following operations,

- 1: $(2^{\text{nd}} \text{ col.}) - a'_{12} \times (1^{\text{st}} \text{ col.})$
- 2: $(3^{\text{rd}} \text{ col.}) - a'_{13} \times (1^{\text{st}} \text{ col.})$
- 3: $(4^{\text{th}} \text{ col.}) - a'_{14} \times (1^{\text{st}} \text{ col.})$

yields a reduction in the

order of the determinant;

$$|A| = a_{11} \begin{vmatrix} a''_{22} & a''_{23} & a''_{24} \\ a''_{32} & a''_{33} & a''_{34} \\ a''_{42} & a''_{43} & a''_{44} \end{vmatrix} = a_{11} a''_{22} \begin{vmatrix} 1 & a'''_{23} & a'''_{24} \\ a''_{32} & a''_{33} & a''_{34} \\ a''_{42} & a''_{43} & a''_{44} \end{vmatrix} = a_{11} a''_{22} \begin{vmatrix} 1 & 0 & 0 \\ a'''_{32} & a'''_{33} & a'''_{34} \\ a'''_{42} & a'''_{43} & a'''_{44} \end{vmatrix}$$

- 1: $(2^{\text{nd}} \text{ col.}) - a'''_{23} \times (1^{\text{st}} \text{ col.})$
- 2: $(3^{\text{rd}} \text{ col.}) - a'''_{24} \times (1^{\text{st}} \text{ col.})$

$$|A| = a_{11} a''_{22} \begin{vmatrix} a'''_{33} & a'''_{34} \\ a'''_{43} & a'''_{44} \end{vmatrix} = a_{11} \cdot a''_{22} \cdot \left[(a'''_{33} \times a'''_{44}) - (a'''_{43} \times a'''_{34}) \right]$$

The procedure is repeated till a $(2,2)$ determinant is finally reached.

(Yc-73, Ay-62).

APPENDIX F-DESCRIPTION OF THE PROGRAMS

CORGAM is the main program through which the flow of the program is controlled. This program is used to:

1. Read the program flow parameters.
2. Define many of the data parameters.
3. Read the input data which describes the experimental conditions, such as irradiation time, counting times, etc.
4. Read the complex spectrum, i.e., the spectrum to be analyzed.
5. Subtract background from the complex spectrum, normalize it, and shift it to compensate for electronic instabilities in the MCA.
6. Calculate the irradiation and decay time correction factors.
7. Form the (X^0WX) matrix.
8. Calculate the concentration estimators.
9. Delete any and all non-significant reference isotopes.
10. Print or punch the output information.

The following 19 subprograms are called by CORGAM, their description are given in the following pages, and they are listed in order called.

- | | |
|------------|------------|
| 1. INIT | 17. CHI |
| 2. PHOTO | 18. VARNCE |
| 3. SMINV | 19. WRIT1 |
| 4. INDEX | |
| 5. SHIFT | |
| 6. SHIFTS | |
| 7. WATE | |
| 8. REFS | |
| 9. REFIN | |
| 10. XFORM | |
| 11. PEAKS | |
| 12. SAVE | |
| 13. DET | |
| 14. DELETE | |
| 15. STAT | |
| 16. WRIT | |

The following is the listing of the subprograms called by CORGAM. The description of the subprograms are also given together with the variables used and their options.

1. INIT:

This subprogram is used to initialize the irradiation and decay correction factors and many of the program control parameters.

```
SUBROUTINE INIT (NITER,RAT,SAV,C,ISOCHN,MODE,NBKGD,NUBKG,NSHFT,NPK,LPP,NORM,
NCTIN,NAREA,NCHCU,NCULL,NCUUL,NRHO,NUMVAR,NVAR,NREFS,ITER,NR,NW,LOCHN,NHICHN,
NCHAN,MC,MVAR,T,AREA,BKGTIM,TIMIRR,PHRL,UP,XNCOM)
```

```
DIMENSION C(15)
```

NITER: Number of iterations used in variance calculations

RAT: Correction factor

SAV: Correction factor

C(I): Correction factor for the Ith reference isotope, if -1.0 is entered for C(I) value, the Ith isotope is deleted from the analysis.

ISOCHN: Number of channels in the complex spectrum.

MODE: 1 Read by 5E14.8 format

2 Read by 6X,12F6.0,2X format

NBKGD: 0 no background subtraction

Other will subtract background

NUBKG: 0 no new background will be read

Other, a new background will be read

NSHFT: 0, no spectrum shifting

Other, will shift spectrum

NPK: Number of peaks in complex spectrum used in shifting

LPP: Index of peak used in shifting ratio

NORM: 0, no normalization of complex spectrum is needed

Other, normalize the complex spectrum

NCTIN: 0, read precalculated correction factors

Other, read unity (or less than zero for deletion)

NAREA: 0, read photopeak area for copper reference

1, calculate pp area for Cu ref., read Cu spectrum (read any)

2, use same area as previous spectrum.

NCHCU: Number of channels in Cu reference spectrum.
 NCULL: Lower fit limit on Cu reference photopeak.
 NCUUL: Upper fit limit on Cu reference photopeak.
 NRHO: 0, will not punch shifted output
 Other, will punch shifted output
 NOMVAR: Number of variances to be averaged
 NVAR: 1, read variance by 5E14.8 format
 2, variance: 1.0
 3, variance: RHO
 4, use variance previously read
 NREFS: 0, new set of reference spectra are read
 1, no new reference spectra are to be read
 ITER: Maximum number of iterations on variance
 NR: 0, calculate average weight variance from the long way
 Other, ratio: YAVE/YAVEAEVE
 NW: 0, will not punch shifted output for reference spectra
 Other, will punch shifted output for reference spectra
 LOCHN: Lower channel of least squares fit
 NHICHN: Upper channel of least squares fit
 NCHAN: Number of channel in variance spectrum if variance are to be read
 MC: Number of reference spectra which have a set of decay spectra. These
 spectra must be in order and they must be the first of the reference
 spectra to be read in.
 MVAR: 0, variance of reference spectrum; reference spectrum
 Other, read variance of reference spectrum
 T: Student's t value for null hypothesis test
 AREA: Copper reference photopeak normalized area
 BKGTIM: Counting time of background (minute)
 TIMIRR: Complex sample irradiation time (minute)
 FRHL: Flux reference half-life (minute)
 UP: U_p factor of Chi-squared test (confidence interval factor)
 XNCOM: Complex spectrum normalization constant.

This subprogram is read only for the complex spectrum whose data are not given in the beginning of the main program. Generally the first complex spectrum data is given in DATA statement and in NAMELIST. The complex spectra variables following the first one are initialized by this subprogram.

2. PHOTO:

This program is used to fit the photopeak data of a spectrum to a linearized form of the Gaussian function. The fitting technique is discussed in the Appendix C.

```
SUBROUTINE PHOTO (RES,XO,IPPLL,IPPUL,EPP,AREA)
DIMENSION B(3),Q(15,15),RES(400),RE(3),BZ(60),C(10)
```

RES(I): Counts registered at the I^{th} channel of the flux reference spectrum.
 XO: x_0 (x sub o) of the equation C-1 of appendix C.
 IPPLL: NCULL(defined in INIT)
 IPPUL: NCUUL(defined in INIT)
 EPP: Midpoint energy of the photopeak of interest (MeV).
 AREA: defined in INIT

3. SMINV:

This subprogram is the scientific subroutine designed for the IBM 360 to invert symmetric matrices. It is modified by the author by its UNIVAC version in order to use in Boğaziçi University computer.

```
SUBROUTINE SMINV (R,N)
DIMENSION A(230),R(15,15)
```

R(I,J): I^{th} row, J^{th} column element of the matrix
 N: Order of the matrix

The subprogram is used to obtain the inverse of a symmetry matrix A of order N. Only the upper triangular part of A is stored. On exit the inverse replaces A in storage. The inverse matrix is found by successive congruent transformations to obtain the diagonal. Inverting the diagonal elements and performing the congruent transformations in reverse gives the inverse matrix. In this code A is the (X^0WX) matrix.

4. INDEX:

This subprogram is apart of the subroutine SMINV and is used to store a two-dimensional matrix as a row vector. It is applicable only for symmetrical matrices. It allows reference to a two-dimensional matrix with subscripts (I,J) while the matrix is stored as a vector.

FUNCTION INDEX (I8,J8,N)

I8: Row of matrix

J8: Coloumn of matrix

N: Order of matrix (maximum value 15)

While a matrix of order N has $N \times N$ elements, the same matrix stored as a vector will have $(N^2 + N)/2$ elements, provided that the matrix is symmetric. In this way storage space is reduced.

5. SHIFT:

This program is used to calculate the input parameters to SHIFTS.

SUBROUTINE SHIFT (NCHN,NPK,LPP,NWRITE,Y,PO)

NCHN: ISOCHN (defined in INIT)

NPK: defined in INIT

LPP: defined in INIT

NWRITE: NRHO (defined in INIT)

Y(I): RHO(I), counts registered at the I^{th} channel of the complex spectrum
($I_{\text{max}}: 400$, i.e., up to 400 channels can be used).

PO: Identification number of the spectrum to be shifted.

6. SHIFTS:

This program is used to shift a spectrum to a new gain and baseline, hence it will compensate for electronic instabilities in the MCA.

SUBROUTINE SHIFTS (SPECT,S,RATIO,NCHN,NCHN2,BLSHFT)

DIMENSION SPECT(400),S(400)

SPECT(I): Counts registered at the I^{th} channel of the unshifted spectrum.

S(I): Counts registered at the I^{th} channel of the shifted spectrum by using
SPECT(I).

RATIO: Shifting ratio

NCHN: ISOCHN (defined in INIT), unshifted channel number.

NCHN2: The shifted new channel number.

BLSHFT: Baseline shift.

7. WATE:

This program is used to establish the original form of the weighting matrix. It calculates or reads the weight factors and read or set variances using (A) as storage.

```
SUBROUTINE WATE (NVAR, NUMVAR, NCHAN, RHO, XNCOM, III, OMG, A, RES, ISOCHN)
DIMENSION RES(400), RHO(400), OMG(400), A(400)
```

NVAR: Defined in INIT

NUMVAR: Defined in INIT

NCHAN: Defined in INIT

RHO(I): Counts registered at the Ith channel of the complex spectrum.

XNCOM: Defined in INIT

III: Identification number of the complex spectrum (if several complex spectra are to be analyzed).

OMG(I): Ith element of the variance vector.

A(I): Ith element of the vector X in (X⁰WX) matrix.

RES(I): Defined in PHOTO

ISOCHN: Defined in INIT.

8. REFS:

This program is used to read all pertinent reference spectra concerning each spectrum. Options are provided for each spectrum to have a background subtraction, to be normalized, and to be corrected for decay. In addition, a set of reference spectra (up to five) for an element which upon irradiation produces several non separable isotopes, such as Br Br⁸⁰, Br⁸², may be read in. This program uses these data by interpolation to obtain the reference spectrum at the decay time of the complex spectrum.

```
SUBROUTINE REFS (NISO, NHICHN, ISO, XNORM, O, AT, BKG, NW, DECAY, COUNT, III, NFAC,
FRRHL, D, H, MC, NO, RHO, A)
```

```
DIMENSION ISO(15), H(15), D(15), XNORM(15), O(15), AT(400, 15), BKG(400), RES(400),
P(15), CALC(400), NFAC(15), CT(400, 15), T(5), C(5), RHO(400), A(400)
```

NISO: Number of reference isotopes used in the analysis of the complex spectrum

NHICHN: Defined in INIT

ISO(I): Number of channels in the Ith reference spectrum

XNORM: Normalization constant

O(I): Identification name of the reference spectrum

AT(I,J): Counts registered at the I^{th} channel of the J^{th} reference spectrum
 BKG(I): Counts registered at the I^{th} channel of the background spectrum.
 NW: Defined in INIT
 DECAY: Decay time for complex spectrum (minute)
 COUNT: Counting time for complex spectrum (minute)
 III: Defined in WATE
 NFAC(I): Decay time specification for the I^{th} reference isotope
 FRRHL: Reference spectrum, flux reference isotope half-life (minute)
 D(I): Irradiation time, in minutes, of reference sample spectrum
 H(I): Half-life, in minutes, of reference isotope spectrum
 MC: Defined in INIT
 NO: Number of decay spectra of the reference isotope (max 5)
 RHO(I): Defined in WATE
 A(I): Defined in WATE

9. REFIN:

This program is used to interpolate, channel by channel between those spectra discussed in REFS, by Lagrangian method. The method is discussed in the appendix D.

SUBROUTINE REFIN (AT,III,T,C,CT,NO,M,DECAY,COUNT,ISO,RHO,A)
 DIMENSION AT(400,15),CT(400,15),T(5),C(5),ISO(15),IS(15),RHO(400),A(400)
 AT(I,J): Defined in REFS
 III: Defined in REFS
 T(K): Decay time in minutes of the K^{th} decay spectra of the J^{th} reference
 C(K): Counting time in minutes of the K^{th} decay spectra of the J^{th} reference
 CT(I,K): Counts registered at channel I of the K^{th} decay spectra for J^{th}
 reference isotope
 NO: Defined in REFS
 M: Tag name of the reference isotope
 DECAY: Defined in REFS
 COUNT: Defined in REFS
 ISO(J): Defined in REFS
 RHO(I): Defined in WATE
 A(I): Defined in WATE

10. XFORM:

This program is used to form the $(X'WX)$ matrix, its inverse, and the matrix correlation coefficients. A provision is included to evaluate the determinant of the matrix of correlation coefficients which is used as a measure of the efficiency for extracting the maximum information from the analysis problem. Further, the calculated identity matrix $(X'WX)^{-1}(X'WX)$ is formed and the error of average element can be found. Finally, the accuracy of the inverse matrix can be improved by an iteration method.

SUBROUTINE XFORM (NFORM,NISO,R,RI,MAXCON,P,O,LOCHN,NHICHN,A,AT,NCORR,NWRIT,
NIDEN,NINTF,RII,BETA,THETA,OI,RHO,III)
DIMENSION R(15,15),RI(15,15),RII(15,15),P(15),O(15),A(400),AT(400),OI(15),
Q(15,15),S(15,15),BETA(15),THETA(15),RHO(400)

NFORM: Specification for the $(X'WX)^{-1}$ matrix to be read or formed
NISO: Defined in REFS
R(I,J): The inverse cross product matrix $(X'WX)^{-1}$
RI(I,J): The cross product matrix $(X'WX)$
MAXCON: The remaining number of reference isotopes
P(I): Tag name of the i^{th} reference isotope
O(I): Defined in REFS
LOCHN: Defined in INIT
NHICHN: Defined in INIT
A(I): Defined in WATE
AT(I): Defined in REFS
NCORR: Control variable which specifies formation of correlation coefficients
NWRIT: Control variable which specifies writing options for the $(X'WX)$ and
its inverse
NIDEN: Control variable which specifies formation of identity matrix
NINTF: Control variable for interference calculation
RII(I,J): $R(I,J)$, the $(X'WX)^{-1}$ matrix
BETA(J): Concentration estimators (ppm) of the j^{th} reference isotope
THETA(J): Interferences in percent
OI(J): Intermediate vector
RHO(I): Defined in WATE
III: Defined in REFS

11. PEAKS:

This program is used to select the data near each photo-peak which is to be used in the area-of-interest unfolding procedure.

SUBROUTINE PEAKS (AT,A,RHO,LOCHN,NHICHN,NISO,III)

AT(I,J): Defined in REFS

A(I): Defined in WATE

RHO(I): Defined in WATE

LOCHN: Defined in INIT

NHICHN: Defined in INIT

NISO: Defined in REFS

III: Defined in REFS

12. SAVE:

This program is used to store the original $(X^0WX)^{-1}$ matrix and the corresponding reference spectra identification tags in order to allow stacking of the complex spectra

SUBROUTINE SAVE (NISO,O,OI,RI,RII)

NISO: Defined in REFS

O(J): The tag name of the reference spectrum

OI(J): O(J)

RI(I,J): The $(X^0WX)^{-1}$ matrix

RII(I,J): RI(I,J)

13. DET:

This program is used to evaluate the determinant by pivotal condensation (Chio's method) of the matrix composed of the correlation coefficients of the $(X^0WX)^{-1}$ matrix. The method is discussed in the appendix E.

SUBROUTINE DET (R,N,DETERM)

R: The matrix to be used $(X^0WX)^{-1}$

N: Order of the matrix

DETERM: The determinant of the matrix R.

14. DELETE:

This program is used to delete from the analysis the reference spectra which are not significant at a pre-selected level

SUBROUTINE DELETE (NISO,REMOVE,ISOCHN,BETA,R,C,O,THETA,L)

NISO: Defined in REFS

REMOVE: Intermediate value for the reference isotope

ISOCHN: Defined in INIT

BETA(I): New concentration estimator for Ith reference isotope

R(I,J): The $(X^0WX)^{-1}$ matrix

C(J): Defined in REFIN

O(J): Defined in REFS

THETA(J): Defined in XFORM

L: Tag name of the deleted isotope

15. STAT:

This program is used to calculate the standard deviations of the concentration estimators. In addition if some average weighting matrix is used in the analysis, this program is used to correct the standard deviations for this calculations.

SUBROUTINE STAT (REMOVE,BETA,RHOSQD,NISO,LOCHN,NHICHN,R,O,AT,A,RES,RHO,MVAR,NR,RAT,ST,NITER,F,RCORR,P,MAXCON,RHOSUM,XNORM,MVAR,ISO,III)

REMOVE: Defined in DELETE

BETA: Defined in DELETE

RHOSQD: $\sum (RHO(I))^2$

NISO: Defined in REFS

LOCHN: Defined in INIT

NHICHN: Defined in INIT

R(I,J): Defined in DELETE

O(J): Defined in REFS

AT(J): Defined in REFS

A(I): Defined in WATE

RES(I): Defined in PHOTO

RHO(I): Defined in WATE
 NVAR: Defined in INIT
 NR: Defined in INIT
 RAT: Defined in INIT
 ST: T -the student's t value
 NITER: Number of iterations to be performed
 F: F value for null hypothesis
 RCORR: Correlation coefficient
 P: Tag name for the reference isotope
 MAXCON: Remaining number of isotopes after deletions
 RHOSUM: $\sum (RHO(I))$
 XNORM: Defined in REFS
 MVAR: Defined in INIT
 ISO: Defined in REFS
 III: Defined in REFS

16. WRIT:

This program is used to print the concentration estimators, standard deviations, t values, etc.

SUBROUTINE WRIT (NITER, ITER, O, BETA, STDEV, ST, NISO, F, RCORR)

NITER: Iteration number
 ITER: Maximum iterations
 O(I): Tag number of the reference isotope
 BETA: Concentration estimators (ppm)
 STDEV: Standard deviations of BETA
 ST: Calculated t value
 NISO: Order of the isotope whose values are going to be printed
 F: Calculated F value
 RCORR: Correlation coefficients

This program is composed only of WRITE and FORMAT statements.

17. CHI:

This program is used to calculate the value of Chi-squared divided by the degrees of freedom for each analysis

SUBROUTINE CHI (CALC,RES,MAXCON,P,O,LOCHN,NHICHN,BETA,AT,C,RHO,NISO,QUAL,A)

CALC: Intermediate value for QUAL

RES(I): Defined in PHOTO

MAXCON: Defined in STAT

P(J): Defined in STAT

O(J): Defined in REFS

LOCHN: Defined in INIT

NHICHN: Defined in INIT

BETA(J): Defined in DELETE

AT(I): Defined in REFS

C(I): Defined in REFIN

RHO(I): Defined in WATE

NISO: Defined in REFS

QUAL: Quality of fit number

A(I): Defined in WATE

UP: Confidence interval of Chi-squared

DF: Degrees of freedom

18. VARNCE:

This program is used to adjust the weighting matrix to account for the variance in the reference spectra and the concentration estimators

SUBROUTINE VARNCE (A,OMG,STDEV,AT,LOCHN,NHICHN,NISO,MAXCON,C,P,O,BETA,XNORM)

All of the variables are previously defined.

19. WRIT1:

This program is used to write the significant concentrations estimators and their standard deviations, onto an intermediate storage.

SUBROUTINE WRIT1 (O,BETA,STDEV,NISO)

All of the variables are previously defined.

APPENDIX G

- LISTING OF THE INPUT DATA AND INPUT OPTIONS

Listing of input data and input options.

The following cards and decks are read by CORGAM:

A.1 Card One (15A4 format): Identification card for the set of data which may contain more than one complex spectrum.

A.2 Card Two (25I3 format):

NISO = number of isotopes used in analyzing all complex spectra of the data set. Any analysis for which a specific isotope is not desired may be removed by entering a negative unity in the proper location of the irradiation and decay times correction factor card.

NCASES = number of complex spectra contained in the data set.

Six other control parameters are carefully defined in the comment cards of the program.

A.3 Card Three (25I3 format):

NCHG1 = 0; no change in NAM1. See the comment cards in CORGAM for the definition of the variables in NAM1

NCHG1 = 1; change in NAM1. Below is a list of the standard values of the variables of NAM1. Read one or more cards with the necessary input data

NCHG2 = 0; no change in NAM2. This namelist contains the irradiation and decay time correction factors

NCHG2 = 1; change in NAM2. The standard value for all of these correction factors is unity. Read one or more cards with the necessary input data

NCHG3 = 0; no change in NAM3. See the comment cards in CORGAM for the definition of the variables in NAM3.

NCHG3 = 1; change in NAM3. This is the standard value for NCHG3 because not all of the necessary input data is defined. Below is a list of the standard values for the variables of NAM3. Read one or more cards with the necessary input data

A.4. Card Four (15A4 format): Identification card of a specific complex spectrum from the group which is to be analyzed.

A.5 Deck One (5E14.8 or 6X,12F6.0,2X format): This is the complex spectrum.

Note: Card Five and Deck Two are not needed if NBKGD = 0 or
NUBKGD = 0

A.6. Card Five (15A4 format): Identification card for the background spectrum.

A.7 Deck Two (6X,12F6.0,2X format): This is the background spectrum.

Note: Card Six and Deck Three are not needed unless NAREA = 1

A.8 Card Six (15A4 format): Identification card for the flux reference spectrum

A.9 Deck Three (6X,12F6.0,2X format): This is the flux reference spectrum

Note: Card Seven and Cards Eight are not needed if NSHFT = 0

A.10 Card Seven (8F10.0 format): This card contains the gain (MeV/ch) to which the complex spectrum is to be shifted

A.11 Cards Eight (4(I3,7X,F10.0) format): These cards contain the approximate mid point and energy of each photopeak used in shifting the complex spectrum

Note: If NVAR = 1, Deck Four is needed

A.12 Deck Four (5E14.8 format): This deck contains a variance spectrum corresponding to the complex spectrum.

The following cards and decks are read by subprogram REFS.

A disk is needed for intermediate storage.

Note: There will be NISO decks consisting of Card One and Card two plus a deck of control parameters and a reference spectrum

B.1 Card One (A4,9I3 format): This card contains an identification tag and several control parameters for a reference spectrum. See subprogram REFS comment cards for definitions

B.2 Card Two (8F10.0 format): This card contains the half life (in minutes), the irradiation time (in minutes), flux reference isotope half life (in minutes), and the reference spectrum normalization constant. This normalization constant is read as unity if the reference spectrum is to be normalized.

Note: Card Three is needed only if NO, the number spectra composing a set of reference decay spectra, is > unity.

B.3 Card Three (8F10.0 format): This card contains the decay time (in minutes) and counting time (in minutes) for each spectrum in the set of reference decay spectra. There is a maximum of five spectra allowed in each set of reference decay spectra; all the sets of reference decay spectra must come first in reference spectra decks; and each spectrum in a set of reference decay spectra must be in order of the decay times.

Note: Cards Four, Five, Deck One, Card Six, Deck Two, are not needed if NO is zero or unity

B.4 Card Four (25I3 format): This card contains several control parameters for the set of decay reference spectra.

- B.5 Card Five (8F10.0 format): This card contains the background counting time (in minutes), the flux reference decay time (in minutes), the sample weight (in grams), the weight of the flux reference (in grams), and the flux reference counting time (in minutes).
- B.6 Deck One (5E14.8;6X,12F6.0,2X; or 8F10.0 format): This deck contains the set of decay reference spectra.
 Note: If NORF is zero, Card Six, Deck Two, Card Seven, Card Eight, and Card Nine are not needed. If NNBKG is yew, Card Six and Deck Two are not needed.
- B.7 Card Six (15A4 format): Identification card for the background spectrum
- B.8 Deck Two (6X,12F6.0, 2X format): This deck contains the background spectrum.
 Note: There will NO decks composed of Card Seve, Card Eight, and Cards Nine
- B.9 Card Seven (25I3 format): This card contains the number of peaks and the pivotal peak used in shifting the reference spectrum.
- B.10 Card Eight: See Card Seven of CORGAM
- B.11 Card Nine: See Card Eight of CORGRAM
 Note: If NO is zero, some or all of the following cards or decks are needed. If NORF is unity, Card Ten and Card Eleven are needed.
- B.12 Card Ten: See Card Four of REFS
- B.13 Card Eleven (8F10.0 format): This card contains the counting time (in minutes) and the information contained on Card Five of REFS for each reference spectrum
- B.14 Deck Three (5E14.8;6X,12F6.0,2X; or 8F10.0 format): This deck contains the reference spectrum.
 Note: If NORF is not equal to unity, Card Twelve, Deck Four, Cards Fourteen, Card Fifteen and Deck Five are not needed. If NUBKG is zero, Card Twelve and Deck Four are not needed.
- B.15 Card Twelve (15A4 format): Identification card for the background spectrum.
- B.16 Deck Four (6X,12F6.0,2X format): This deck contains a background spectrum
- B.17 Card Thirteen: See Card Seven of CORGAM.
- B.18 Card Fourteen: See Card Eight of CORGAM.
- B.19 Card Fifteen (15A4 format): Identification card for the flux reference spectrum
- B.20 Deck Five (6X,12F6.0,2X format): This deck contains a flux reference spectrum

The following cards and decks are read by subprogram XFORM

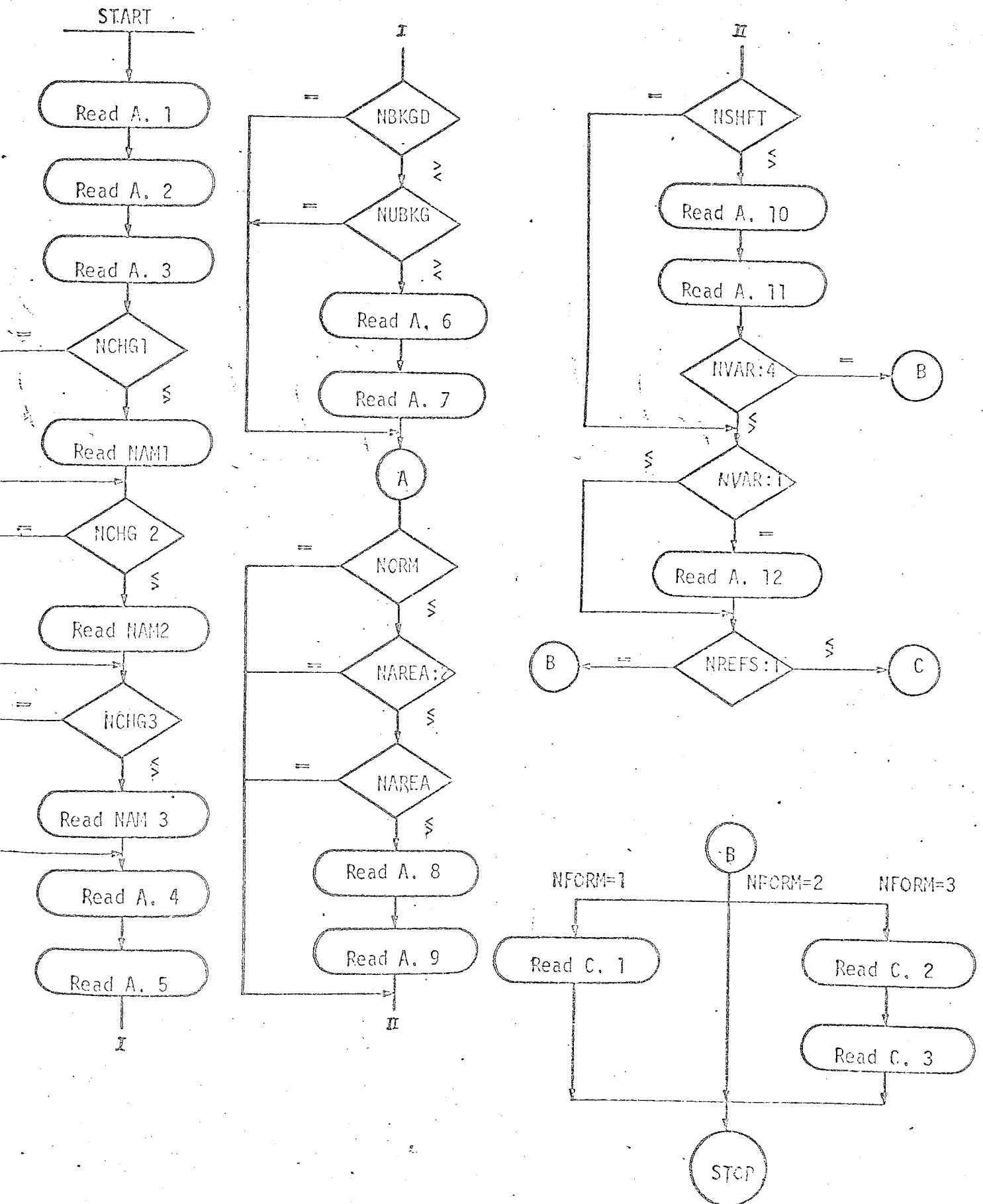
Note: If NFORM = 1, the following deck is needed:

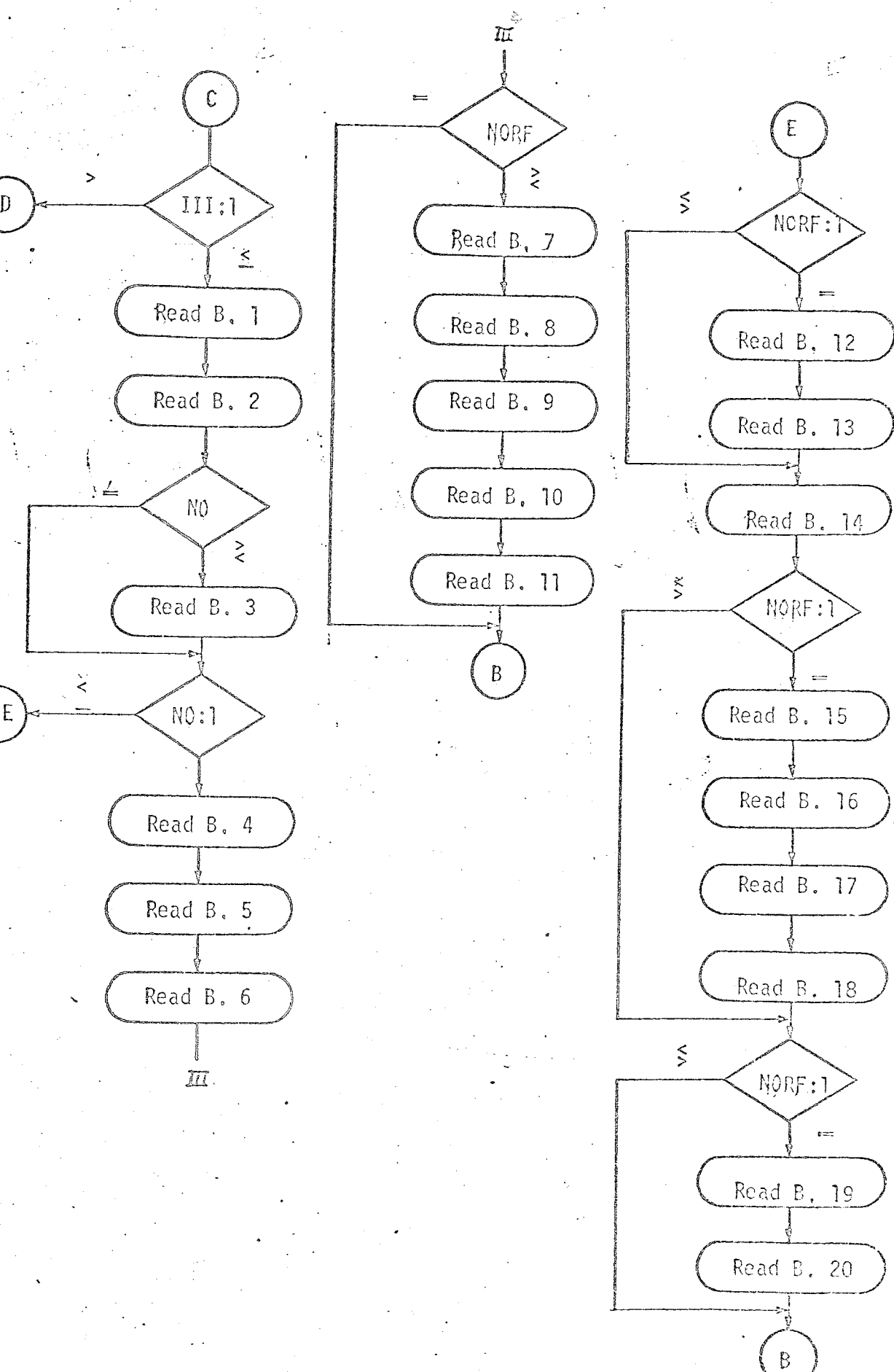
- C.1 Deck One (3E24.18 format): This deck contains the $(X'W X)^{-1}$ matrix which has been formed previously

Note: If NFORM = 2, no other input is required

If NFORM = 3, the following two cards are needed.

- C.2 Card One (25I3 format): This card contains the number of peaks needed for the area of interest (AOI) unfolding procedure and the number of channels on either side of the mid-point channel of the photopeak used in the AOI unfolding procedure.
- C.3 Card Two (25I3 format): This card contains the channel numbers which correspond to each peak used in the AOI unfolding procedure.





APPENDIX H

- LISTING OF THE UNIVAC-1106 VERSION OF THE CODE (CORAM)


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1  .MAIN
2  DIMENSION RHO(400), AT(400,15), A(400), THETA(15), BETAL(15), P(15), R(15), CORG
3  115), C(15), O(15), RES(400), CALC(400), RI(15,15), H(15), BKG(400), Q(15,1), CORG
4  115), D(15), ISO(15), S(15,15), SI(400), OMG(400), STDEV(400), ST(15), NFAC(CORG
5  115), XNORM(15), OI(15), RII(15,15)
6  NAMELIST /NAM1/ ISO, CHN, MODE, NBKGD, NUBKG, NSHFT, NPK, LPP, NORM, NCTIN,
7  1 NAREA, NCHCU, NCULL, NCUUL, NRHO, NUMVAR, NVAR, NREFS, ITER, NR, NW, LOCHN,
8  2 NHICHN, NCHAN, MC, MVAR/ NAM2/ C/ NAM3/ T, DECAY, COUNT, WT, CUCT, WTCU, AREA,
9  3 CUDEC, BKG TIM, TIMIRR, FRHL, UP, XNCOM
10 DATA NITER, RAT, SAV, C/ 0, 1.0, 0.0, 15*1.0/
11 DATA ISO, CHN, MODE, NBKGD, NUBKG, NSHFT, NPK, LPP, NORM, NCTIN,
12 1 NAREA, NCHCU, NCULL, NCUUL, NRHO, NUMVAR, NVAR, NREFS, ITER, NR,
13 2 VW, LOCHN, NHICHN, NCHAN, MC, MVAR/ 256, 2, 1, 1, 1, 3, 1, 1, 1, 1, 48, 33, 40, 1
14 3, 1, 3, 0, 0, 0, 1, 7, 250, 256, 1, 0/
15 DATA T, AREA, BKG TIM, TIMIRR, FRHL, UP, XNCOM/ 1.645, 1.0, 60.0, 15.0/
16 1774.0, 2.5758, 1.0/
17 FORMAT( 1H1 )
18 FORMAT( 25I3 )
19 FORMAT( 5E14.8 )
20 FORMAT( 8F10.0 )
21 FORMAT( /24HL (ATrans = * OMEGA * RHO) / )
22 FORMAT( 11H T VALUE = , F7.4 )
23 FORMAT( 15A4 )
24 FORMAT( /35HL DECAY AND IRR CORRECTION FACTORS / )
25 FORMAT( /23HL SOLUTION VECTOR (PPM) / )
26 FORMAT( 14, (1X, 10E12.5) )
27 FORMAT( 2, (1X, 13, 1X, E12.5, 1X, E12.5, 1X, E12.5) )
28 FORMAT( 1H1, 2, (1X, 3, 4CHN, 5X, 3HEXP, 10X, 4HCALC, 10X, 3HRES, 4X) )
29 FORMAT( 1X, A4, (1X, 9E12.5) )
30 FORMAT( A4, 9I3 )
31 FORMAT( 14, 6(2X, A4, 3H = , E12.5) )
32 FORMAT( 3E24.18 )
33 FORMAT( 6X, 12F6.0, 2X )
34 FORMAT( /35H NO VARIABLES SIGNIFICANT AT A T = , F5.1 )
35 FORMAT( /15H CU REF AREA = , E14.8/ )
36 FORMAT( /18H ABS DEV PER PT = , E14.7, 13H NO OF PTS = , I3 / )
37 FORMAT( /6X, 9(4X, A4, 4X) )
38 FORMAT( /17H SAMPLE T(GM) = , E12.5, 17H IRR TIME(MIN) = , E12.5, 19H DC
39 1 ECAY TIME(MIN) = , E12.5, 14H COUNT TIME = , E12.5/ 19H FLUX REF WT(GM)
40 2 ) = , F12.5, 23H REF DECAY TIME(MIN) = , E12.5, 23H REF COUNT TIME(MIN)
41 3 ) = , F12.5, 18H REF HLIFE(MIN) = , E11.4/ 17H BKG TIME(MIN) = , E12.5 )
42 50 FORMAT( /19H Y NORM CONSTANT = , E15.8/ )
43 51 FORMAT( 8F10.3 )
44 52 READ( 5, 15 ) ( P(I), I=1, 15 )
45 53 READ( 5, 10 ) NISO, NCASES, NRES, NFORM, NWRIT, NCORR, NINTF, NIDEN
46 54 NRES=0 NO RES CALC
47 55 =1 RES CALC BUT NOT WRITTEN OUT, JUST UND OUTSIDE ABS(2)
48 56 =2 RES CALC AND WRITTEN OUT
49 57 NFORM = 1 READ INV COR MATRIX
50 58 = 2 FORM INV COR MATRIX
51 59 = 3 TAKE ONLY PEAK CHAN VALUES FOR LST SQRS FIT
52 60 NWRIT = 0 WRITE R AND RINV MATRICES
53 61 = 1 OTHER DO NOT WRITE R AND RINV MATRICES
54 62 NCORR = 0 FORM CORRELATION COEFF
55 63 = 1 OTHER DO NOT FORM CORRELATION COEFF
56 64 NINTF = 0 INTERFERENCES WILL BE CALCULATED
57 65 = 1 OTHER INTERFERENCES WILL NOT BE CALCULATED
58 66 NIDEN = 0 CALC THE IDENTITY MATRIX FROM THE INVERSE
59 67 = 1 OTHER DO NOT CALC THE IDENT
60 68 IF( NISO.EQ.0 ) CALL EXIT
61 69 NHI=NHICHN
62 70 WRITE( 6, 9 )
63 71 WRITE( 6, 15 ) ( P(I), I=1, 15 )
64 72 ISO, CHN = NO OF CHN IN COMPLEX SPECTRUM
65 73 MODE = 1 READ BY 5E14.8
66 74 = 2 READ BY 6X, 12F6.0, 2X
67 75 MAXCON=NISO
68 76 NBKGD = 0 NO BKG SUBTRACTION
69 77 = 1 OTHER WILL SUBTRACT BKG
70 78 NUBKG = 0 NO NEW BKG TO BE READ
71 79 = 1 OTHER A NEW BKG WILL BE READ
72 80 NSHFT = 0 NO SPECTRUM SHIFTING
73 81 = 1 OTHER WILL SHIFT SPECTRUM
74 82 NPK = NO OF PEAKS IN SPECT FOR SHIFTING
75 83 LPP = INDEX OF PK USED IN SHIFT RATIO
76 84 NORM = 0 NO NORMALIZATION OF COMPLEX NEEDED
77 85 = 1 OTHER NORMALIZE THE COMPLEX
78 86 NCTIN = 0 READ PRECALC CORRECTION FACTORS
79 87 = 1 OTHER READ UNITY (OR LT ZERO FOR DELETION)
80 88 NAREA = 0 READ PP AREA FOR CU REF
81 89 = 1 UNITY CALC PP AREA FOR CU REF, READ CU SPECT(READ ANY)
82 90 = 2 USE SAME AREA AS PREVIOUS SPECTRUM

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[illegible]

	READ(5,34)(RES(I),I=1,NCHCU)	CORG	164
	CALL PHOTO(RES,XO,NCOLL,NCUUL,0.511,AREA)	CORG	165
	CUDEC=CUDEC+CUCT/2.	CORG	166
	AREA=AREA*EXP(CUDEC*ALOG(2.)/FRHL)/(WTCU*CUCT)	CORG	167
570	WRITE(6,36)AREA	CORG	168
171	XNCOM=AREA*WT*1.0E+06*COUNT*SF	CORG	169
	DO 131 I=1,ISOCHN	CORG	170
131	RHO(I)=RHO(I)/XNCOM	CORG	171
	WRITE(6,50)XNCOM	CORG	172
133	IF(NSHFT.EQ.0) GO TO 3013	CORG	173
	ICHN=ISOCHN	CORG	174
	CALL SHIFT(ISOCHN,NPK,LPP,NRHO,RHO,PO)	CORG	175
	RATIO=(FLOAT(ISOCHN)-0.5)/FLOAT(ICHN)	CORG	176
	NHICHN=FLOAT(NHICHN)*RATIO+0.5	CORG	177
	LOCHN=FLOAT(LOCHN)*RATIO+0.5	CORG	178
	IF(NVAR.EQ.4) GO TO 3190	CORG	179
013	CALL WATE(NVAR,NUMVAR,NCHAN,RHO,XNCOM,III,OMG,A,RES,ISOCHN)	CORG	180
	IF(DECAY.EQ.SAV) GO TO 3190	CORG	181
	IF(III.GT.1) GO TO 3195	CORG	182
	SAV=DECAY	CORG	183
195	IF(NRFEES.EQ.1) GO TO 3190	CORG	184
	CALL REFS(NISO,NHICHN,ISO,XNORM,0,AT,RKG,NW,DECAY,COUNT,III,NFAC,	CORG	185
1	FRRHL,D,H,MC,NO)	CORG	186
190	DO 978 I=1,MAXCON	CORG	187
	IF(NCTIN.EQ.0) GO TO 978	CORG	188
	XN=(1.-EXP(-ALOG(2.)*15./FRRHL))	CORG	189
	SF=XN/(1.-EXP(-ALOG(2.)*D(I)/FRRHL))	CORG	190
	XL=ALOG(2.)/2H(I)	CORG	191
	IF(NFAC(I).EQ.0) GO TO 3337	CORG	192
	FACT=1.0	CORG	193
337	GO TO 130	CORG	194
	TB=DECAY*ALOG((1.-EXP(-XL*COUNT))/(COUNT*XL))/XL	CORG	195
	FACT=EXP(XL*TB)	CORG	196
130	C(I)=FACT*C(I)*1.0E+06*SF*(1.-EXP(-XL*D(I)))/(1.-EXP(-XL*15.))	CORG	197
978	P(I)=C(I)	CORG	198
	WRITE(6,16)	CORG	199
	WRITE(6,27)NISO,(C(I),I=1,NISO)	CORG	200
	IF(NVAR.EQ.4) GO TO 319	CORG	201
99	CALL XFORM(NFORM,NISO,R,RI,MAXCON,P,0,LOCHN,NHICHN,A,AT,NCORR,NWRIC	CORG	202
1	I,NIDFN,NINTF,RII,BETA,THETA,OI,RHO,III)	CORG	203
119	RHOSUM=0.	CORG	204
132	RHOSQD=0.	CORG	205
	REMOVE=0.	CORG	206
	DO 120 I=LOCHN,NHICHN	CORG	207
	IF(A(I).EQ.0.0) A(I)=1.0	CORG	208
	RHOSQD=RHOSQD+(RHO(I)**2)/A(I)	CORG	209
120	RHOSUM=RHOSUM+RHO(I)/A(I)	CORG	210
266	RAT=RHOSUM/FLOAT(NHICHN-LOCHN+1)	CORG	211
	FORM ATRANS * OMEGA * RHO	CORG	212
253	DO 117 K=1,NISO	CORG	213
117	THETA(K)=0.0	CORG	214
	L=1	CORG	215
	DO 4050 K=1,MAXCON	CORG	216
	IF(P(K).NE.0(L)) GO TO 4050	CORG	217
	DO 1000 I=LOCHN,NHICHN	CORG	218
000	THETA(L)=THETA(L)+AT(I,K)*RHO(I)/A(I)	CORG	219
	L=L+1	CORG	220
	IF(L.GT.NISO) GO TO 4051	CORG	221
050	CONTINUE	CORG	222
051	WRITE(6,13)	CORG	223
	WRITE(6,18)NISO,(THETA(I),I=1,NISO)	CORG	224
	WRITE(6,9)	CORG	225
701	DO 106 J=1,NISO	CORG	226
	BETA(J)=0.0	CORG	227
	DO 106 I=1,NISO	CORG	228
006	BETA(J)=BETA(J)+R(J,I)*THETA(I)	CORG	229
	DO 125 I=1,NISO	CORG	230
25	BETA(I)=BETA(I)*C(I)	CORG	231
	DO 500 I=1,NISO	CORG	232
000	REMOVE=REMOVE+BETA(I)*THETA(I)/C(I)	CORG	233
	ISOCHN=NISO	CORG	234
	L=1	CORG	235
002	IF(C(I)) 601,600,600	CORG	236
001	CALL DELETE(NISO,REMOVE,ISOCHN,BETA,R,C,0,THETA,L)	CORG	237
	L=L-1	CORG	238
000	L=L+1	CORG	239
	IF(L.LE.NISO) GO TO 602	CORG	240
	CALL STAT(REMOVE,BETA,RHOSQD,NISO,LOCN,NHICHN,R,C,0,AT,A,STDEV,RH	CORG	241
1	0,NVAR,NR,RAT,ST,NITER,F,RCORR,P,MAXCON,RHOSUM,XNORM,MVAR,ISO,III)	CORG	242
	CALL WRIT(NITER,ITER,0,BETA,STDEV,ST,NISO,F,RCORR)	CORG	243
52	IF(ITER.EQ.0) GO TO 262	CORG	244
	IF(NITER.GE.ITER) GO TO 262	CORG	245

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CALL CHI(CALC,RES,MAXCON,P,O,LOCHN,NHICHN,BETA,AT,C,RHO,NISO,CHIS,CORG 246
1A) NITER=NITER+1 CORG 247
NCTIN=0 CORG 248
JPMX=JP*SQRT(2./FLOAT(NHICHN-LOCHN-NISO))+1. CORG 249
IF(CHIS.LE.JPMX)GO TO 252 CORG 250
CALL VARNCE(A,OMG,STDEV,AT,LOCHN,NHICHN,NISO,MAXCON,C,P,O,BETA,XNO CORG 251
1RM) NFORM=2 CORG 252
GO TO 99 CORG 253
262 ISOCHN=NISO CORG 254
NITER=0 CORG 255
AMIN=ST(1) CORG 256
DO 950 I=1,NISO CORG 257
IF(AMIN.LT.ST(I))GO TO 950 CORG 258
L=I CORG 259
AMIN=ST(I) CORG 260
950 CONTINUE CORG 261
IF(AMIN.GT.T)GO TO 951 CORG 262
IF(NISO.GT.1)GO TO 953 CORG 263
WRITE(6,35)T CORG 264
GO TO 954 CORG 265
953 CALL DELETE(NISO,REMOVE,ISOCHN,BETA,R,C,O,THETA,L) CORG 266
CALL STAT(REMOVE,BETA,RHOSQD,NISO,LOCHN,NHICHN,R,C,O,AT,A,STDEV,RH CORG 267
10,NVAR,NR,RAT,ST,NITER,F,RCORR,P,MAXCON,RHOSUM,XNORM,MVAR,ISO,III) CORG 268
CALL WRIT(NITER,ITER,O,BETA,STDEV,ST,NISO,F,RCORR) CORG 269
IF(NISO.GT.O)GO TO 951 CORG 270
WRITE(6,35)T CORG 271
NISO=MAXCON CORG 272
CALL SAVE(NISO,OI,O,RII,R) CORG 273
GO TO 1002 CORG 274
51 IE(NISO.LT.ISOCHN)GO TO 952 CORG 275
954 DEG=NHICHN-LOCHN=NISO CORG 276
IF(NRFS.EQ.O)GO TO 959 CORG 277
CALL CHI(CALC,RES,MAXCON,P,O,LOCHN,NHICHN,BETA,AT,C,RHO,NISO,CHIS,C CORG 278
1A) REMOVE=0. CORG 279
DO 971 J=LOCHN,NHICHN CORG 280
REMOVE=REMOVE+RES(J)**2 CORG 281
REMOVE=SQRT(REMOVE) CORG 282
NOP=NHICHN-LOCHN+1 CORG 283
TOTAL=0.0 CORG 284
DO 980 J=LOCHN,NHICHN CORG 285
TOTAL=TOTAL+ABS(RES(J)) CORG 286
TOTAL=TOTAL/FLOAT(NOP) CORG 287
WRITE(6,38)TOTAL,NOP CORG 288
IF(NRFS.NE.2)GO TO 959 CORG 289
WRITE(6,21) CORG 290
WRITE(6,20)(J,RHO(J),CALC(J),RES(J),J=LOCHN,NHICHN) CORG 291
59 CALL WRIT1(O,BETA,STDEV,NISO) CORG 292
NISO=MAXCON CORG 293
WRITE(6,14)T CORG 294
WRITE(6,9) CORG 295
CALL SAVE(NISO,OI,O,RII,R) CORG 296
NHICHN=NH CORG 297
02 CONTINUE CORG 298
GO TO 198 CORG 299
END CORG 300
SUBROUTINE REFS(NISO,NHICHN,ISO,XNORM,O,AT,BKG,NW,DECAY,COUNT,III, CORG 301
1NFAC,FRRHL,D,H,MC,NO,RHO,A) CORG 302
DIMENSIONISO(15),H(15),D(15),XNORM(15),O(15),AT(400,15),BKG(400), CORG 303
1RES(400),P(15),CALC(400),NFAC(15),CT(400,5),T(5),C(5),RHO(400),A(4 CORG 304
200) CORG 305
10 FORMAT( 25I3 ) CORG 306
11 FORMAT( 5E14.8 ) CORG 307
12 FORMAT(8F10.0 ) CORG 308
13 FORMAT( 15A4 ) CORG 309
14 FORMAT( 14,(1X, 10E12.5 ) ) CORG 310
24 FORMAT( A4,9I3 ) CORG 311
34 FORMAT( 6X,12F6.0,2X ) CORG 312
36 FORMAT(/154 CU REF AREA = ,E14.8/) CORG 313
39 FORMAT(/6X,9(4X,A4,4X)) CORG 314
51 FORMAT(8F10.3) CORG 315
REWIND 10 CORG 316
MM = 1 CORG 317
DO 121 I=1,NISO CORG 318
IF(III.GT.1)GO TO 3194 CORG 319
READ(5,24)O(I),ISO(I),NPK,LPP,NORF,MOHE,NFAC(I),NO CORG 320
READ(5,12)H(I),D(I),FRRHL,XNORM(I) CORG 321
IF(NO.EQ.O)GO TO 91 CORG 322
READ(5,12)(T(J),C(J),J=1,NO) CORG 323
ISOCHN = NO OF CHN IN REF CORG 324

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NP = TAG NAME OF REF SPECT
 LPP = INDEX OF PIVOTAL PK IN REF SPECT FOR SHIFTING
 NORF = 1 NORM OF REF REQD
 MODE = 1 5E14.8 INPUT FORMAT
 2 6X.12F6.0,2X INPUT FORMAT
 3 8F10.0 INPUT FORMAT
 NFAC = 0 REF IS AT TIME ZERO
 NFAC = 1 REF NEEDS DECAY CORRECTION
 2 1 REF IS AT TIME OF COMPLEX
 NO = NO OF SPECT IN THE SET OF REF DECAY SPECT
 H = HALF LIFE OF REF SPECT
 D = IRRAD TIME OF REF SPECT (MIN)
 FRPHL = FLUX REF HALF LIFE FOR REF (MIN)
 T = DECAY TIME (MIN) OF REF SPECT
 C = COUNT TIME (MIN) OF REF SPECT

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91 PO=0(1)
   ISOCHN=ISO(I)
   DO 1114 J=1,400
114 AT(J,I)=0.0
   IF(NO.LE.1)GO TO 256
   READ(5,10)NURKG,NCUUL,NCUUL,NCHCU,NCHRK
   READ(5,12)COUN,DECA,BKGTIM,CUDEC,WT,WTCU,CUCT
   DO1114 ME=1,NO
   DO1115 J=1,ISOCHN
15 CT(J,M)=0.0
   GO TO(116,117,118),MODE
16 READ(5,11)(CT(J,M),J=1,ISOCHN)
   GO TO 114
17 READ(5,34)(CT(J,M),J=1,ISOCHN)
   GO TO 114
18 READ(5,12)(CT(J,M),J=1,ISOCHN)
14 CONTINUE
   FACT=0.0
   IF(NORF.EQ.0)GO TO 257
   IF(NURKG.EQ.0)GO TO 262
   READ(5,15)(P(J),J=1,15)
   READ(5,34)(BKG(J),J=1,NCHBK)
62 DO 259 K=1,NO
   FACT=C(K)/BKGTIM
   READ(5,10)NPK,LPP
   DO 258 J=1,ISOCHN
   CALC(J)=CT(J,K)-FACT*BKG(J)
58 IF(CALC(J).LT.0.)CALC(J)=0.0
59 ICHN=ISOCHN
   CALL SHIFT(ICHN,NPK,LPP,0,CALC,PO)
   IF(ICHN.GT.NHICHN)ICHN=NHICHN
   DO 259 J=1,ICHN
59 CT(J,K)=CALC(J)
   ISOCHN=ICHN
   ISO(I)=ISOCHN
   GO TO 257
56 IF(NORF.NE.1)GO TO 93
   READ(5,10)NURKG,NCUUL,NCUUL,NCHCU,NCHRK
   READ(5,12)COUN,DECA,BKGTIM,CUDEC,WT,WTCU,CUCT
93 GO TO(21,22,23),MODE
21 READ(5,11)(AT(J,I),J=1,ISOCHN)
   GO TO 224
22 READ(5,34)(AT(J,I),J=1,ISOCHN)
   GO TO 224
23 READ(5,12)(AT(J,I),J=1,ISOCHN)
24 IF(NORF.NE.1)GO TO 910
   FACT=0.0
   FACT=COUN/BKGTIM
   IF(NURKG.EQ.0)GO TO 264
   READ(5,15)(P(J),J=1,15)
   READ(5,34)(BKG(J),J=1,NCHBK)
   GO TO 264
54 DO 260 J=1,ISOCHN
   CALC(J)=AT(J,I)-FACT*BKG(J)
50 IFT(CALC(J).LT.0.)CALC(J)=0.0
   CALL SHIFT(ISOCHN,NPK,LPP,0,CALC,PO)
   IF(ISOCHN.GT.NHICHN)ISOCHN=NHICHN
   DO 261 J=1,ISOCHN
51 AT(J,I)=CALC(J)
   ISO(I)=ISOCHN
57 IF(NO.LE.1)GO TO 910
94 CALL REFIN(AT,III,T,C,CT,NO,I,DECA,COUNT,ISO,RHO,A)
   WRITE(6,39)O(I)
   IC=ISO(I)
   WRITE(6,18)ISO(I),(AT(J,I),J=1,IC)
   IF(III.LE.1)GO TO 910
  
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17 FORMAT(F6.3,7X,F8.3,7X,F8.3,7X,E12.5,7X,E12.5) FOT0 9
18 FORMAT(9X,4H+OR=,F8.3,3X,4H+OR=,F8.3,3X,4H+OR=,E12.5,3X,4H+OR=,E12.5) FOT0 10
1 5 FOT0 11
1 5 FOT0 12
1 5 FOT0 13
1 5 FOT0 14
212 XN=0 FOT0 15
212 DO 321 I=1,3 FOT0 16
212 3(I)=0 FOT0 17
212 DO 321 J=1,3 FOT0 18
321 3(I,J)=0 FOT0 19
321 DO 30 I=IPPLL,IPPUL FOT0 20
XN2=XN*XN FOT0 21
XN3=XN2*XN FOT0 22
XN4=XN3*XN FOT0 23
ZN=ALOG( RES(I)) FOT0 24
Q(1,1)=Q(1,1)+XN4*RES(I) FOT0 25
Q(1,2)=Q(1,2)+XN3*RES(I) FOT0 26
Q(1,3)=Q(1,3)+XN2*RES(I) FOT0 27
Q(2,3)=Q(2,3)+XN*RES(I) FOT0 28
Q(3,3)=Q(3,3)+RES(I) FOT0 29
B(1)=B(1)+XN2*ZN*RES(I) FOT0 30
B(2)=B(2)+XN*ZN*RES(I) FOT0 31
3(3)=B(3)+ZN*RES(I) FOT0 32
30 XN=XN+1 FOT0 33
Q(2,1)=Q(1,2) FOT0 34
Q(3,1)=Q(1,3) FOT0 35
Q(2,2)=Q(1,3) FOT0 36
Q(3,2)=Q(2,3) FOT0 37
CALL SMINV(0,3) FOT0 38
DO 110 J=1,3 FOT0 39
RE(J)=0 FOT0 40
DO 110 I=1,3 FOT0 41
106 RE(J)=RE(J)+Q(J,I)*R(I) FOT0 42
XO=(-RE(2)/(2.*RE(1))) FOT0 43
XO=-1./RE(1) FOT0 44
YO=EXP(XO*XO/BO+RE(3)) FOT0 45
IF(BO.LT.0.)BO=ABS(BO) FOT0 46
AREA=SQRT(3.1416*BO)*YO FOT0 47
XO=XO+FLOAT(IPPULL) FOT0 48
DO 800 I=1,3 FOT0 49
800 B(I)=RE(I) FOT0 50
N=0 FOT0 51
RESI=0 FOT0 52
STDE=0 FOT0 53
XN=0 FOT0 54
DO 40 I=IPPLL,IPPUL FOT0 55
STDE=STDE+(ALOG( RES(I))-B(3)-B(2)*XN-B(1)*XN*XN)**2) FOT0 56
RESI=RESI+( RES(I)-F(FLOAT(I)))**2 FOT0 57
40 XN=XN+1 FOT0 58
IF(RESI.LT.0.)RESI=ABS(RESI) FOT0 59
STDE=SQRT(RESI/FLOAT(IPPUL-IPPLL-2)) FOT0 60
IF(1.5*STDE.GT.ABS( RES(IPPULL)-F(FLOAT(IPPULL))))GO TO 50 FOT0 61
IPPULL=IPPULL+1 FOT0 62
N=N+1 FOT0 63
50 IF(STDE.GT.ABS( RES(IPPUL)-F(FLOAT(IPPUL))))GO TO 60 FOT0 64
IPPUL=IPPUL-1 FOT0 65
J=1 FOT0 66
60 IF(N.F0.1)GO TO 212 FOT0 67
IF(IPPLO.NE. IPPULL)GO TO 70 FOT0 68
IF(IPPJ0.E0. IPPUL)GO TO 71 FOT0 69
70 WRITE(6,4) IPPLO,IPPLL,IPP00,IPPUL FOT0 70
71 ZN=1./(4.*B(1)**2) FOT0 71
XN=(B(2)/B(1))**2 FOT0 72
XN2=1./B(1)**4 FOT0 73
XN3=XN/4 FOT0 74
THE FOLLOWING STATEMENT HAS BEEN CHANGED BY THE ENEA CPL SO THAT IT
CORRESPONDS TO THE FORMULA WHICH IS IN THE REPORT.
XN4=(XN**2)/FLOAT(NCHN) FOT0 75
XN4=(XN**2)/16. FOT0 76
C(1)=ZN*(Q(2,2)+XN*Q(1,1)) FOT0 77
C(2)=XN2*Q(1,1) FOT0 78
C(3)=(YO**2)*(Q(3,3)+XN3*Q(2,2)+XN4*Q(1,1)) FOT0 79
C(4)=3.1416*(BO*C(3)+C(2)*YO**2/(2.*BO)) FOT0 80
DO 100 I=1,4 FOT0 81
100 C(I)=SQRT(C(I)) FOT0 82
WRITE(6,16) FOT0 83
WRITE(6,17)EPP,XO,BO,YO,AREA FOT0 84
WRITE(6,18)C(1),C(2),C(3),C(4) FOT0 85
RETURN FOT0 86
SUBROUTINE SHIFT(NCHN,NPK,LPP,NWRITE,Y,PO) SHIFT 1

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10 DIMENSION Y(400), IX0(15), X(15), E(15), X5(15), RES(400)
11 FORMAT( 6X, 12F6.0, 2X )
12 FORMAT( 10I3 )
13 FORMAT( 4(I3, 7X, F10.0) )
16 FORMAT( 8F10.0 )
26 FORMAT( /1X, 12H OLD GAIN = , E14.7, 13H INTERCEPT = , E14.7,
11X, 18H BASE LINE SHFT = , E14.7, 12H NEW GAIN = , E14.7, 9H RATIO = ,
2E14.7 )
42 FORMAT( 14, (1X, 10E12.5) )
44 FORMAT( 1H1, 1X, 17H NON SHIFTED SPECT , 3X, A4 )
45 FORMAT( 1X, 13H SHIFTED SPECT , 3X, A4 )
47 FORMAT( 5E14, 8 )
48 FORMAT( 1H1 )
WRITE(6, 48)
READ(5, 16) GAIN
READ(5, 12) (IX0(I), E(I), I=1, NPK)
IX0 = APPROX MID PT OF PP
E = ENERGY OF GAMMA PP
DO 100 I=1, NPK
IPPULL=IX0(I)-3
IPPUL=IX0(I)+3
CALL PHOTO(Y, X0, IPPULL, IPPUL, E(I), AREA)
100 X(I)=X0
IF(NPK.GT.1) GO TO 800
B1=E(1)/X(1)
BLSHFT=0.
800 XNPK=NPK
EM=0.
XM=0.
IF(NPK.EQ.1) GO TO 103
DO 807 J=1, NPK
EM=EM+E(J)
XM=XM+X(J)
807 EM=EM/XNPK
XM=XM/XNPK
TP=0.
BT=0.
DO 808 J=1, NPK
TP=TP+(X(J)-XM)*(E(J)-EM)
808 BT=BT+(X(J)-XM)**2
B1=TP/BT
EO=EM-B1*XM
IF(NPK.EQ.1) GO TO 103
BLSHFT=-EO/B1
103 RATIO=(E(LPP)-EO)/(GAIN*X(LPP))
WRITE(6, 26) B1, EO, BLSHFT, GAIN, RATIO
DO 809 J=1, NPK
XP(J)=RATIO*(X(J)-BLSHFT)
809 NCHN2=FLOAT(NCHN)*RATIO+0.5
CALL SHIFTS(Y, RES, RATIO, NCHN, NCHN2, BLSHFT)
DO 900 I=1, NPK
IPPULL=XP(I)-3.
IPPUL=XP(I)+5.
CALL PHOTO(RES, X0, IPPULL, IPPUL, E(I), AREA)
900 CONTINUE
WRITE(6, 44) P0
WRITE(6, 42) NCHN, (Y(J), J=1, NCHN)
WRITE(6, 45) P0
WRITE(6, 42) NCHN2, (RES(J), J=1, NCHN2)
NCHN=NCHN2
DO 905 I=1, NCHN
905 Y(I)=RES(I)
IF(NWRITE.EQ.0) RETURN
WRITE(2, 45) P0
WRITE(2, 47) (RES(J), J=1, NCHN2)
RETURN
END
SUBROUTINE SHIFTS(SPECT, S, RATIO, NCHN, NCHN2, BLSHFT)
DIMENSION SPECT(400), S(400)
X=0.
11=0
** TEST DATA FOR ZERO COUNTS IN CHANNELS 1, 2, OR 3
IF(SPECT(1).NE.0.) GO TO 20
SPECT(1)=SPECT(2)
20 IF(SPECT(2).NE.0.) GO TO 21
SPECT(1)=SPECT(3)
SPECT(2)=SPECT(3)
21 IF(SPECT(3).NE.0.) GO TO 22
SPECT(1)=SPECT(4)
SPECT(2)=SPECT(4)
SPECT(3)=SPECT(4)
** FIT 3 POINTS OF SPECTRUM WITH PARABOLA AND EVALUATE

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22	X=X+1. I1=I1+1 AD=(X/RATIO)*RLSHFT IF(XP.LE.1.)GO TO 24 IF(XP.GE.2.)GO TO 25 GO TO 26	SHIFT	16
24	S(I1)=SPECT(1)/RATIO GO TO 22	SHIFT	17
26	X1=1. X2=2. X3=3. Y1=SPFCT(1) Y2=SPFCT(2) Y3=SPFCT(3) GO TO 27	SHIFT	18
25	IX2=XD+.5 IF(IX2.GE.NCHN)GO TO 28 IX1=IX2-1 IX3=IX2+1 Y1=SPFCT(IX1) Y2=SPFCT(IX2) Y3=SPFCT(IX3) X1=IX1 X2=IX2 X3=IX3	SHIFT	19
27	AA=(Y3-2.*Y2+Y1)/2. BB=(-Y3*(X2+X1)+2.*Y2*(X1+X3)-Y1*(X3+X2))/2. CC=((X1*X2*Y3)-2.*(X1*X3*Y2)+(X2*X3*Y1))/2. S(I1)=(AA*XP+BB*XP+CC)/RATIO IF(S(I1).LT.0.)S(I1)=0.0 IF(I1.LT.NCHN2)GO TO 22 RETURN END	SHIFT	20
40	SUBROUTINE WRIT1(O,BETA,STDEV,NISO) DIMENSION O(15),BETA(15),STDEV(15) FORMAT(8X,6(4X,A4,4X)) FORMAT(8HSOL(PPM),6(E12.4)) FORMAT(8HSTD DEV ,6(E12.4)) LO=1 MAX=0	SHIFT	21
44	IF(NISO.LT.MAX)MAX=NISO WRITE(2,40)(O(I),I=LO,MAX) WRITE(2,42)(BETA(I),I=LO,MAX) WRITE(2,43)(STDEV(I),I=LO,MAX) IF(NISO.EQ.MAX)GO TO 50 LO=LO+6 MAX=MAX+6 GO TO 44	SHIFT	22
50	RETURN END	SHIFT	23
105	SUBROUTINE VARNCE(A,OMG,STDEV,AT,LOCHN,NHICHN,NISO,MAXCON,C,P,O,BE 1IA,XNORM) DIMENSION RES(400),OMG(400),STDEV(400),AT(400,15),P(15),O(15),BETA 1(15),C(15),A(400),XNORM(15) DO 105 J=LOCHN,NHICHN RES(J)=0.0 K=1 DO 101 I=1,MAXCON IF(P(I).NE.0(K))GO TO 101 DO 102 J=LOCHN,NHICHN RES(J)=RES(J)+((BETA(K)/C(K))**2)*AT(J,I)/XNORM(I)+(AT(J,I)*STDEV(1K)/C(K))**2 K=K+1 IF(K.GT.NISO)GO TO 103 CONTINUE DO 104 J=LOCHN,NHICHN A(J)=OMG(J)+RES(J) RETURN END	SHIFT	24
101		SHIFT	25
103		SHIFT	26
104		SHIFT	27
30	SUBROUTINE DELETE(NISO,REMOVE,ISOCHN,BETA,R,C,O,THETA,L) DIMENSION RES(400),BETA(15),C(15),O(15),THETA(15),R(15,15) FORMAT(/174 ISOTOPE REMOVED , A4 /) WRITE(6,30)O(L) NISO=NISO-1 BETAR=BETA(L)/C(L) DO 601 J=1,ISOCHN RES(J)=R(J,L) REMOVE=REMOVE-(BETA(L)/C(L))**2/R(L,L) DO 604 K=1,NISO BETA(K)=(BETA(K)/C(K)-RES(K)*BETAR/RES(L))*C(K) DO 604 J=1,NISO R(K,J)=R(K,J)-RES(K)*RES(J)/RES(L)	SHIFT	28
601		SHIFT	29
604		SHIFT	30
		SHIFT	31
		SHIFT	32
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		SHIFT	96
		SHIFT	97
		SHIFT	98
		SHIFT	99
		SHIFT	100

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DO 602 K=L,NISO
C(K)=C(K+1)
S(K)=S(K+1)
THETA(K)=THETA(K+1)
BETA(K)=BETA(K+1)
DO 602 J=1,NISOCHN
R(J,K)=R(J,K+1)
DO 603 K=L,NISO
DO 603 J=1,NISO
R(K,J)=R(K+1,J)
RETURN
END
SUBROUTINE DET(R,N,DETERM)
DIMENSION R(15,15)
DETERMINANT EVALUATED USING PIVOTAL CONDENSATION
K = 2
L = 1
DO 20 I=K,N
RATIO = R(I,L)/R(L,L)
DO 20 J=K,N
R(I,J) = R(I,J)-R(L,J)*RATIO
CONTINUE
IF(K=N) 15,21,21
L = K
K = K+1
GO TO 5
21 DETERM = 1
DO 25 L=1,N
25 DETERM = DETERM*R(L,L)
RETURN
END
SUBROUTINE WRIT(NITER,ITER,0,BETA,STDEV,ST,NISO,F,RCORR)
DIMENSIONO(15),BETA(15),STDEV(400),ST(15)
401 FORMAT(/10X,10(4X,A4,4X))
421 FORMAT(/11H ITERATION,13,4H OF,13,9H MAX ITER /)
431 FORMAT(10H SOL(PPM),10(E12.4))
441 FORMAT(10H STD DEV,10(E12.4))
451 FORMAT(12H F VALUES,10(E12.4))
WRITE(6,41)NITER,ITER
MAX=NISO
IF(NISO.LE.10)GO TO 4450
MAX=10
WRITE(6,40)(O(I),I=1,MAX)
WRITE(6,42)(BETA(I),I=1,MAX)
WRITE(6,43)(STDEV(I),I=1,MAX)
WRITE(6,44)(ST(I),I=1,MAX)
IF(NISO.LE.10)GO TO 4451
WRITE(6,40)(O(I),I=11,NISO)
WRITE(6,42)(BETA(I),I=11,NISO)
WRITE(6,43)(STDEV(I),I=11,NISO)
WRITE(6,44)(ST(I),I=11,NISO)
51 WRITE(6,45)F,RCORR
RETURN
END
SUBROUTINE SAVE(NISO,0,OI,RI,RII)
DIMENSIONO(15),OI(15),RI(15,15),RII(15,15)
DO 3180 I=1,NISO
OI(I)=O(I)
DO 3180 J=1,NISO
80 RII(I,J)=RI(I,J)
RETURN
END
SUBROUTINE XFORM(NFORM,NISO,R,RI,MAXCON,P,0,LOCHN,NHICHN)
1R,NWRIT,NIDEN,NINTF,RII,BETA,THETA,OI,RHO,III)
DIMENSION R(15,15),RI(15,15),RII(15,15),P(15),O(15),A(400)
115),OI(15),Q(15,15),S(15,15),BETA(15),THETA(15),RHO(400)
THIS SUB. FORMS OR READS A=TRANS * W * A
9 =FORMAT(1H1)
13 =FORMAT(14,1X,10(E12.5))
23 =FORMAT(1X,A4,(1X,9E12.5))
25 =FORMAT(/18H CORRELATION COEFF /)
28 =FORMAT(/26H INTERFERENCES IN PER CENT /)
29 =FORMAT(/21H CROSS PRODUCT MATRIX /)
31 =FORMAT(/25H INV CROSS PRODUCT MATRIX /)
32 =FORMAT(/16H IDENTITY MATRIX /)
33 =FORMAT(/13H INV ERROR =,E14.7 /)
37 =FORMAT(/20H EFF(IN PER CENT) =,E18.12 /)
39 =FORMAT(/6X,9(4X,A4,4X))
GO TO (98,99,40),NFORM
40 CALL PEAKS(AT,A,RHO,LOCHN,NHICHN,NISO,III)

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DETR	1
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WRIT	1
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SAVE	1
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98 GO TO 99
  READ(5,29)((R(I,J),I=1,NISO),J=1,NISO)
  CALL SAVE(NISO,0,0I,R,RII)
  GO TO 322
99 DO 102 J=1,NISO
  DO 102 I=1,NISO
  RI(I,J)=0.
102 R(I,J)=0.
  LL=1
  DO 4052 J=1,MAXCON
  IF(P(J).NE.0(LL))GO TO 4052
  L=1
  DO 4053 K=1,MAXCON
  IF(P(K).NE.0(L))GO TO 4053
  DO 100 I=LOCHN,NHICHN
  IF(A(I).LE.0.001)A(I)=1.0
100 R(LL,L)=R(LL,L)*AT(I,J)*AT(I,K)/A(I)
  L=L+1
  IF(L.GT.NISO)GO TO 4054
4053 CONTINUE
4054 LL=LL+1
  IF(LL.GT.NISO)GO TO 4055
4052 CONTINUE
4055 WRITE(6,23)
  IF(NCORR.NE.0) GO TO 97
  WRITE(6,23)
  DO 311 J=1,NISO
  DO 311 I=1,NISO
311 RI(I,J)=(R(I,J)**2)/(R(I,I)*R(J,J))
  WRITE(6,18)NISO,((RI(I,J),I=1,NISO),J=1,NISO)
  CALL DET(RI,NISO,DETERM)
  DETERM=100.*DETERM
  WRITE(6,37)DETERM
97 CALL SAVE(NISO,0,0I,R,RII)
  IF(NWRIT.NE.0) GO TO 107
  WRITE(6,9)
  WRITE(6,28)
  WRITE(6,18)NISO,((R(I,J),I=1,NISO),J=1,NISO)
107 CALL SMINV(R,NISO)
  IF(NWRIT.NE.0) GO TO 313
  WRITE(6,31)
  WRITE(6,18)NISO,((R(I,J),I=1,NISO),J=1,NISO)
  CALL SAVE(NISO,0I,0,RRI,RI)
  CALL SAVE(NISO,0,0I,R,RII)
313 IF(NIDEN.NE.0)GO TO 322
  LL=0
001 ERROR=0.
  DO 324 K=1,NISO
  DO 324 J=1,NISO
  Q(K,J)=0.
  DO 324 I=1,NISO
324 Q(K,J)=Q(K,J)+RI(K,I)*R(I,J)
  DO 323 K=1,NISO
  DO 323 J=1,NISO
323 ERROR=ERROR+ABS(Q(K,J))
  ERROR=(ERROR+FLOAT(NISO))/((FLOAT(NISO))**2)
  IF(LL.GT.3)GO TO 3360
  IF(ERROR.LT.0.000050)GO TO 3360
  *** ITERATE TO IMPROVE ACC
  DO 127 I=1,NISO
  DO 127 J=1,NISO
127 S(I,J)=Q(I,J)
  DO 128 J=1,NISO
128 S(J,J)=2.0+S(J,J)
  DO 129 K=1,NISO
  DO 129 J=1,NISO
  Q(K,J)=0.0
  DO 129 I=1,NISO
129 Q(K,J)=Q(K,J)+R(K,I)*S(I,J)
  DO 130 J=1,NISO
  DO 130 K=1,NISO
130 R(K,J)=Q(K,J)
  LL=LL+1
  GO TO 4001
4001 WRITE(6,33)ERROR
  WRITE(6,32)
  WRITE(6,18)NISO,((Q(J,K),J=1,NISO),K=1,NISO)
322 IF(NINTF.NE.0)RETURN
  WRITE(6,9)
  WRITE(6,25)
  MIN=2
  MAX=NISO-1

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DO 315 I=1,MAX
DO 316 J=MIN,NISO
BETA(J)=0(J)
316 THETA(J)=((R(I,J)**2)/(R(I,I)*R(J,J)))*100.
WRITE(6,39)(BETA(J),J=MIN,NISO)
WRITE(6,22)O(I),(THETA(J),J=MIN,NISO)
315 MIN=MIN+1
RETURN
END
SUBROUTINE WATE(NVAR,NUMVAR,NCHAN,RHO,XNCOM,III,OMG,A,RES,ISOCHN;
11 DIMENSION RES(400),RHO(400),OMG(400),A(400)
147 FORMAT(1X,14.8)
48 FORMAT(/22H AVE WT FACTORS==USES,13.4H IN NO /)
49 FORMAT(/19H WT FACTORS = UNITY /)
FORMAT(/15H WT FACTORS = Y /)
THIS SUB CALCULATES OR READS THE WT FACTORS
READ OR SET VARIANCES USING (A) AS STORAGE
GO TO (201,203,3010),NVAR
201 DO 2202 J=1,400
2202 RES(J)=0.0
WRITE(6,47)NUMVAR
DO 2201 J=1,NUMVAR
READ(5,11)(A(I),I=1,NCHAN)
DO 2222 K=1,NCHAN
2222 RES(K)=RES(K)+A(K)
2201 CONTINUE
DO 2224 I=1,NCHAN
2224 RES(I)=RES(I)/FLOAT(NUMVAR)
WRITE(2,11)(RES(I),I=1,NCHAN)
DO 2223 I=1,NCHAN
2223 A(I)=RES(I)
GO TO 203
203 DO 213 I=1,ISOCHN
213 A(I)=1.0
WRITE(6,48)
GO TO 205
3010 DO 3014 I=1,ISOCHN
3014 A(I)=RHO(I)/XNCOM
IF(A(I).EQ.0.)A(I)=1.0
WRITE(6,49)
205 IF(NVAR.EQ.2)GO TO 254
IF(III.GT.1)GO TO 254
256 DO 255 I=1,ISOCHN
255 OMG(I)=A(I)
254 CONTINUE
RETURN
END
SUBROUTINE CHI(CALC,RES,MAXCON,P,O,LOCHN,NHICHN,BETA,AT,C,RHO,NISO
1,QUAL,A)
DIMENSION CALC(400),RES(400),P(15),O(15),BETA(15),AT(400,15),C(15),
1RHO(400),A(400)
10 FORMAT(1X,2A4)
14 FORMAT(18H DEG OF FREEDOM = ,F4.0,15H QUAL OF FIT = ,E10.3)
18 FORMAT(/14,(1X,10E12.5))
DO 105 I=LOCHN,NHICHN
105 CALC(I)=0.
RES(I)=0.
K=1
DO 956 I=1,MAXCON
956 IF(P(I).NE.0(K))GO TO 956
DO 970 J=LOCHN,NHICHN
970 CALC(J)=BETA(K)*AT(J,I)/C(K)+CALC(J)
K=K+1
IF(K.GT.NISO)GO TO 957
CONTINUE
957 QUAL=0.
DO 104 I=LOCHN,NHICHN
104 RES(I)=RHO(I)-CALC(I)
DO 971 J=LOCHN,NHICHN
971 QUAL=QUAL+(RES(J)**2)/A(J)
QUAL=QUAL/FLOAT(NHICHN-LOCHN-NISO)
DF=NHICHN-LOCHN-NISO
WRITE(6,14)DF,QUAL
RETURN
END
SUBROUTINE PEAKS(AT,A,RHO,LOCHN,NHICHN,NISO,III)
1 DIMENSION AT(400,15),A(400),RHO(400),NK(40),T(5),C(5),CT(400,5),ISOCHN(15)
41 FORMAT(/14H COMPLEX SPECT /)
42 FORMAT(25I3)
43 FORMAT(1X,5E14.7)

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FORM	103
FORM	104
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FORM	106
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FORM	108
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FORM	110
WATE	1
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WATE	4
WATE	5
WATE	6
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WATE	8
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WATE	33
WATE	34
WATE	35
WATE	36
WATE	37
WATE	38
CHI	1
CHI	2
CHI	3
CHI	4
CHI	5
CHI	6
CHI	7
CHI	8
CHI	9
CHI	10
CHI	11
CHI	12
CHI	13
CHI	14
CHI	15
CHI	16
CHI	17
CHI	18
CHI	19
CHI	20
CHI	21
CHI	22
CHI	23
CHI	24
CHI	25
CHI	26
CHI	27
CHI	28
PEAK	1
PEAK	2
PEAK	3
PEAK	4
PEAK	5
PEAK	6
PEAK	7


```

106 R(J,I)=R(I,J)
115 MIN=MTN+1
RETURN
300 WRITE (3,6)
STOP
END
FUNCTION INDEX(I8,J8,N)
FOR SYMMETRICAL MATRICES ONLY.
THIS SUBPROGRAM ALLOWS THE PROGRAMMER TO REFER TO A TWO-DIMENSIONAL
MATRIX WITH SUBSCRIPTS (I,J) WHILE THE MATRIX IS STORED AS A VECTOR.
I9= ROW OF MATRIX
JI= COLUMN OF MATRIX
N = ORDER OF MATRIX

I9=I8
JI=J8
IF(I9.LE.JI)GO TO 2
J9=JI
JI=I9
I9=J9
2 MI=0
IF(I9.LT.2)GO TO 4
DO 5 LI=2,I9
5 MI=MI+N-LI
4 INDEX=I9+JI-1+MI
RETURN
END
SUBROUTINE STAT(REMOVE,BETA,RHOSQD,NISO,LOCHN,NHICHN,R,C,O,AT,A,RES,
15,RHO,NVAR,NR,RAT,ST,NITER,F,RCORR,P,MAXCON,RHOSUM,XNORM,MVAR,ISO,STAT
21(I))
DIMENSION RES(400),BETA(15),R(15,15),C(15),O(15),AT(400,15),A(400),
15,RHO(400),S2(15),ST(15),P(15),XNORM(15),ISO(15),ATT(400,15)
28 FORMAT(/12H STD DEV OF ,A4,8H IS NEG /)
34 FORMAT( 6X,12F6.0,2X )
IF(IIT.GT.1)GO TO 525
DO 526 J=1,MAXCON
DO 527 I=1,NHICHN
527 ATT(I,J)=0.0
LI=ISO(J)
DO 524 I=1,LI
524 ATT(I,J)=AT(I,J)
526 CONTINUE
VAREST=1.0
RCORR= REMOVE/RHOSQD
IF(RCORR.GT.0.9999)GO TO 502
DF=FLOAT(NHICHN-LOCHN+1)
VAREST=(RHOSQD-RHOSUM/DF)/DF
502 IF(MVAR.EQ.0)GO TO 522
DO 523 J=1,NISO
LI=ISO(J)
523 READ(5,34)(ATT(I,J),I=1,LI)
522 DO 123 I=1,NISO
S2(I)=0.0
LI=1
DO 122 J=1,MAXCON
IF(P(J).NE.0(L))GO TO 122
DO 102 K=LOCHN,NHICHN
102 S2(I)=S2(I)+(R(I,L)*RHO(K)/A(K))*2)*ATT(K,J)/XNORM(J)
LI=LI+1
IF(LI.GT.NISO)GO TO 123
122 CONTINUE
123 CONTINUE
IF(NVAR.EQ.2)GO TO 100
IF(NITER.GT.0)GO TO 107
IF(NVAR.NE.3)GO TO 111
DO 103 I=1,NISO
IF(R(I,I).GE.0.)GO TO 104
WRITE(6,28)O(I)
R(I,I)=ABS(R(I,I))
104 RES(I)=SORT(R(I,I),S2(I))*C(I)
103 ST(I)=BETA(I)/RES(I)
IF(NVAR.EQ.3)GO TO 105
111 IF(NR.EQ.0)GO TO 107
VAREST=RAT
GO TO 100
107 DO 131 I=1,NISO
RES(I)=0.0
MI=1
DO 110 J=1,MAXCON
IF(P(J).NE.0(M))GO TO 119
MI=1
DO 120 LI=1,MAXCON

```

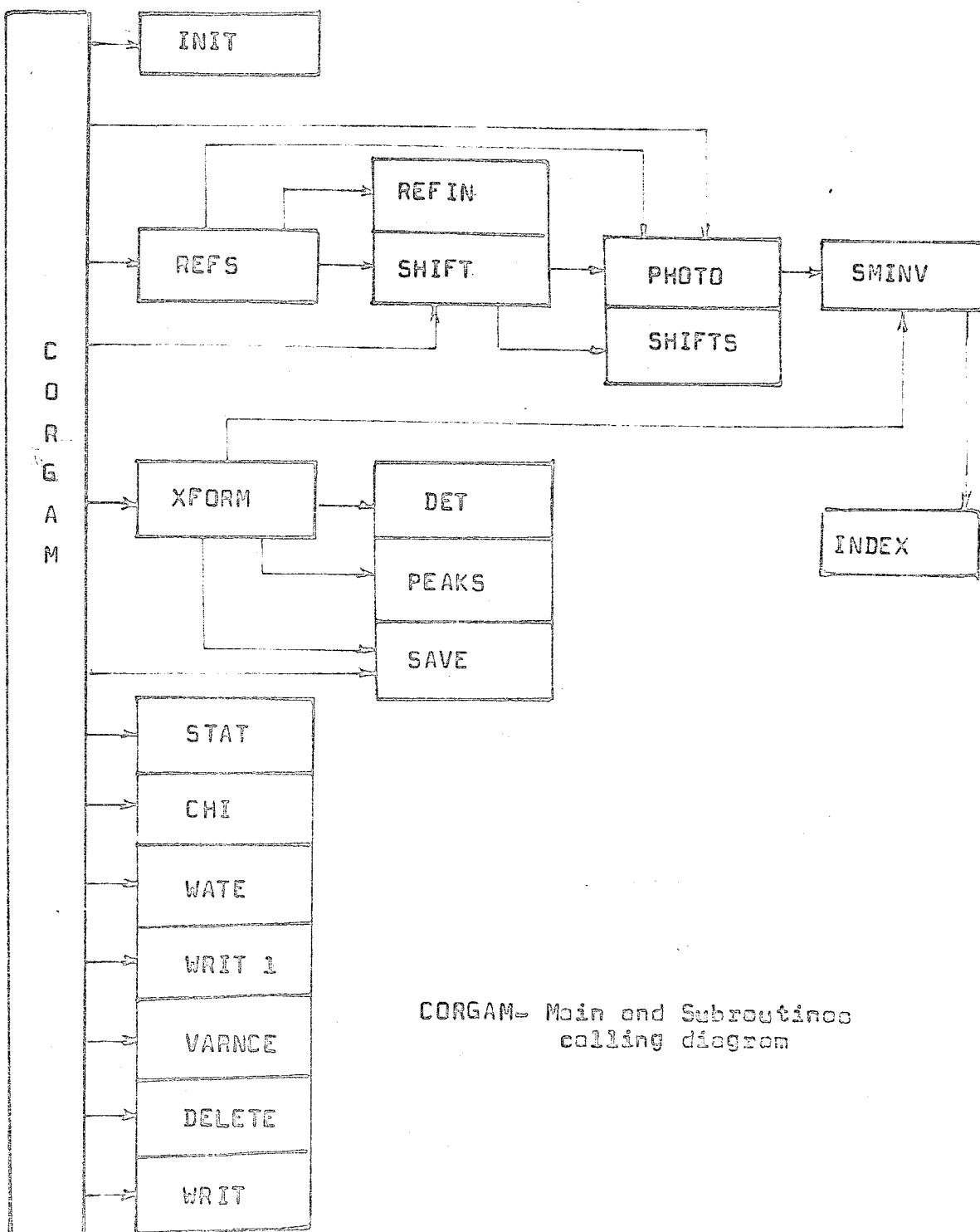
```

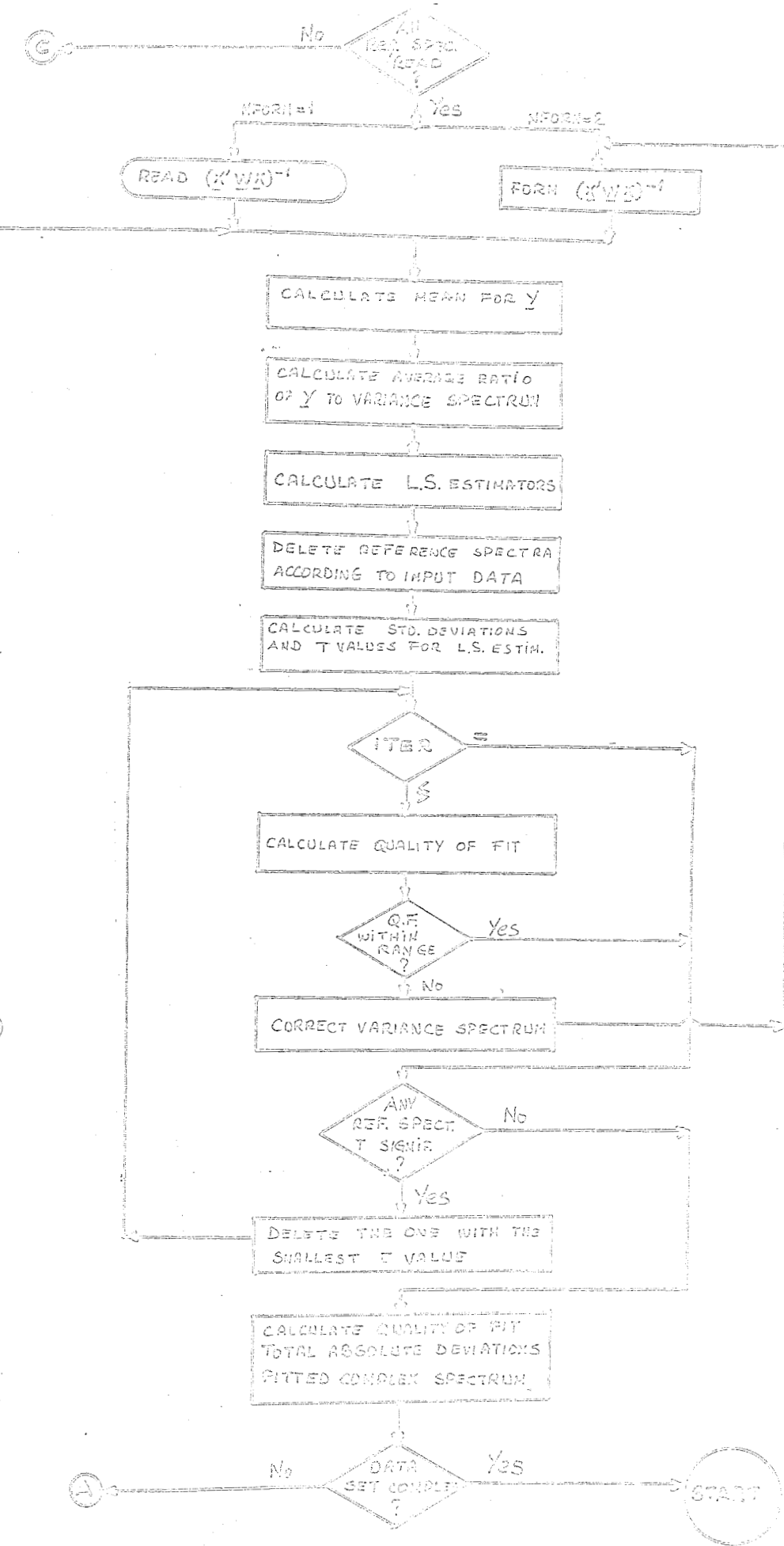
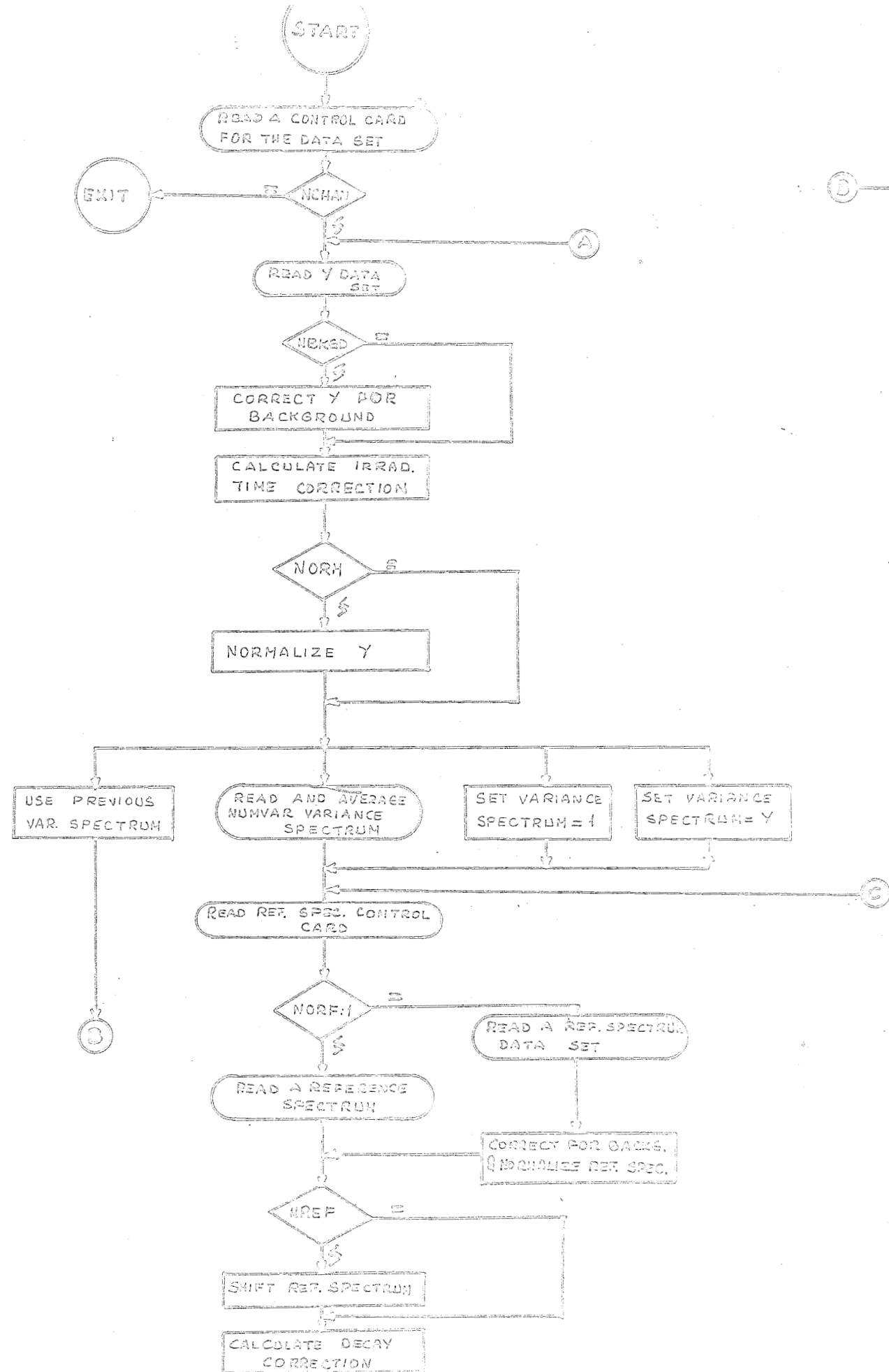
MIN 140
MIN 141
MIN 142
MIN 143
MIN 144
MIN 145
INDEX 1
INDEX 2
INDEX 3
INDEX 4
INDEX 5
INDEX 6
INDEX 7
INDEX 8
INDEX 9
INDEX 10
INDEX 11
INDEX 12
INDEX 13
INDEX 14
INDEX 15
INDEX 16
INDEX 17
INDEX 18
INDEX 19
INDEX 20
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INDEX 39
INDEX 40
INDEX 41
INDEX 42
INDEX 43
INDEX 44
INDEX 45
INDEX 46
INDEX 47
INDEX 48
INDEX 49
INDEX 50
INDEX 51
INDEX 52
INDEX 53
INDEX 54
INDEX 55

```


APPENDIX J

-FLOW DIAGRAM OF THE CODE





APPENDIX K

- LISTING OF THE INPUT DATA FOR SAMPLE PROBLEM

The following is the listing of the input data cards used for the analysis of the sample problem data. They are listed in order of appearance in the program. For further use change of some of the control cards is sufficient. The data can be read from punched cards as well as from a storage file or from a magnetic tape. The listing of the input data is also given together with the read formats. The options are given in the comments cards of CORGAM and in the appendix F.

1. Card: (15A4) ID card for the complex spectrum

2. Card: (25I3)

NISO: Number of isotopes in complex spectra used in the analysis

NCASES: Number of complex spectra to be analyzed

NRES: Resonance calculation control parameter (optional)

NFORM: Least-squares fit control parameter (optional)

NWRIT: (X^0WX) matrix writing control parameter (optional)

NCORR: Correlation coefficient control parameter (optional)

NINTF: Interferences calculation control parameter (optional)

NIDEN: Identity matrix control parameter (optional)

3. Card: (25I3)

NCHG1: Change in NAM1 (optional)

NCHG2: Change in NAM2 (optional)

NCHG3: Change in NAM3 (optional)

(NAM1, NAM2, NAM3 are the NAMELIST variables)

4. Card: If change in NAM1 is required, new values are given by this card

5. Card: " NAM2 " " "

6. Card: " NAM3 " " "

7. Card: " " " " "

NAM1 contains ISOCHN, MODE, NBKGD, NUBKG, NSHFT, NPK, LPP, NORM, NCTIN

NHICHN, NCHAN, MC, MVAR

NAM2 contains C(I)

NAM3 contains T, DECAY, COUNT, WT, CUCT, WTCU, AREA, CUDEC, BKGTIM, TIMIRR,

FRHL, UP, XNCOM

The definitions of these variables are given in the comments of

CORGAM. These variables are entered in the program by a DATA statement, if a change is required, this is done in the 3. card and the new values are given in 4., 5., 6. and 7. cards. If a specific isotope won't be used in the analysis -1.0 will be entered in NAM2 for the C(I) value of the Ith isotope. For the complex spectra following the first one (if any), the input parameters are read from the subprogram INIT.

8. Card: (15A4) Complex spectrum ID card

9. Card up to 30. Card (included) (6X, 12(F6.0, 2X)) :

This is the complex spectrum data set. The variable name is RHO(I) where I is from 1 to ISOCHN. ISOCHN is the number of the channel contained in the complex spectrum. Maximum value of I can be 400, and 12 values are punched on each card. If the channel numbers are less than 400 (as in the case of sample problem 256), only the values prespecified are read.

31. Card: (15A4) Background ID card

32. Card up to 53. Card (included) (6X, 12(F6.0, 2X)): Background spectrum deck,

The variable name is BKG(I) where I is from 1 to ISOCHN

54. Card: Flux reference spectrum ID card

55. Card up to 58. Card (included) (6X, 12(F6.0, 2X)): Flux reference spectrum data set. The variable name is RES(I) where I is from 1 to NCHCU.

NCHCU is the channel number contained in the flux reference spectrum.

59. Card: (8F10.0) The gain of the system in MeV/ch. The variable name is GAIN

60. Card: (4(I3, 7X, F10.0)) IXO(I), E(I) I from 1 to NPK, where the variable

IXO is the approximate mid-point of photopeak, E is the energy of the gamma photopeak in MeV. Both values are for the complex spectrum. NPK

being the number of the photopeaks in the complex spectrum.

61. Card: (A4, 9I3) O(I), ISO(I), NPK, LPP, NORF, MODE, NFAC(I), NO

O(I): Tag name of the Ith isotope

ISO(I): Number of channels in the Ith reference isotope

NPK: is the photo-peaks contained in the complex spectrum

LPP: Index of photo-peak used in shifting

NORF: Specification for normalization of reference spectra

MODE: Reference spectrum input specification

NFAC(I): Decay time specification of reference spectrum

NO: Number of decay spectra of a specific reference isotope

62. Card: (8F10.0) H(I), D(I), FRRHL, XNORM(I)

H(I): Half-life, in minutes, of reference isotope spectrum

D(I): Irradiation time, in minutes, of reference sample spectrum

FRRHL: Reference spectrum, flux reference isotope half-life, in minutes

XNORM(I): Normalization constant of the Ith reference isotope

63.and64.Cards:(8F10.0) T(J),C(J) J from 1 to NO

These data are for the reference decay spectra. Where T(J) is the decay time in minutes of the Jth decay spectra and C(J) is the count time in minutes of the Jth decay spectra. NO being the number of the decay spectra.

65.Card:(25I3) NUBKG,NCULL,NCUUL,NCHCU,NCHBK

NUBKG:Background spectra specification

NCULL:Lower fit limit on copper reference photopeak

NCUUL:Upper " " " " "

NCHCU:Number of channels in copper reference spectrum

NCHBK:Number of channels in background spectrum

66.Card:(8F10.0) COUN,DECA,BKGTIM,CUDEC,WT,WTCU,CUCT

COUN:Counting time,in minutes,for reference spectrum

DECA:Decay time,in minutes,for reference spectrum

BKGTIM:Background counting time,in minutes,for reference spectrum

CUDEC:Decay time,in minutes,for flux reference spectrum

WT:Weight,in grams,of the reference isotope

WTCU:Weight,in grams,of the flux reference isotope

CUCT:Counting time,in minutes,for the reference spectrum,flux referenc spectrum.

67.Card up to 186.Card (5E14.8) CT(J,M) J from 1 to ISOCHN, M from 1 to NO

These are the decay spectra of the reference isotopes,where CT(J,M)

is the counts registered at Jth channel of the reference isotope

Mth decay time.NO is the number of decay spectra.If an isotope doesn't have a decay spectra M is assumed to be equal to 1.

187.Card:same as card 61

188.Card:same as card 62

189.and 190.Cards:same as cards 63 and 64

191.Card:same as card 65

192.Card:same as card 66

193.Card and the following deck:same as 67. card and the following deck.

The same order repeats itself till all the reference isotopes are read in.In the sample problem data this repetition ends at the 458. card.From this point on the next complex spectrum data is given, using the same formats as in the first spectrum.

459.Card:same as card 3

460.Card:same as card 4

461.Card:same as card 5

462.Card:same as card 6

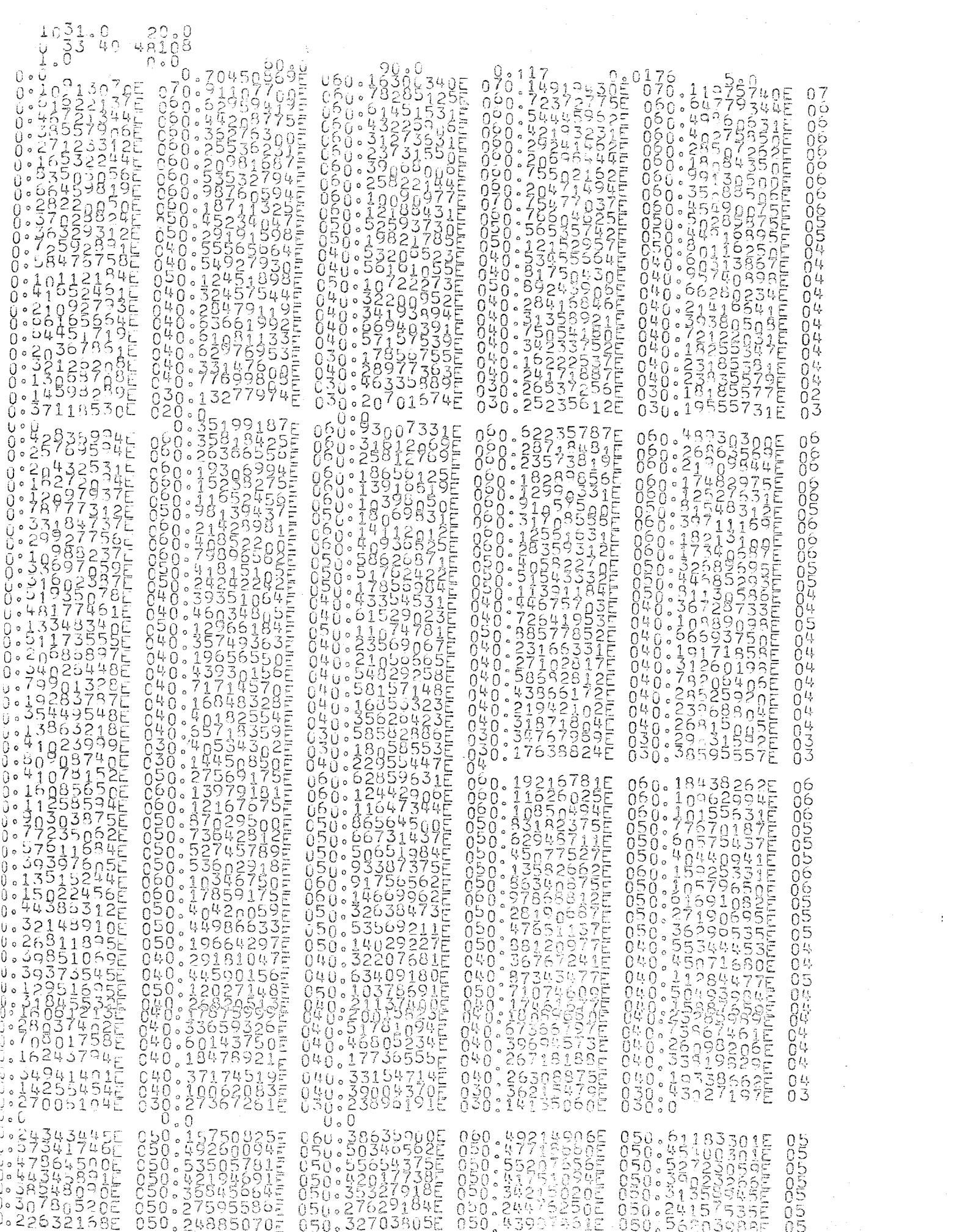
463.Card:same as card 7

464.Card:same as card 8

465.Card up to 486.Card:same as the 9. card up to 30. card

The same order repeats itself till all the complex spectra are read in.

	3597	5590	10056	8062	7501	7429	7323	7390	7557	7383	6471	4822
	11843	2296	2705	2427	2401	2400	2804	5929	18481	42037	53059	35133
			417	195	152	146	139	150	154	156	146	139
0.00145		0.845	115		1.81	135		2.12				
R=11115	1	1	1	5								
	1.000	15.0	774.000	0.007								
6.0		2.0	31.0	5.0	62.0	5.0			145.0	10.0		



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[illegible]

INTERFERENCES IN PER CENT

BR-1	CU64 .33129+002	AL28 .34040+000	S370 .58111+002	NA24 .42128-001	CA49 .12584-001	K420 .30729+000	CL38 .52735-003	MN56 .50116+001	MG27 .16896+001
CU64	AL28 .98761-002	S370 .58347+000	NA24 .27170+000	CA49 .61236+000	K420 .95915-002	CL38 .14568+000	MN56 .68828-001	MG27 .19022+000	
AL28	S370 .41628+000	NA24 .69045+001	CA49 .10878+001	K420 .78202+001	CL38 .94716+001	MN56 .11703+002	MG27 .27300+001		
S370	NA24 .16899+002	CA49 .66725+002	K420 .21513+000	CL38 .12249+002	MN56 .69020+000	MG27 .32810+000			
NA24	CA49 .30084+002	K420 .16606+000	CL38 .34992+001	MN56 .13486+001	MG27 .21339+001				
CA49	K420 .26257+000	CL38 .13208+002	MN56 .10819+001	MG27 .66034+000					
K420	CL38 .26989+001	MN56 .12830+000	MG27 .25414+001						
CL38	MN56 .14538+001	MG27 .11412-001							
MN56	MG27 .35122+002								

(ATTRANS * OMEGA * RHO)

10	.31905+007	.24420+007	.19313+009	.28651+005	.63610+007	.28482+006	.51989+005	.57712+007	.17032+009	.15614+007
----	------------	------------	------------	------------	------------	------------	------------	------------	------------	------------

ISOTOPE REMOVED AL28

ISOTOPE REMOVED S370

ISOTOPE REMOVED CA49

ITERATION, 0 OF 0 MAX ITER

	BR-1	CU64	NA24	K420	CL38	MN56	MG27
SOL (PPM)	.1256+003	-.6845+002	.9456+001	.2940+005	.2755+004	.2571+003	.5669+005
STD DEV	.8029+002	.5875+002	.8508+001	.2306+004	.1321+003	.3382+001	.2245+006
T VALUES	.1565+001	-.1131+001	.1112+001	.1231+002	.2066+002	.7601+002	.4549+000

F VALUE = .1647+002 CORR COEF = .9936+000

ISOTOPE REMOVED CU64

ITERATION, 0 OF 0 MAX ITER

	BR-1	NA24	K420	CL38	MN56	MG27
SOL (PPM)	.7461+002	.9575+001	.2845+005	.2759+004	.2569+003	.5669+005
STD DEV	.5330+002	.8508+001	.2305+004	.1321+003	.3384+001	.1245+006
T VALUES	.1400+001	.1125+001	.1234+002	.2089+002	.7570+002	.4554+000

F VALUE = .1921+002 CORR COEF = .9934+000

ISOTOPE REMOVED MG27

ITERATION, 0 OF 0 MAX ITER

	BR-1	NA24	K420	CL38	MN56
SOL (PPM)	.7762+002	.1109+002	.2864+005	.2760+004	.2578+003
STD DEV	.5268+002	.8176+001	.2283+004	.1322+003	.2582+001
T VALUES	.1474+001	.1357+001	.1255+002	.2088+002	.9986+002

F VALUE = .2305+002 CORR COEF = .9934+000

ISOTOPE REMOVED NA24

ITERATION, 0 OF 0 MAX ITER

	BR-1	K420	CL38	MN56
SOL (PPM)	.7980+002	.2896+005	.2788+004	.2578+003
STD DEV	.5260+002	.2269+004	.1306+003	.2581+001
T VALUES	.1517+001	.1276+002	.2134+002	.9986+002

F VALUE = .2681+002 CORR COEF = .9934+000

ISOTOPE REMOVED BR-1

ITERATION, 0 OF 0 MAX ITER

	K420	CL38	MN56
SOL (PPM)	.2932+005	.2780+004	.2578+003
STD DEV	.2255+004	.1305+003	.2317+001
T VALUES	.1300+002	.2130+002	.1113+003

F VALUE = .3841+002 CORR COEF = .9932+000

DEG OF FREEDOM = 112. QUAL OF FIT = .204+001

ABS DEV PER PT = .7490734+001 NO OF PTS = 116

8
SAMPLE WT(GM) = .38600-001 IRR TIME(MIN) = .15000+002 DECAY TIME(MIN) = .12658+003 COUNT TIME = .10000+002
FLUX REF WT(GM) = .33800-001 REF DECAY TIME(MIN) = .10586+004 REF COUNT TIME(MIN) = .20000+001 REF HLIFE(MIN) = .77000+001
BKG TIME(MIN) = .60000+002
Y NORM CONSTANT = .25088707+001

E .845	+OR- 55.292 .138	+OR- BO 6.082 .182	+OR- YO .13030+004 .10611+003	+OR- AREA .26959+004 .73599+003
E 1.810	+OR- XO 115.015 .733	+OR- BO 14.820 2.503	+OR- YO .13337+003 .34285+002	+OR- AREA .91004+003 .25706+003
E 2.120	+OR- XO 134.848 1.326	+OR- BO 18.353 5.758	+OR- YO .55091+002 .20351+002	+OR- AREA .42569+003 .18110+003

OLD GAIN = 1605694-001 INTERCEPT = -.4161721-001
 BASE LINE SHIFT = .2591852+001 NEW GAIN = .1450000-001 RATIO = .1105872+001

E .845	+OR- XO 58.312 .126	+OR- BO 7.691 .193	+OR- YO .11605+004 .11402+003	+OR- AREA .57041+004 .56950+003
E 1.810	+OR- XO 124.372 .695	+OR- BO 19.695 2.609	+OR- YO .11896+003 .25040+002	+OR- AREA .93571+003 .22279+003
E 2.120	+OR- XO 146.336 1.328	+OR- BO 25.668 6.476	+OR- YO .58180+002 .18070+002	+OR- AREA .45962+003 .18319+003

INTERFERENCES IN PER CENT

BR71	CU64 .31393+002	AL28 .33853+000	S370 .71415+002	NA24 .55203+001	CA49 .15209+001	K420 .29233+000	CL38 .77592+002	MN56 .54066+001	MG27 .16927+001
CU64	AL28 .96617+002	S370 .50425+000	NA24 .21223+000	CA49 .54022+000	K420 .60307+002	CL38 .16549+000	MN56 .74224+001	MG27 .18237+000	
AL28	S370 .47196+000	NA24 .83994+001	CA49 .12023+001	K420 .85460+001	CL38 .83429+001	MN56 .11327+002	MG27 .23355+001		
S370	NA24 .14227+002	CA49 .96799+002	K420 .11551+000	CL38 .16755+002	MN56 .62402+000	MG27 .27654+000			
NA24	CA49 .25855+002	K420 .76683+001	CL38 .48933+001	MN56 .12103+001	MG27 .22690+001				
CA49	K420 .14319+000	CL38 .18490+002	MN56 .99180+000	MG27 .58122+000					
K420	CL38 .20343+001	MN56 .97560+001	MG27 .26394+001						
CL38	MN56 .16975+001	MG27 .57620+003							
MN56	MG27 .33427+002								

(ATRANS * OMEGA * RHO)

10	.34021+007	.26039+007	.20593+009	.30551+005	.67827+007	.30370+006	.55436+005	.61539+007	.18161+009	.16649+007
----	------------	------------	------------	------------	------------	------------	------------	------------	------------	------------

ISOTOPE REMOVED AL28

ISOTOPE REMOVED S370

ISOTOPE REMOVED CA49

ISOTOPE REMOVED MG27

ITERATION, 0 OF 0 MAX ITER

	BR-1	CU64	NA23	K420	CL38	MN56
SOL (PPM)	.9589+002	.3188+002	.3206+002	.2908+005	.3060+004	.2973+003
STD DEV	.7256+002	.5756+002	.8845+001	.2151+004	.2529+003	.2929+001
T VALUES	.1321+001	.5556+000	.3625+001	.1052+002	.1212+002	.1015+000

F VALUE = .1421+002 CORR COEF = .9933+000

ISOTOPE REMOVED CU64

ITERATION, 0 OF 0 MAX ITER

	BR-1	NA24	K420	CL38	MN56
SOL (PPM)	.1181+003	.3188+002	.2904+005	.3060+004	.2973+003
STD DEV	.4944+002	.8835+001	.2148+004	.2529+003	.2929+001
T VALUES	.2388+001	.3609+001	.1352+002	.1210+002	.1015+000

F VALUE = .2305+002 CORR COEF = .9933+000

DEG OF FREEDOM = 110. QUAL OF FIT = .201+001

ABS DEV PER PT = .6427585+001 NO OF PTS = 116

T VALUE

1.6450

000117000

012-5: 000 2

0297205002

70 592947-000

0.187964002

SAMPLE WT(GM) = .33100-001 IRR TIME(MIN) = .15000-002 DECAY TIME(MIN) = .13858-003 COUNT TIME = .10005-002
FLUX REF WT(GM) = .33800-001 REF DECAY TIME(MIN) = .10588-004 REF COUNT TIME(MIN) = .20000-001 REF HLIFE(MIN) =
BKG TIME(MIN) = .60000-002
Y NORM CONSTANT = .21513891-001

E .845 $\times 0$ 55.274 $\div OR =$.153 $\div OR =$ BO 8.149 $\div OR =$.211 $\div OR =$.99176+003 $\div OR =$.14238+003 $\div OR =$ AREA .5588+004
 1.810 $\div OR =$ 115.051 $\div OR =$ 15.869 $\div OR =$ 3.700 $\div OR =$.99176+003 $\div OR =$.29881+002 $\div OR =$ AREA .72129+003
 E 2.120 $\div OR =$ 134.815 $\div OR =$ 21.825 $\div OR =$ 8.959 $\div OR =$.45162+002 $\div OR =$.17725+002 $\div OR =$ AREA .5396+003
 OLD GAIN = BASE LINE SHIFT = 16.05597-001 INTERCEPT = .2581081+001 NEW GAIN = .4144175-001
 .1430000-001 RATIO = .1106011+001

E .845 $\times 0$ 58.316 $\div OR =$.144 $\div OR =$ BO 7.750 $\div OR =$.223 $\div OR =$.85458+003 $\div OR =$.99316+002 $\div OR =$ AREA .45649+004
 E .810 $\div OR =$ 124.444 $\div OR =$ 23.217 $\div OR =$ 4.085 $\div OR =$.87976+002 $\div OR =$.22449+002 $\div OR =$ AREA .75136+003
 E .120 $\div OR =$ 146.316 $\div OR =$ 35.145 $\div OR =$ 13.085 $\div OR =$.39144+002 $\div OR =$.13593+002 $\div OR =$ AREA .51344+003
 .17957+005

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BR-1	CU64 .32411+002	AL28 .37402+000	S370 .32630-002	NABH .48418-001	CA65 .53556-002	K450 .35052+000	CL51 .10153-001	MA36 .30091+001	MA37 .15246+001
CU64	AL28	S370	NABH	CA65	K450	CL51	MA36	MA37	

MN56 .32414+002
(ATrans * OMEGA * RHO)
10 .29173+007 .22329+007 .17659+009 .26193+005 .58163+007 .26043+006 .47537+005 .52770+007 .15573+009 .14277+007

(ATRANS * OMEGA * RHO)

10 .29173+007 .22329+007 .17659+009 .26193+005 .58163+007 .26043+006 .47537+005 .52770+007 .15573+009 .14277+007

ISOTOPE REMOVED AL28

ISOTOPE REMOVED S370

ISOTOPE REMOVED CA49

ISOTOPE REMOVED MG27

ITERATION, 0 OF 0 MAX ITER

SOL (PPM)	BR-1	CU64	NA24	K420	CL38	MN56
STD DEV	.5051+002	.4285+002	.3240+002	.2822+005	.2530+004	.2405+003
T VALUES	.5909+002	.4629+002	.9474+001	.2121+004	.2928+003	.2723+001
	.9512+000	.9279+000	.3420+001	.1331+002	.8643+001	.8831+002
F VALUE =	.1923+002	CORR COEF =		.9944+000		

ISOTOPE REMOVED CU64

ITERATION, 0 OF 0 MAX ITER

SOL (PPM)	BR-1	NA24	K420	CL38	MN56	
STD DEV	.2559+002	.3267+002	.2828+005	.2536+004	.2405+003	
T VALUES	.4108+002	.9467+001	.2118+004	.2928+003	.2723+001	
	.6229+000	.3451+001	.1335+002	.8663+001	.8831+002	
F VALUE =	.2307+002	CORR COEF =		.9943+000		

ISOTOPE REMOVED BR-1

ITERATION, 0 OF 0 MAX ITER

SOL (PPM)	NA24	K420	CL38	MN56
STD DEV	.3287+002	.2840+005	.2523+004	.2405+003
T VALUES	.9462+001	.2109+004	.2920+003	.2544+001
	.3474+001	.1347+002	.8641+001	.9454+002
F VALUE =	.2884+002	CORR COEF =		.9943+000
DEG OF FREEDOM = 111.		QUAL OF FIT =		.112+001
ABS DEV PER PT =		.4230796+001		NO OF PTS = 110

SAMP-⁵WT(GM) = .34700+001 IRR TIME(MIN) = 15000+002 DECAY TIME(MIN) = .58584+002 COUNT TIME
FLUX RATE WT(GM) = .33800+001 REF DECAY TIME(MIN) = .10586+004 REF COUNT TIME(MIN) = .20000+00
BKG TIME(MIN) = .60000+002
Y NORM CONSTANT = .22553837+001

E .845	+OR-	XO 55.270 .146	+OR-	BO 6.470 .205	+OR-	YO .12431+004 .15673+003	+OR-	AREA .56045+004 .71751+003
E 1.810	+OR-	XO 115.012 .894	+OR-	BO 18.544 3.817	+OR-	YO .13245+003 .33133+002	+OR-	AREA .10109+004 .29259+003
E 2.120	+OR-	XO 135.616 2.102	+OR-	BO 31.956 13.915	+OR-	YO .77483+002 .29524+002	+OR-	AREA .77635+003 .38033+003

OLD GAIN = 1593234-001 INTERCEPT = -.3289121-001
 BAS- LINE SHFT = .2064431+001 NEW GAIN = .1450000-001 RATIO = .1095427+001

E .845	+OR-	XO 58.311 .132	+OR-	BO 8.073 .211	+OR-	YO .11186+004 .10986+003	+OR-	AREA .56235+004 .56299+003
E 1.810	+OR-	XO 123.744 .821	+OR-	BO 22.843 3.375	+OR-	YO .12022+003 .25637+002	+OR-	AREA .10184+004 .26490+003
E 2.120	+OR-	XO 146.161 1.351	+OR-	BO 32.909 8.606	+OR-	YO .71904+002 .17654+002	+OR-	AREA .73112+003 .22529+003

CROSS PRODUCT MATRIX

[illegible]

INV CROSS PRODUCT MATRIX

[illegible]

INV ERROR = .8257627=005

IDENTITY MATRIX

[illegible]

INTERFERENCES IN PER CENT

BR-1	CU64 .31370+002	AL28 .29777+000	S370 .12578-002	NA24 .32211-001	CA49 .78065-002	K420 .33378+000	CL38 .15423-001	MN56 .43482+001	MG27 .16772+001	
CJ04	AL28 .75818-002	S370 .33985+000	NA24 .23203+000	CA49 .37415+000	K420 .25378-002	CL38 .68469-001	MN56 .95285-001	MG27 .17587+000		
AL28	S370 .13087+001	NA24 .69437+001	CA49 .25843+001	K420 .70934+001	CL38 .11727+002	MN56 .11415+002	MG27 .30461+001			
S370	NA24 .30098+002	CA49 .95149+002	K420 .99334-001	CL38 .75423+001	MN56 .33584+000	MG27 .42914+000				
NA24	CA49 .49066+002	K420 .92524-001	CL38 .29996+001	MN56 .11807+001	MG27 .20849+001					
CA49	K420 .12595+000	CL38 .79903+001	MN56 .74939+000	MG27 .92140+000						
K420	CL38 .34394+001	MN56 .20004+000	MG27 .27401+001							
CL38	MN56 .15568+001	MG27 .30668-001								
MN56	MG27 .38096+002									
(ATRANS * OMEGA * RHO)										
10	.30583+007	.23408+007	.18512+009	.27464+005	.60974+007	.27302+006	.49835+005	.55321+007	.16326+009	.14967+007

ISOTOPE REMOVED AL28

ISOTOPE REMOVED S370

ITERATION, 0 OF 0 MAX ITER

	BR-1	CU64	NA24	CA49	K420	CL38	MN56	MG27
SOL (PPM)	.7947+002	.5153+002	.5327+002	-.2857+005	.3454+005	.2770+004	.2119+003	-.4250+004
STD DEV	.7593+002	.5682+002	.1525+002	-.5142+005	.2401+004	.9354+002	.3031+001	.2359+005
T VALUES	.1046+001	.9069+000	.3278+001	-.4552+001	.1443+002	.2958+002	.6902+002	-.1802+000

F VALUE = .1434+002 CORR COEF = .9891+000

ISOTOPE REMOVED CA49

ITERATION, 0 OF 0 MAX ITER

	BR-1	CU64	NA24	K420	CL38	MN56	MG27
SOL (PPM)	.8202+002	.4785+002	-.1536+002	.3567+005	.2772+004	.2112+003	-.4250+004
STD DEV	.7596+002	.5680+002	.7274+001	.2398+004	.9364+002	.3022+001	.2350+005
T VALUES	.1080+001	.8425+000	-.2112+001	.1462+002	.2960+002	.6988+002	-.1808+000

F VALUE = .1638+002 CORR COEF = .9884+000

ISOTOPE REMOVED NA24

ITERATION, 0 OF 0 MAX ITER

	BR-1	CU64	K420	CL38	MN56	MG27
SOL (PPM)	.8302+002	.4828+002	.3480+005	.2750+004	.2107+003	-.4250+004
STD DEV	.7595+002	.5680+002	.2397+004	.9319+002	.3001+001	.2350+005
T VALUES	.1093+001	.8500+000	.1456+002	.2951+002	.7019+002	-.1808+000

F VALUE = .1911+002 CORR COEF = .9882+000

ISOTOPE REMOVED MG27

ITERATION, 0 OF 0 MAX ITER

	BR-1	CU64	K420	CL38	MN56
SOL (PPM)	.8184+002	.4857+002	.3482+005	.2750+004	.2103+003
STD DEV	.7520+002	.5663+002	.2371+004	.9336+002	.2181+001
T VALUES	.1088+001	.8577+000	.1469+002	.2945+002	.9642+002

F VALUE = .2293+002 CORR COEF = .9882+000

ISOTOPE REMOVED CU64

ITERATION, 0 OF 0 MAX ITER

	BR-1	K420	CL38	MN56
SOL (PPM)	.1174+003	.3477+005	.2747+004	.2103+003
STD DEV	.5147+002	.2368+004	.9334+002	.2181+001
T VALUES	.2282+001	.1468+002	.2943+002	.9643+002

F VALUE = .2866+002 CORR COEF = .9882+000

DEG OF FREEDOM = 111. QUAL OF FIT = .340+001

ABS DEV PER PT = .7448490+001 NO OF PTS = 116

APPENDIX M-LISTING OF THE UPDATING PROGRAMS

The first program is used to record the content of the magnetic tape obtained from NEA-CPL to the main storage of a UNIVAC-1106 computer used in Boğaziçi University. The main program and the sample problem data were recorded on to the same file. The main program and the sample input data are loaded separately into two different files, CORGAM and DAFCA respectively. The namelist is removed from the 96. line to the 4. line due to the requirements of the UNIVAC computing system. These are done by the help of the 2. and 3. programs. The 4. program is used to update the coding symbols for UNIVAC-1106 Card Reader and Line Printer. In order to execute the program by the sample input data, the 5. program is used to remove the main program into the 2. cycle of the file, because the first cycle contains the program in data form, by removing it to the 2. cycle, it is transformed into an executable form. Finally the 6. program is used to run the program using the sample data as input.

PROGRAM-1 Records the tape in the main storage

```
@RUN
@ASG,T,J      T.,6C9,D80218
@MOVE  T.,7
@DELETE,C     BOGRUN.
@ASG,UP       BOGRUN.
@USE         F.,BOGRUN.
@COB,ISE
    IDENTIFICATION DIVISION .
    PROGRAM-ID. TEYP-OKUMA.
    ENVIRONMENT DIVISION.
    CONFIGURATON SECTION.
    SOURCE-COMPUTER. U-1106
    OBJECT-COMPUTER. U-1106
    INPUT-OUTPUT SECTION.
    FILE-CONTROL.
        SELECT T ASSIGN TO UNISERVO T.
    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.

@MAP,IN
@XQT
@DATA,L      BOGRUN.
@FIN
```

PROGRAM - 2 1. Update of main program

```
@RUN
@ASG,A        BOGRUN.
@DELETE,C     CORGAM.
@ASG,UP       CORGAM.
@DATA,L       BOGRUN.,CORGAM.
-4
      NAMELIST /NAM1/ISOCHN,MODE,NBKGD,NUBKG,NSHFT,LPP,NORM,NCTIN
1NAREA,NCHCU,NCULL,NCUUL,NRHO,NUMVAR,NVAR,NREFS,ITER,NR,NWW,
2LOCHN,NHICHN,NCHAN,MC,MVAR/NAM2/C/NAM3/T,DECAY,COUNT,WT,CUC
3T,WTCU,AREA,CUDEC,BKGTIM,FHRL,UP,XNCOM
-93,96
-1296,1851
@END
@FIN
```

PROGRAM - 3 Load sample problem data

```
@RUN
@ASG,A        BOGRUN.
@DELETE,C     DAFCA.
@ASG,UP       DAFCA.
@DATA,L       BOGRUN.,DAFCA.
-1,1295
@END
@FIN
```

PROGRAM - 4 2. Update of main program

```
@RUN
@ASG,A        CORGAM.
@ED,L         CORGAM.,CORGAM.
C /READ(1,/READ(5,/ ALL
C /WRITE(3,/WRITE(6,/ ALL
@END
@FIN
```


PROGRAM - 5

3. Update of main program.

```
@RUN
@ASG,A      CORGAM.
@ASG,UP     CORGAM(+1).
@FTN,US     CORGAM(+1)
@ADD,DP     CORGAM.
@FIN
```

PROGRAM - 6

Run of main program with
sample problem inputdata.

```
@RUN
@ASG,A      CORGAM.
@ASG,A      DAFCA.
@DELETE,C 2.
@DELETE,C 10.
@ASG,UP     2.
@ASG,UP     10.
@FTN,S      CORGAM.MAIN
@PREP       CORGAM.
@MAP,I      ,CORGAM.MAIN
IN CORGAM.MAIN
LIB CORGAM.
@XQT        CORGAM.MAIN
@ADD,DP     DAFCA.
@FIN
```

APPENDIX N

The following is a list of the computer programs coded for experimental data processing, used in common neutron activation analysis.

A-Computer codes available in ARGONNE NATIONAL LABORATORY (ANL-7411)

- 1- TOAD : "A computer code for processing gamma-ray spectra"
Reactor code abstract: 333, Coded for: UNIVAC-1108
Language: Fortran IV Issued at: June, 1968
- 2- CORGAM : "A correlation algorithm for gamma-ray spectra"
Reactor code abstract: 390, Coded for: IBM 360/50
Language: Fortran IV-G Issued at: May, 1969
- 3- ALPHA-M : "Resolution of gamma-ray spectra" (improved version of ALPHA)
Reactor code abstract: 413, Coded for: IBM 360
Language: Fortran IV, CPL Issued at: December 1970
- 4- GSSLRN1B : "Least squares photopeak spectra code"
Reactor code abstract: 457, Coded for: UNIVAC-1108
Language: Fortran IV, CPL Issued at: June 1972
- 5- GASPAN : "Complex gamma-ray spectra analysis"
Reactor code abstract: 485, Coded for: CDC 6600
Language: Fortran IV Issued at: January 1972

B-Computer codes available in NEA-CPL, Ispra

- 6- GRETEL : "Ge(L1) gamma spectrum unfolding"
Program abstract: E 433 Coded for: IBM 370
Language: Fortran IV, CPL, Assembler
- 7- RADAK : "Neutron and gamma spectrum unfolding"
Program abstract: E 487 Coded for: IBM 370
Language: Fortran IV