

ANALYSIS OF GAMMA RAY SPECTRA
FROM NEUTRON ACTIVATION STUDIES

by

H. Levent Akın

B.S. in A.E., Istanbul Technical University, 1982

Submitted to the Institute for Graduate Studies in
Science and Engineering in partial fulfillment of
the requirements for the degree of

Master of Science

in

Nuclear Engineering

Bogazici University Library



39001100315046

14

Boğaziçi University

1984

ACKNOWLEDGEMENTS

I would like to express my special thanks to Doç.Dr. Özer Çiftçioğlu whose continual interest helped in preparing the programs. I would also like to thank Doç.Dr.Vural Altın, my thesis advisor, for his invaluable and encouraging guidance and assistance throughout this work. Special thanks are extended to Prof.Dr.Turan B.Enginöl and Doç.Dr.A.Nezihi Bilge for their constructive criticisms and suggestions.

Finally my thanks are due to OECD NEA DATA BANK for supplying program SAMPO80 and GAMDAT-78 gamma ray data collection.

Levent Akın

ABSTRACT

Neutron activation analysis coupled with Gamma Ray Spectrometry is a powerful and highly precise, non-destructive elemental analysis method.

In this work a program package, BUCAASA, was developed for the analysis of gamma ray spectra.

The first program of the package BUCAASA/FIND, using an improved version of the method of the smoothed first derivative identifies the peaks in the spectrum.

The second program BUCAASA/FIT is then used for fitting a function to the peaks for the accurate determination of peak location and peak area. The function used for fitting was developed by Çiftçioğlu.

The third program BUCAASA/CALIBR performs energy and efficiency calibration.

The constituent nuclides together with their activities are identified by the fourth program BUCAASA/NUCLIDE which is an adapted version of SAMPO80 PART III.

All of the programs are interactive and can be used for both routine and academic work. Since they are coded in standard FORTRAN 77 programming language their implementation on other computers is easy. Implementation on microcomputers requires overlaying however.

Ö Z E T

Gamma spektrometri ile birlikte yapılan nötron aktivasyon analizi güçlü, tahribatsız bir element analizi yöntemidir.

Bu çalışmada gamma spektrumlarının analizi için bir program paketi, BUCAASA geliştirilmiştir.

İlk program BUCAASA/FIND, düzgünleştirilmiş birinci türev yönteminin geliştirilmiş bir şeklini kullanarak spektumdaki fotopiklerin tanınması işlevini yerine getirir.

İkinci program BUCAASA/FIT, hassas kanal ve fotopik alanı saptaması için fotopiklere eğri uydurmada kullanılır. Gözönüne alınan fonksiyon Çiftçioğlu tarafından geliştirilmiştir.

Üçüncü program BUCAASA/CALIBR, enerji ve verim kalibrasyonunu yapar.

Spektrumu meydana getiren nüklitlerin tanınması SAMPO80 PART III ün uyarlanmış bir şekli olan dördüncü program BUCAASA/NUCLIDE tarafından yapılır.

Bütün programlar etkileşimlidir ve rutin ve akademik çalışmalar için kullanılabilir. Bütün programlar standard FORTRAN 77 programlama dilinde yazıldığı için başka sistemlere uyarlanmaları kolaydır. Mikrobilgisayarlara uyarlamak için örtme gereklidir.

TABLE OF CONTENTS

	<u>Page</u>
ACKNOWLEDGEMENTS	iii
ABSTRACT	iv
ÖZET	v
LIST OF FIGURES	viii
LIST OF TABLES	ix
LIST OF SYMBOLS	x
1. INTRODUCTION	1
2. GAMMA RAY SPECTROMETRY	3
2.1. Interactions of Gamma Rays With Matter	4
2.2. Detection Systems	6
2.2.1. The Detectors	7
2.2.2. Comparison of Santillation and Semiconductor Detectors	13
3. COMPUTER ANALYSIS OF GAMMA RAY SPECTRA	18
3.1. Peak Identification	22
3.1.1. Peak Location by Finding Relative Maxima	23
3.1.2. Method of Smoothed First Derivative	24
3.1.3. Generalized Second Differences	24
3.2. Dedector Response Functions for the Determination of Peak Position and Area	26
3.2.1. Analytical Approach for Detector Response Functions	27
3.3. Energy and Efficiency Calibration	33
3.4. Nuclide Identification	34
3.4.1. Simple Line Matching	35
3.4.2. Identification With Associated Lines	35
4. PROGRAM PACKAGE BUCAASA	38
4.1. Organization of BUCAASA	39
4.2. Program BUCAASA/FIND	41
4.3. Program BUCAASA/FIT	42
4.4. Program BUCAASA/CALIBR	43
4.5. Program BUCAASA/NUCLIDE	44
5. DISCUSSIONS AND CONCLUSIONS	46

	<u>Page</u>
APPENDIX A. THE VARIABLE METRIC MINIMIZATION METHOD	52
APPENDIX B. ERROR ESTIMATION IN FITTING	60
B.1. Error Estimates of the Parameters in Fitting	60
B.2. Error Estimates for Areas	64
APPENDIX C. USERS' GUIDE FOR BUCAASA	67
C.1. Input Data Structure for BUCAASA/FIND	67
C.2. Input Data Structure for BUCAASA/FIT	68
C.3. Input Data Structure for BUCAASA/CALIBR	70
C.4. Input Data Structure for BUCAASA/NUCLIDE	71
APPENDIX D. IMPLEMENTATION GUIDE FOR BUCAASA	73
D.1. The File Structure of BUCAASA	73
D.2. Description of the Important Variable of The Program Units of BUCAASA	75
D.2.1. Program FIND	75
D.2.2. Subroutine SMOOTH	76
D.2.3. Subroutine PEAKID	76
D.2.4. Program FIT	77
D.2.5. Subroutine VARMET	78
D.2.6. Subroutine DERIVS	79
D.2.7. Subroutine CUBINT	79
D.2.8. Subroutine RINT	79
D.2.9. Program CALIBR	79
D.2.10. Subroutine POLIN	80
D.2.11. Subroutine MATIN	80
D.2.12. Subroutine POLIX	80
D.2.13. Subroutine INTRP	80
D.2.14. Program NUCLIDE	80
D.2.15. Subroutine CORR	81
D.2.16. Subroutine DIAG	81
D.2.17. Subroutine GLSQ	81
D.2.18. Subroutine IDENT	81
D.2.19. Subroutine INTRF	82
D.2.20. Subroutine LIBRAR	82
D.2.21. Subroutine MATRIX	83
D.2.22. Subroutine ORDER	83
APPENDIX E. LISTINGS OF BUCAASA	84
APPENDIX F. OUTPUT EXAMPLES	133
REFERENCES	138

LIST OF FIGURES

<u>Figure</u>	<u>Page</u>
2.1. Regions of domain of photoelectric, Compton and pair production absorption processes ⁽⁹⁾	6
2.2. Schematic representation of the outer electronic bands of an insulator at rest (a), and after the absorption of an ionizing radiation (b) ⁽¹⁶⁾	10
2.3. Schematic representation of the outer electronic bands of an n-type semiconductor (a), and of a p-n junction at rest (b), and after a reverse bias has been applied (c) ⁽¹⁶⁾	11
2.4. Schematic arrangement of a gamma spectrometry system	16
3.1. Theoretical gamma ray spectrum from a monoenergetic ray E_γ , a: Dirac δ -function, b: Compton distribution with Compton Edge E_c ^(15,18)	18
3.2. A typical Gamma Ray spectrum ⁽¹⁹⁾	18
3.3. Comparison of $D(x)$ and $T(x)$	29
3.4. Schematical representation of step effect	30
3.5. Schematic representation of the components of the photopeak function $F(x)$	31
3.6. The structure of the working matrix. Non zero elements of the matrix are marked with crosses ⁽²⁹⁾	36
4.1. Schematical organization of BUCAASA with associated input and output files	40
4.2. Subroutine structure of BUCAASA/FIND	41
4.3. Subroutine structure of BUCAASA/FIT	42
4.4. Subroutine structure of BUCAASA/CALIBR	43
4.5. Subroutine structure of BUCAASA/NUCLIDE	45
A.1. Schematic representation of $f_i(x, p+\lambda\Delta s_i)$ for the cubic interpolation	57

LIST OF TABLES

<u>Table</u>		<u>Page</u>
2.1	Classification of Scintillation Detectors ⁽¹⁵⁾	8
2.2	Comparison of Scintillation and Semiconductor Detectors ⁽³⁾	14
5.1	Comparison of the results of the peak identification routines of BUCAASA and SAMPO80 ⁽³⁰⁾ for the IAEA G-2 program Source No.2 spectrum ⁽³⁰⁾	48
5.2	Comparison of the results of peak fitting routines of BUCAASA* and SAMPO ⁽³⁰⁾ for the IAEA G-2 program Source No.2 spectrum ⁽³⁰⁾	48
5.3	Comparison of different fitting functions used by BUCAASA. Data obtained from the analysis of IAEA G-2 program Source No.2 spectrum	50
D.1	Files used by BUCAASA/FIND	73
D.2	Files used by BUCAASA/FIT	74
D.3	Files used by BUCAASA/CALIBR	74
D.4	Files used by BUCAASA/NUCLIDE	74

LIST OF SYMBOLS

A	Height of the Gaussian function, peak area, activity, mass number
\underline{A}_i	Matrix
A_G	Area of the Gaussian function
A_T	Area of the tailing function
A_g	Height of the Gaussian function
A_t	Coefficient of the tailing function
A_v	Avogadro's number
B	Background, tailing function parameter
\underline{B}	Interference matrix
C	Tailing function parameter
$C(x)$	Compton continuum polynomial
C_i	Counts in channel i
D	Tailing function parameter
$D(x)$	Distortion function
\underline{D}	Experimental intensity vector
E	Energy absorbed
E_B	Binding energy of the electron
E_c	Energy of the Compton edge
E_k	Kinetic energy of the electron
E_o	Energy of the incident photon
E_p	Energy of the light photons
E_{tol}	Energy tolerance in nuclide identification
E_1	Energy transferred to a charged particle
F	Fano factor
$F(x), F(x,p)$	Photopeak function
FWHM	Full width at half maximum
G	Internal gain
$G(x)$	Gaussian function
\underline{G}	Hessian matrix
J	Transparency parameter
\underline{H}	Inverse of the Hessian matrix
K	Proportionality constant, geometrical factor
M	Atomic mass
M_A	Mass
N	Number of disintegrations

N_m	Normalization factor in data convolution
Q	Total charge
R	Error correlation
S	Significance value
S^2	Variance of the energy calibration function
$S(x)$	Step function
S_i	Second difference
T	Time
$T(x)$	Tailing function
U	Overall amplification
V	Volume
\underline{V}	Variance covariance matrix
Y	Conversion efficiency
Z	Atomic number
\underline{a}	Derivative vector
a_i	Coefficient of Compton polynomial
a_j	convolution integers
e_i	Photopeak energy
f	Isotopic abundance
$f(p,x)$	Photopeak function
\underline{g}	Gradient vector
h	Step function parameter
h_{\max}	Pulse height
i,j,k,l	Index
m	Order of the Compton polynomial, number of points in data convolution, order of the energy calibration polynomial, number of channels in fit
n	Number of parameters in fit
p	Number of light photons
\underline{p}	Parameter vector
t	Time
\underline{v}	Variance-covariance matrix
x	Independent variable (channels)
x_o	Peak channel
\underline{x}	Unknown activities vector
ΔE	Energy difference
$\Delta h_{1/2}$	Pulse height interval
$\Delta \bar{n}^2$	Mean square value of the statistical variations in the number of the total ionization events

Δp	Increase in p
Δt	Cooling time
χ^2	Independent variable of the Chi-square distribution
χ_R^2	Reduced χ^2
Σ_C	Macroscopic cross section for Compton interaction
Σ_{ph}	Macroscopic cross section for photoelectric effect
α	Coefficient of the step vector
$\underline{\alpha}$	Matrij of second derivatives
$\underline{\beta}$	Derivative vector
$\delta(x)$	Dirac function
ε	Average energy necessary for an ionization energy
$\underline{\underline{\varepsilon}}$	Error matrix
λ	Dummy variable
ν	Degree of freedom
σ	Standard deviation
σ^2	Variance of the energy calibration function
σ_e	Standard deviation of the Gaussian noise
σ_g	Standard deviation of the Gaussian function
σ_t	Tailing function parameter
σ_{AG}^2	Variance of the area of the Gaussian function
σ_{AT}^2	Variance of the area of the failing function
$\sigma_{ii'}$	Covariance of counts in i th and i' th channels
$\sigma_{P_j}^2$	Variance of parameter p_j
τ	Dummy variable

1. INTRODUCTION

Activation analysis is a method for determining concentrations of elemental constituents in a given sample by measuring the characteristic radiations emitted by the radioactive nuclei resulting from nuclear transmutations as a consequence of the irradiation of samples with nuclear particles. Mainly all of its applications are of a technological nature: purity control of high purity materials and semiconductors, soil analysis, geological prospecting, analysis of biological material for medicinal purposes, criminological and archaeological studies, etc.

Neutron activation analysis (NAA) was first discovered in 1936 by Hevesy and Levi⁽¹⁾, who determined the contents of Dy and Eu in a rare-earth mixture. Later work until 1950's was based essentially on the use of post-irradiation chemical separations involving the use of carriers to separate the elements of interest. These chemical separations are generally time consuming and various problems, such as the necessity of ensuring the isotopic exchange of the carrier with the trace element in the sample and the determination of the chemical yield of the separation, exist.

The chemical separations were necessary because the samples were usually counted with Gerger-Mueller counters making qualitative identification difficult. Decay and absorption measurements were the only means of improving the selectivity of the measurement.

The development of NaI scintillation spectrometry provided the birth of Instrumental Neutron Activation Analysis (INAA) which is a non destructive analysis method. In 1960's INAA was restricted by the rather poor resolution obtained with NaI scintillation detectors, making the interpretation of complex spectra difficult.

After the introduction of semiconductor detectors such

as Ge(Li) accompanied with the improvement in the coupled electronic systems such as amplifiers, Analog to Digital Converters, etc., the resolution was greatly improved and INAA took great strides. But the amount of data produced was very extensive and computers had to be introduced to process the spectra. Later with the developments in electronics and computer hardware and software engineering, rather inexpensive and highly precise systems consisting of detectors, multichannel analyzers and microcomputers became available and INAA could be performed, in most cases automatically, in a routine manner⁽²⁻¹⁰⁾.

A gamma ray spectrum is an information complex consisting of basically signals of interest and noise whose character depends on the electronics of the system and is also statistical. The relevant information is represented by shapes called peaks superposed over an underlying continuum. The location of the peak channel contains information about the identity of the element and the area under the peak is a measure of the amount present in the sample.

The human-computer interface interactively tries to separate the signal from the noise as accurately as possible. However as the quality of the results expected decreases, the analysis can be made in a more automated manner.

The subject of this thesis is a computer program package BUCAASA, based on an earlier program CAASA by Çiftçi-oğlu⁽³⁾ developed with basic intentions of keeping human intervention as minimal and the analysis as accurate as possible.

2. GAMMA RAY SPECTROMETRY

Activation analysis is based on the principle that when a material is irradiated by the nuclear particles produced in a suitable source such as a nuclear reactor or particle accelerator, some of the atoms present in the material will interact with the incident particles and undergo nuclear transformations producing isotopes of the same element or a different element which are usually radioactive. The subsequent emission of radiations from these nuclei is a characteristic of the particular isotope. If each different induced radioactivity can be distinguished or separated from all other radioactivities produced, then the amount of each radioactivity is a measure of the quantity of the parent isotope present in the material⁽⁴⁻¹⁰⁾.

A radionuclide can decay to a daughter product by various ways: (a) Beta or beta and gamma ray emission, (b) positron or positron and gamma ray emission, (c) electron capture, (d) gamma ray emission (isomeric transition), (e) internal conversion, (f) alpha particle emission.

In general, the majority of the radionuclides formed by the radiative capture (n, γ) process undergo beta decay, and in most cases beta decay is associated with the emission of one or more gamma rays. Positron decay and electron capture are more probable in radionuclides that have an excess number of protons. Electron capture and internal conversion result from interactions of the nucleus with orbital electrons of the atom and these processes in general lead to the emission of X rays. In contrast γ ray emission results from nucleon configurational changes within the nucleus. However, the electron capture decay of some radionuclides is accompanied by γ ray emissions along with the X ray emissions. Alpha particle emission is favourable only in elements with a high mass number ($Z > 83$) and, although it is frequently accompanied by γ ray emission, the detection of alpha particles in NAA is extremely limited because of their very short range. Overall,

most of the radionuclides that undergo decay by alpha, beta or positron emission and by electron capture also emit γ rays as a result of readjustment of energy content in the radionuclides from excited states to more stable states⁽⁵⁻⁹⁾.

The γ energy spectrum, although specific for a radionuclide, is continuous, thus its use in multielemental analysis by INAA in a sample matrix is impractical. On the other hand, the energies of X and γ ray photons are discrete and characteristic of the radionuclides. Because of this important property γ and X ray measurements are widely used in multielemental NAA. Gamma ray measurements have, in general much wider applications in NAA than X ray measurements because γ rays emitted from most radionuclides have a wider range of energies (40-3000 keV) and have greater penetrating range than X rays (2-90 keV) thus their absorption in a sample is minimal. This property, coupled with recent developments in high-resolution and high efficiency semiconductors such as Ge(Li) detectors and the availability of high output neutron sources makes NAA-gamma spectrometry a powerful multielemental analysis technique.

2.1. Interactions of Gamma Rays With Matter

The quantitative detection of gamma ray photons is based upon their interactions with matter.

There are several ways in which gamma rays interact with an absorbing material; three, namely the photoelectric effect, the Compton effect, and pair production are the most important ones for the utilization of gamma spectrometry in NAA^(2-3,5,7-10).

a) Photoelectric effect: For photons of low energy, i.e. less than 1 MeV, the most important interaction is the photoelectric effect (see fig.2.1). In this process the gamma photon interacts with the atoms of the matter and transfers

the whole of its energy to an orbital electron, which is consequently ejected with kinetic energy E_k

$$E_k = E_o - E_B \quad (2.1)$$

here E_o is the energy of the incident photon, and E_B is the binding energy of the electron.

The extent of the photoelectric interaction depends on both the energy E_o of the gamma radiation and the atomic number Z of the absorbing material. Photoelectric macroscopic absorption cross section is proportional to Z^5/E_o^3 (3,12). For this reason gamma ray detector materials must have a high atomic number (3,9).

b) Compton effect (Scattering): In a Compton interaction a gamma ray photon makes an elastic collision with an electron of the absorbing material. Since, usually, the energy of the incident photon is much greater than the binding energy of the electron, the electron may be accepted as free. Only part of the energy of the incoming photon is transferred to the electron. And as a result of this process, the photon is deflected from its original path. The energy E_θ of a photon scattered at an angle θ can be approximately evaluated with the equation

$$E_\theta = \frac{E_o}{1 + \frac{E_o}{mc^2} (1 - \cos \theta)} \quad (2.2)$$

where E_o is the initial energy of the photon and mc^2 the rest energy of the electron (0.511 MeV).

The scattered electron loses its excess energy in the normal ionization process, however, the scattered photon either interacts with matter again (almost in every case photoelectric interaction) or escapes from the material (detector). This incomplete absorption of energy produces a disturbing effect called Compton continuum which makes the

detection of lower energy photons difficult.

Compton macroscopic cross section is roughly proportional to Z/E_0 . Since Σ_{ph}/Σ_C increases in proportion to Z^4 , detector material must have high Z ⁽³⁾.

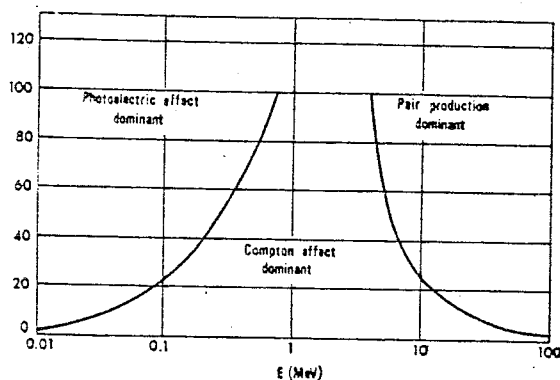


Fig.2.1. Regions of domain of photoelectric, Compton and pair production absorption processes⁽⁹⁾.

c) Pair production: When a γ ray photon with energy in excess of 1.02 MeV passes near the nucleus of an atom, the photon can be annihilated in the strong electrical field with the formation of an electron-positron pair. The kinetic energy of the pair, i.e., the energy excess of 1.02 MeV, is absorbed as a result of the ionization process. The positron will be annihilated after an interaction with an electron, giving two 0.511 MeV gamma rays. The absorption probability of these γ ray photons, in general, is not high relatively, and depends on the detector geometry⁽³⁾.

Pair production macroscopic cross section, increases over the threshold value of 1.02, and for energies greater than 4 MeV it is approximately proportional to $\ln E$. For this reason this interaction forms the basis of detection of high energy photons.

2.2. Detection Systems

Any instrumentation for the detection of gamma photons

consists essentially of two parts: a detector and an amplifying-counting system^(3,16). The detector is the part where the interaction of photons with the matter occurs and an output pulse is generated, whereas the amplifying and counting system increases the detector's output pulse, counts the events and, eventually discriminates them according to their energies.

2.2.1. The Detectors

The main gamma ray detectors can be classified into the following groups (a) gas filled detectors (b) scintillation detectors (c) semiconductor detectors. However in NAA the most widely used detector types are scintillation and semiconductor detectors and only they will be examined.

Scintillation Detectors: Since 1896 some substances (called "phosphors") were known to have the property of emitting light flashes when bombarded with heavily ionizing particles^(13,14,16). Where the counting rates were not too high, the individual light flashes could be visually observed and counted under a microscope. These early scintillation detecting assemblies were called spintharoscopes⁽¹⁶⁾. The development of modern scintillation detectors was started in mid 1940s with the introduction of the photomultiplier tube to convert the light flashes into electrical signals^(7,13,16).

The events leading to charge collection in a scintillation photomultiplier tube system can be summarized as follows. A gamma photon of energy E_0 passing through gives an amount at E_1 of energy ($E_1 \leq E_0$) to a charged particle, usually an electron. The electron dissipates a fraction AE_1 of its energy ($A \leq 1$) in the phosphor the energy AE_1 is converted by the phosphor, with a conversion efficiency $Y (Y = pE_p / AE_1)$, into p light photons, each having an average energy E_p , a fraction G of the emitted photons goes toward the photocathode of the photomultiplier. Moreover, because of the imperfect transparency $J (J < 1)$ of the crystal to its own fluorescence radiation a fraction of them will be absorbed by the phosphor

itself⁽⁵⁾ the photons reaching the photocathode are converted into photoelectrons with an efficiency P (P =number of photoelectrons per photon).

In conclusion, the total number of photoelectrons (n) produced at the photocathode as a consequence of the absorption of an energy E from a gamma ray is

$$n = \frac{E_1 AYJGP}{E_P} \quad (2.3)$$

The photoelectrons are then multiplied by the photo-multiplier and, if U is the overall amplification of the tube, the total charge Q at the final collector plate of the phototube is

$$Q = neU \quad (2.4)$$

where e is the electronic charge. The proportionality between Q and E_1 allows the scintillation counter to be used as a spectrometer⁽¹⁸⁾.

Scintillation detectors can be classified into two categories; organic and inorganic. Organic crystals can be subdivided into crystalline, liquid, plastic and glass scintillators, inorganic scintillators can be further subdivided into crystalline and noble gas detectors.

TABLE 2.1. Classification of Scintillation Detectors⁽¹⁵⁾

Organic				Inorganic	
Crystalline	Liquid	Plastic	Glass	Crystalline	Noble gas
Anthracene	(p-terphenyl, PBO	PBD, TP		NaI(Tl)	Xe
Transstilbene	PDP, POPOP) in	PP) in		LiI(Eu)	Kr
	xylene, toluene	polypenyl-		KI(Li)	
	Phenylcyclohexane	benzene			
	trimethylbenzene	polyvinyl			
	deceline	toluene			

Among the desirable properties for good scintillators are high yield of fluorescent (immediately emitted) light, transparency for this emitted light, rapid light emission in combination with the lowest possible phosphorescence and finally, spectral distribution of the light suitable with regard to the sensitivity of existing photomultipliers^(7,13).

The scintillator detector considered in this study is NaI crystal detector which contain 0.1 % thalium as active impurity and which have an emission band maximum at 4200 \AA , decay time $0,25 \times 10^{-6}$ sec energy conversion efficiency 0.10-0.13 and is unusually transparent to its own scintillations^(7,13,14,16). They are relatively inexpensive and very stable during operation and their life span is fairly long (~ 10 years)⁽⁹⁾. Its comparatively high density and the presence of high atomic number iodine atoms ($Z=53$) give rise to large photoelectric, Compton and pair production absorption cross sections. For further information about NaI(Tl) detectors see for example ref.7,13,14.

Semiconductor Detectors: Mc Kay⁽¹⁶⁾ was the first to use a junction device for nuclear particle detection. He demonstrated that the p-n junction in germanium could be used to detect alpha particles, that the collection time for the charge was quite small, and that the energy required to produce an electron-hole pair in germanium was no more than about 3 eV.

The principle of operation of such detectors is basically the collection of the electric charge released in a solid by the absorption of photons or charged particles. The energy bands of the outer electrons in an insulator are schematically represented in Fig.(2.2a) all the electrons are accomodated in the valence and lower energy loads. The conduction band is usually empty and no movement of electric charge occurs. The valence and the conduction bands are separated by an energy gap usually wider than 3 eV. When an ionizing particle or radiation is absorbed by the insulator,

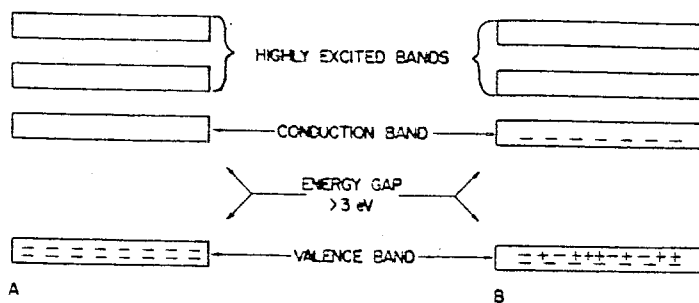


Fig.2.2. Schematic representation of the outer electronic bands of an insulator at rest (a) and after the absorption of an ionizing radiation (b) (16).

it can transfer to a single electron enough energy to raise it from the valence band to the highly excited bands; the removal of a negative charge from the valence band appears as a positive hole in the valence band. The highly excited states exist only about one picosecond after which the electrons are lowered to the conduction band, many more electron-hole pairs being formed in the process. The final situation is that of Fig.2.2b with positive holes at the valence band and an equal number of electrons in the bottom conduction band. When two electrodes are placed on two parallel faces of the crystal and a voltage is applied, the charge carriers move to the appropriate electrodes and the induced charge can be detected.

Fig.2.3a shows the energy band of outer electrons in a semiconductor. It differs from the energy bands in an insulator in two aspects (1) The energy gap between conduction and valence bands is usually lower than 3 eV; and (2) impurity energy states are present close to the crystal's energy bands. The impurities, the presence of which allows a semiconductor to conduct, can be schematically gathered into two types (1) Donors who give electrons to the conduction band; and (2) Acceptors who accept electrons from the conduction band (Fig.2.3a). When a p-n junction is formed the distribution of free holes, conduction electrons, and impurity sites is that shown in Fig.(2.3b). When a reverse bias is applied, all the charge carriers move towards the electrodes

and a depleted region is formed where a space charge due to the ionized impurity sites exists (Fig.2.3c). This depleted region is the sensitive area of a p-n junction detector^(3,16).

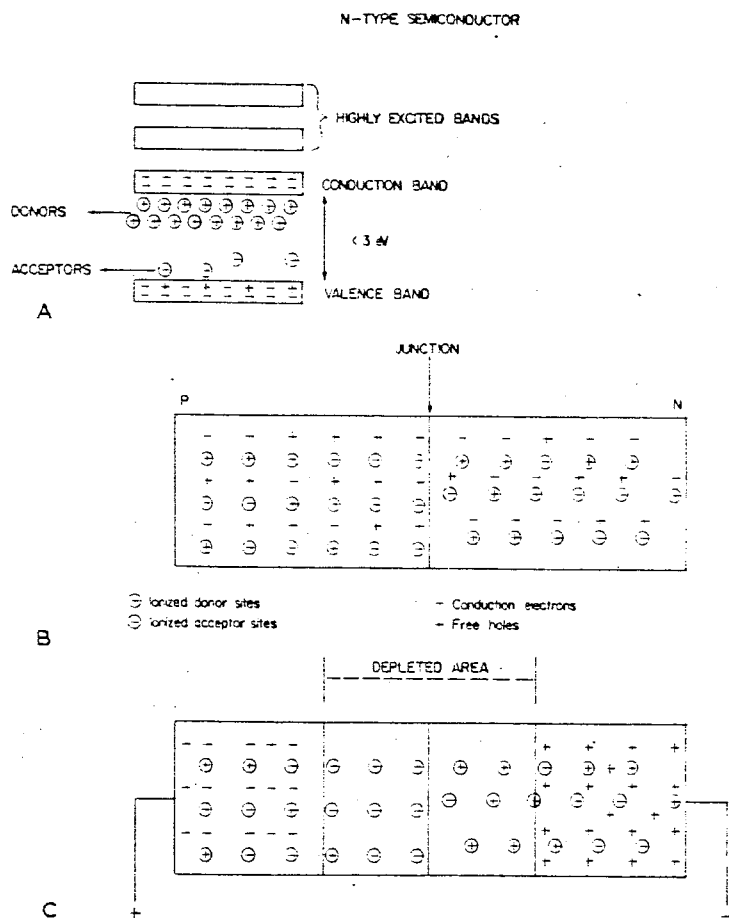


Fig.2.3. Schematic representation of the outer electronic bands of an n-type semiconductor (a) and of a p-n junction at rest (b) and after a reverse bias has been applied (c)⁽¹⁶⁾.

In order to have good detection characteristics, the detector material should fulfill the following requirements as closely as possible

a) It should contain very few free electric charge carriers in the operating condition; such carriers may form a current and will tend to conceal or to spread the desired signal.

b) It should not contain a significant number of trapping centers capable of holding electrons or holes and

therefore giving rise to an incomplete charge collection. Furthermore, trapped electrons and holes produce an electric field in the crystal which, being opposite to the applied field, causes the current to decrease with time (polarization effect).

c) Recombination of holes and electrons during the charge collection process must be very small.

d) Charge collection must be as fast as possible; holes and electrons must therefore have high mobility.

e) In order to have a good resolution, the average energy to produce an electron-hole pair must be as low as possible.

Today the most commonly used semiconductor detectors are Ge(Li), Si(Li), and high purity Ge.

Since the depletion area is generally small in a pure semiconductor this region can be extended by adding Li to the semiconductor (Si and Ge). This process is called drifting. The drifted Li decreases the net density of holes in the depleted region and a wider depleted region is obtained in this region the free charge carriers formed as a result of ionization can move to p or n side of the system and thus form a current.

Since ΔE , the energy difference between the valence and conduction band, decreases with increasing temperature, Ge(Li) detectors can not be operated at room temperature, the reason for this is that the 0.6 eV energy is supplied with the available heat energy and a great number of hole-electron pairs are formed, in order to stop the diffusion of the drifted Li at the necessary level Ge(Li) detectors must be kept and operated under -200°C .

This problem can be avoided to some extent in high purity Ge detectors which need cooling only under operation

conditions.

2.2.2. Comparison of Scintillation and Semiconductor Detectors

Here the basis of comparison will be their application to gamma spectrometry

a) Energy Resolution: The resolution of a detection 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. The degree of the uniformity of the pulse heights is usually described by the quantity FWHM, the full width at half maximum⁽¹³⁾. The quantity FWHM is calculated as

$$\text{FWHM} = \frac{\Delta h_{1/2}}{h_{\max}} \quad (2.5)$$

where h_{\max} is the pulse height corresponding to the maximum in the curve while $\Delta h_{1/2}$ is the pulse height interval between the points at which one-half of the maximum value occurs. Since as it will be seen in the succeeding chapters that the peak is generally represented by a Gaussian function, another definition of the FWHM can be given as

$$(\text{FWHM})^2 = 4 \ln 4 \frac{\text{Variance}}{(\text{mean})^2} \quad (2.6)$$

The resolution is important because as the spread in the peak gets smaller, peaks whose average energies are very close can be distinguished and interferences will be minimized and even very complex spectra can be analyzed easily. Semiconductor detectors have a very definite advantage over scintillation detectors in this respect.

In both kinds of detectors, only part of the energy of the incident gamma ray photon is used for useful ionization leading to detection. This causes statistical variations in scintillation detectors in the number of electrons reaching

the first cathode and in semiconductor detectors in the number of electron hole pairs formed.

The ratio of the mean square value of the statistical variations observed in the number of total ionization events ($\Delta\bar{n}^2$) to the number of total ionization events is defined as Fano factor⁽³⁾ and is given as

$$F = \frac{\Delta\bar{n}^2}{\bar{n}} = \frac{\Delta\bar{n}^2}{E} \epsilon \quad (2.7)$$

Here E is the energy absorbed and ϵ is the average energy necessary for an ionization event.

Combining eq.(2.6) and (2.7) a new definition

$$\Delta E = \text{FWHM} = 2\sqrt{2\ln 4} \epsilon \sqrt{F, \bar{n}} \quad (2.8)$$

is obtained.

Fano factor for scintillation detectors is 1, and for Ge(Li) detectors is less than 0.13⁽³⁾.

TABLE 2.2. Comparison of Scintillation and Semiconductor Detectors⁽³⁾

	Symbol	Type of Detector	
		Semiconductor	Scintillation
Necessary energy for an ionization event (eV)		3	300
The number of electrons formed at energy E (eV)	\bar{n}	E/3	E/300
Standard deviation of \bar{n} ($\sigma = \sqrt{F\bar{n}}$)		$\sqrt{F \cdot E/3}$	$\sqrt{F \cdot E/300}$
Resolution	FWHM	$2.335\sqrt{3} F \cdot E$	$2.335\sqrt{300} F \cdot E$
Internal gain	G	1	10^6
Charge (Coulomb)	Q	$E \times 0.5 \times 10^{-19}$	$E \times 0.5 \times 10^{-15}$

The resolution calculated from eq.(2.8) takes into consideration only the detector. However, since the detector

and the coupled electronic system are the sources of independent statistical variations that affect the total resolution obtained from gamma spectrometry they will be added as

$$(\Delta E)_{\text{total}}^2 = (\Delta E)_{\text{detector}}^2 + (\Delta E)_{\text{electronics}}^2 \quad (2.9)$$

In Ge(Li) detectors at low energies, the statistical spread in charge production is small and in most cases it is less than the spread contributed by the electronic noise. At higher energies, detectors frequently show insufficient charge collection due to trapping and or recombination. This results in a larger noise contribution from the detector than the estimated contribution, causing the FWHM vs photon energy characteristic to be linear rather than parabolic⁽¹⁷⁾. In semiconductor detectors, because of the vacancies and impurities in the crystal structure trapping regions are formed and some of the charge carriers are either lost from the current or they are retarded, this leads to a fluctuation in the current. The resolution decreases and in the lower energy side of the nearly Gaussian spectrum line shape an assymmetric region is formed.

The other factors affecting the resolution are detector noise (Shot, Johnson, superficial leakage current noise) and detector capacity. For further information see for example ref⁽³⁾.

b) Detector Efficiency: Another important parameter is detection efficiency. Although efficiency can be defined with respect to peaks produced in different interactions; in the range used in this study (40 keV-2 MeV) the photoelectric interaction cross section is considerably greater than Compton and pair production cross sections and only full energy photopeak efficiencies will be considered.

Every efficiency can be expressed as intrinsic, absolute or relative.

Total energy photopeak efficiency is the probability of counting a gamma ray photon of a given energy in the photopeak energy region.

Absolute total energy photopeak efficiency is defined as the probability of counting the photons from a source of known activity in the total energy photopeak region.

However the most frequently used definition of efficiency is the relative efficiency which is defined as the ratio of total energy photopeak efficiency to the efficiency in a different energy.

2.2.3. Auxillary Electronic Equipment

In general the amplifying-counting system consists of the high voltage supply, preamplifier, amplifier and the multichannel analyzer.

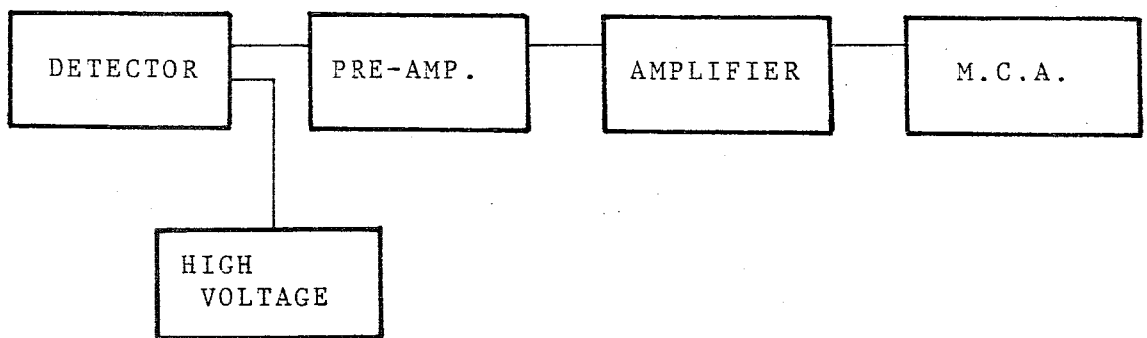


Fig.2.4. Schematic arrangement of a gamma spectrometry system.

Highvoltage power supply: Both scintillation and semiconductor detectors need high voltage for different reasons; while high voltage is used in the photomultiplier tube for the amplification of electron current, it is used in the semiconductor detector for the application of reverse bias.

Preamplifier: The signals obtained from detectors have very small amplitudes. For this reason they have to be amplified in, order to be analyzed. This can be performed in

three ways: (1) Voltage amplification (2) Current amplification (3) Charge amplification.

Amplifier: is used for obtaining variable voltage gain, reducing pulse pile up to a minimum.

Multichannel (pulse height) analyzer: is used for obtaining the frequency distribution histogram of the heights of the incoming pulses. The amplitude of each signal is measured, and with an Analog to Digital Converter, is transformed to an integer approximately proportional to the amplitude. And the information thus obtained is kept in the memory area in cells called channels. The counts in every channel shows the number of pulses whose amplitude value is in between the limits of each channel.

3. COMPUTER ANALYSIS OF GAMMA RAY SPECTRA

The phenomenon of a gamma photon dissipating all or part of its energy in the detector and eventually giving rise to a digital signal representing the γ -ray energy is called an event. The collection of numbers of events corresponding to a specific digital channel for a given radioactive source and measurement time is called the gamma ray spectrum⁽¹⁸⁾ (GRS).

The term gamma ray spectrum is somewhat misleading because the detection of gammarays is indirect and the spectrum is actually the spectrum of the fast electrons produced by the interactions of the gamma photons with the detector material. As a result the spectrum contains continuous parts and escape peaks in addition to peaks corresponding to the mono energetic gamma rays.

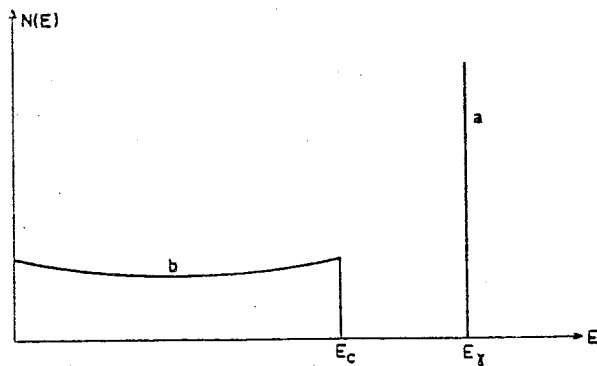


Fig.3.1. Theoretical gamma ray spectrum from a monoenergetic ray E_γ a) Dirac δ -function, b) Compton distribution with Compton edge E_c (15,18).

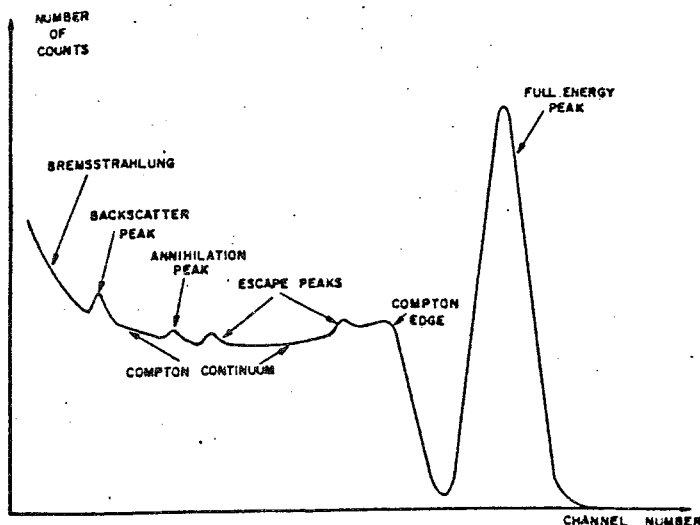


Fig.3.2. A typical Gamma ray spectrum⁽¹⁹⁾.

In gamma ray spectra (GRS) two kinds of statistical phenomena have to be considered. The first is that due to the phenomenon of radioactivity itself because of which the number of events in each channel is governed by Poisson statistics.

$$P(m) = \frac{N^m e^{-N}}{m!} \quad (3.1)$$

where P is the probability of observing m events and N is the expected average of events. The magnitude of the statistical fluctuations is conventionally given by the estimate of the standard deviation on the Poisson distribution^(3,19).

$$\Delta N = \sqrt{N} = \sqrt{m} \quad (3.2)$$

The second kind of statistics is related to the detector system response. The gamma photons emitted by radioactive isotopes are monoenergetic. They have a very small spread in energy determined by Heisenberg's uncertainty relation. In channel units. They can be represented by a Dirac delta function at their specific energy E_γ as shown in Fig.3.1. Photons that do not dissipate all their energy are those interacting via the Compton effect with quasi-free electrons in the detector, giving the theoretical energy distribution of eq. (2.2). In addition, for energies greater than 1.02 MeV, those that produce pairs lead to single and double escape peaks.

The physical processes that govern the creation of light photons or electron-hole pairs in detectors, those that produce the electrical discharge and finally those that transform the latter into a digital binary number are all statistical in nature^(3,19).

A GRS consists of a large series of integer numbers, a few hundred to a few thousand depending on the kind of detector used, arranged in a certain sequence. The extraction of the information that is of value from the numbers and their sequence is the art of analysis of a spectrum. Throughout the text sought after information will be denoted as signal,

and noise (background), denotes the bits of data that obscures the recognition of the presence of the valuable information. In a GRS the noise has partly a composite statistical and partly a continuous nature which is due to Compton effect, pulse pile-up, Bremsstrahlung, etc .

In regions of the spectrum, hereafter denoted as peaks, the signal-to-noise ratio is stronger than in continuum parts, at least with respect to a given specimen. In the following the concept of complex will be used for a group of channels in an observed GRS that are related by the fact that several sources of information contribute to such a group of channels, e.g., true detector background, Compton distributions from several gamma lines, statistical fluctuations of different origin and one or more unique signals belonging to γ rays. If a complex contains several unique signals, each of them experiences the sum of others as part of the noise.

The signal has a qualitative as well as a quantitative aspect. The first is the information about the species (isotopes or elements) that have contributed to the complex and the second, about the species (isotopes or elements) that have contributed to the complex and the second, about the amount of each specimen present. The exact position of the peak maximum determines the qualitative aspect, whereas the integrated area under the peak determines the quantitative aspect. Both these values can be determined only after the presence of a peak region has been recognized. The latter involves the concept of peak shape in numerical terms, such that signal and background can be accurately separated. The recognition of the peak shape is also important for a judgement of the uniqueness of the signal.

All numerical values extracted from the GRS are influenced by the statistical part of the noise. As a result only estimates of the true value can be given, accompanied by standard deviations representing a measure for the precision of the estimate. The statistical part of the noise also puts

a limit on the ability to recognize a peak region, which leads to the concept of limit of detection.

However, the amount of valuable information that can be extracted from a given GRS is determined by the nature and the quality of the measurement. The signal-to-noise ratio cannot be improved after the measurement, no matter how sophisticated or powerful the mathematical techniques used for the analysis⁽¹⁹⁾:

Especially with the starting of wide spread use of Ge(Li) detectors, because of their high resolution; multichannel analyzers with 4096, even with 8192 channels became common place; such vast amount of data could not be manually analyzed in a reasonable time, thoroughly and in an efficient manner. With parallel advances in computer hardware and software, the introduction of computers and computer codes into the field of gamma ray spectra analysis was not only logical but became a must.

Many computer codes have been written for the analysis of NaI(Tl) spectra these generally require a knowledge of the possible component isotopes in the spectrum and also the availability of standard pulse height spectra of these components^(18,19). However because of their high resolution Ge(Li) spectra need a special treatment which is, in most cases easier, faster, and more automatic than analyzing NaI(Tl) spectra^(3,19,22-26).

A computer code developed for the analysis of gamma ray spectra must have the following qualifications^(3,26).

- (a) The method must be programmable to be able to perform an automatic analysis.
- (b) The code must be able to handle data obtained under various experimental conditions.
- (c) The code must be able to analyze highly complex spectra.
- (d) It must include information about error limits.

- (e) The execution time and memory requirements should be kept to a minimum.

In general the steps in computer analysis are as follows:

- a) Peak identification
- b) Fitting a function to the peaks
- c) Energy and efficiency calibration
- d) Identification of nuclides producing the spectrum.

3.1. Peak Identification

In order to minimize statistical variations in count rate various filtering methods are used to smooth the spectral data the earliest and the most commonly used is the method of Savitzky and Golay⁽²⁰⁾ which is a least squares fitting of a polynomial to the data points carried out by their convolution with properly chosen sets of integers.

$$C'_i = \frac{1}{N_m} \sum_{j=-m}^{+m} a_j C_{i+j} \quad (3.3)$$

Here C_i represents counts in channel i , a_j are the convolution integers, N_m is the normalisation factor (which are given tabulated form in ref⁽²⁰⁾) and C'_i is the smoothed value of channel i . Here for the smoothing process $2m+1$ points are used. Smoothing the whole spectrum can be carried out by taking channel $i+m+1$ and dropping channel $i-m-1$. In this way not only a smoothed spectrum but the derivatives of the spectrum can also be obtained.

The number of channels used in convolution and the order of polynomial are the important parameters. For optimum performance the number of channels included in smoothing should be equal to FWHM and a cubic polynomial for calculating the first derivative for peak detection purposes must be used^(3, 21, 22).

Several authors have used Fourier transformations. However, these are method relatively complex to be programmed need more execution time and memory and by no means much superior considering their complexity. For a discussion of these methods see ref⁽¹⁹⁾.

In BUCAASA smoothing is used as an aid in determining the first derivative spectrum.

The methods of peak detection are classified in five groups i.e. those based on (1) The detection of a relative maximum in the spectrum, (2) The use of the first derivative, (3) The use of the second derivative, (4) cross correlation methods and (5) visual methods⁽²⁴⁾.

As a result of the IAEA G-1 Intercomparison of methods for processing Ge(Li) Gamma-ray Spectra⁽²⁴⁾, it was found that in the best hands, visual methods and the use of the second derivative are capable of marginally superior performance.

The performance of a peak detection method can be evaluated by considering its ability to detect true peaks, reject spurious ones, and detect multiplets.

3.1.1. Peak Location by Finding Relative Maxima

This is the simplest method. The spectrum is first scanned and the possible peaks are selected by finding those channels where the counts fulfill the conditions⁽¹⁹⁾:

$$C_{i-2} < C_i - K \sqrt{C_i} \quad \text{and} \quad C_{i+c} < C_i - K \sqrt{C_i(i)} \quad (3.4)$$

Where K is an experimentally determined constant.

This method is fast and can be programmed easily but often overlooks peaks, especially small ones, and cannot separate multiplets⁽¹⁹⁾.

3.1.2. Method of Smoothed First Derivative

If the number of counts is regarded as a continuous function of the channel number, then the first derivative changes sign at the top of the peaks. In approaching a peak it is positive and after the peak it becomes negative in the next few adjacent channels. This can also be used for locating peaks. The computer looks for groups of channels such that the smoothed first derivative C' fulfills the following criteria

$$\begin{aligned} C'_i &\leq 0 \\ C'_{i+j} &< 0 \quad j = 1, 2, \dots, r \\ C'_{i-j} &> 0 \quad j = 1, 2, \dots, l \end{aligned} \quad (3.5)$$

Being able to recognize significant peaks but to disregard statistical fluctuations, r and l must be chosen in accordance with energy resolution⁽¹⁹⁾.

This method with a few extensions and checks for detecting multiplets is used in BUCAASA for peak detection.

3.1.3. Generalized Second Differences

In this method developed by Mariscotti⁽²⁵⁾, the peaks are assumed to be described by Gaussian functions and the background to be approximated by a linear function within short intervals:

$$Y(x) = G(x) + a_1 + a_2x \quad (3.6)$$

where $G(x)$ represents a Gaussian function if a peak is present and is zero otherwise, a_1 and a_2 are constants describing the background.

If it is assumed that $Y(x)$ is a continuous function its second derivative $Y''(x)$ becomes independent of the background and it vanishes for any interval in which there is no peak. Therefore a peak would be located wherever $Y''(x) \neq 0$.

Because of the discrete nature of data, the second derivative must be replaced by the second difference

$$S_i = C_{i+1} - 2C_i + C_{i-1} \quad (3.7)$$

which, like $Y''(x)$ should be only different from zero in the neighborhood of a peak. However, since the data C_i are defined within a statistical error, The S_i values will fluctuate around the expected value according to their standard deviation and, if the expected value S_i is comparable to its standard deviation no peak searching can be attempted.

To detect weaker peaks S_i is replaced by a "smoothed" second derivative expressed by

$$S_i(w) = \sum_{x=i-m}^{i+m} S_j \quad (3.8)$$

where the normalization constant is omitted.

This process is repeated, the averages are averaged and the generalized second difference is defined as

$$S_i(z, w) = \sum_{j=1-m}^{i+m} \dots \sum_{k=1-m}^{i+m} S_k \quad (3.9)$$

z

The optimum pair z, w is found to be $z_0 = 5$ and $w_0 = 0,6$ FWMM thus $S_i(z, w) \approx 0$ at the background and Compton continuum, differs significantly from zero around a peak and is proportional to the second derivative of a Gaussian, if the peak is a full energy peak superimposed on a linear background.

A peak is identified in channel i if $-S_i(z, w) > 2\Delta S_i(z, w)$. It is then tested to determine whether it is a real full energy peak or a Compton shoulder.

3.2. Detector Response Functions for Determination of Peak Position and Area

In order to assess precise values of energy and intensity. The spectrum line shape of a peak must be known, at least approximately. Although, theoretically an event corresponding to a given gamma ray energy is represented by a Dirac δ -function the statistical nature of radioactivity and the detection system as a whole, causes a widening of the line and thus forming the shape called peak as described in sub section 4.1. Here after until otherwise stated only detector response functions for Ge(Li) will be considered Generally, a response function is of the form

$$Y(x) = F(G(x)) + C(x) \quad (3.10)$$

Here $Y(x)$ is the approximate detector response function $G(x)$ is a Gauss function

$$G(x) = A \exp \left[-\frac{(x-x_0)^2}{2\sigma^2} \right] \quad (3.11)$$

and $C(x)$ is a polynomial:

$$C(x) = \sum_{i=1}^n a_i x^{i-1} \quad n=1,2,3 \quad (3.12)$$

However, the main difference lies in the construction of F which is a function of the Gaussian $G(x)$ ⁽³⁾: Usually in order to compensate for trapping effects the Gaussian is modified with the addition of exponential tailing functions. For a general discussion of these methods see ref⁽³⁾.

The requirements for a response function can be summarized as follows.

a) The physical events that affect the shape of the peak must as a whole be represented.

b) Since the resultant function is nonlinear nearly in every case it must have as few parameters as possible in order for the minimisation method (generally a nonlinear least squares fitting) to work reliably and fast. These methods are iterative, so initial guesses must be supplied, as the number of parameters increase this becomes not only tedious but sometimes impossible.

c) And the method must be programmable easily.

In CAASA⁽³⁾ and in BUCAASA an analytical approximation of the form given in eq (3.10) is constructed.

3.2.1. The Analytical Approach for Detector Response Function⁽³⁾

Generally in experiments investigating physical events, the data obtained is distorted due to the effects originating both from the system used and from the event itself. In such a case the variation of a physical quantity can be represented by a convolution integral

$$F(x) = \int_0^x G(x-\tau)D(\tau)d\tau = \int_0^x G(\tau) D(x-\tau)d\tau \quad (3.13)$$

Here $G(x)$ is the function representing the pure data and $D(x)$ is the distortion function, and x is an independent variable. The ideal detector response in the detection of monoenergetic gammarays is a Dirac δ -function. Assuming that $D(x)$ is a Gaussian function (eq.3.11) where x the independent variable representing channels, the detector response can be found as;

$$F_G(x) = A \int_0^{x_0} \delta(\tau-x_0) \exp \left[-\frac{1}{2} \left(\frac{x-\tau}{\sigma_g} \right)^2 \right] d\tau = A \exp \left[-\frac{1}{2} \left(\frac{x-x_0}{\sigma_g} \right)^2 \right] \quad (3.14)$$

Where A is the amplitude, σ_g is the standard deviation being a function of energy (see Table 2.2) and x_0 is the channel where the Gaussian is a maximum.

The distortion due to trapping effects can be represented by the convolution integral of an exponential function with the Gaussian noise:

$$f_1(x) = A_1 \exp[B(x-x_0)] \quad (3.15)$$

$$f_2(x) = A_2 \exp\left(-\frac{1}{2\sigma_e^2} x^2\right) \quad (3.16)$$

$$T(x) = f_1(x) * f_2(x) = A_2 \int_{-\infty}^{x_0} \exp[B(\tau-x_0)] \cdot \exp\left[-\frac{1}{2}\left(\frac{x-\tau}{\sigma_e}\right)^2\right] d\tau \quad (3.17)$$

where B is a constant, $A=A_1.A_2$ and σ_e is the standard deviation of the Gaussian noise.

$$\text{Defining } U = \frac{\tau - \left(\frac{x}{\sigma_e} + B\right)\sigma_e}{\sigma_e} \quad (3.18)$$

and

$$\text{erf}(x) = \frac{1}{(2\pi)^{1/2}} \int_0^x \exp\left(-\frac{1}{2} t^2\right) dt \quad (3.19)$$

and

$$\text{erfc}(x) = \frac{1}{2} - \text{erf}(x) = \frac{1}{2} - \frac{1}{(2\pi)^{1/2}} \int_0^x \exp\left(-\frac{1}{2} t^2\right) dt \quad (3.20)$$

$$T(x) = A(2\pi)^{1/2} \sigma_e \exp\left[B(x-x_0) + \frac{1}{2} B^2 \sigma_e^2\right] \text{erfc}\left(\frac{x-x_0}{\sigma_e} + B\sigma_e\right) \quad (3.21)$$

is obtained

However, in BUCAASA instead of T(x) a new tailing function

$$D(x) = A_t \exp\left[B(x-x_0)\right] \cdot \left\{1 - \exp\left(-\frac{1}{2\sigma_t^2} (x-Cx_0)^2\right)\right\} \cdot \delta \quad (3.22)$$

is considered as can be seen from fig.3.3 D(x) is very similar in nature to T(x) and easier to implement in the program and better error estimates for D(x) can be obtained. Furthermore the time required for the minimisation process is less than the time required for minimising a function containing T(x).

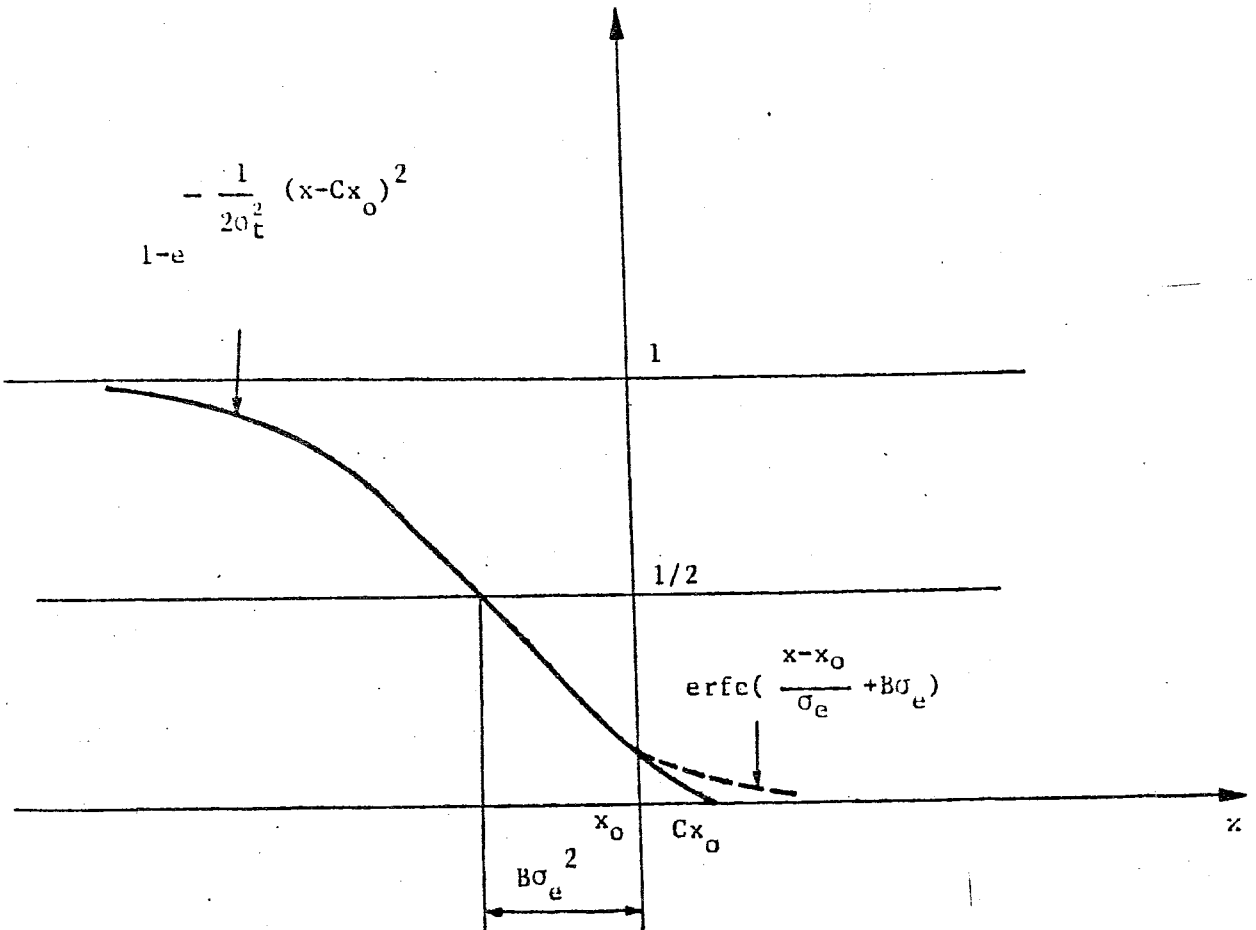


Fig.3.3. Comparison of $T(x)$ and $D(x)$

Here $C > 1$ and

$$A_t = A(2\pi)^{1/2} \sigma_e \exp\left(\frac{1}{2} B^2 \sigma_e^2\right)$$

(3.23)

$$\delta = \begin{cases} 1 & , \quad x < Cx_0 \\ 0 & , \quad x \geq Cx_0 \end{cases}$$

In GRS, although the ideal response is a Dirac δ -function the statistical variations, which are assumed to have a Poisson distribution in the number of ion-pairs cause the line shape to spread and be more or less a Gaussian. However, the probability of detection of monoenergetic photons in the lower energy side of the Gaussian is greater than the

probability of detection in the higher energy side. Because the photon whose initial energy is E_0 and which corresponds to an energy E in the Gaussian, can be detected at any energy level less than or equal to E and however this is not true for energies greater than E . For this reason if it is assumed that the distribution of photoelectron energies is a Gaussian function and the probability of detection of a photon for all energies less than or equal to E is constant equal to a step function component over the Compton continuum is formed see fig.3.4.

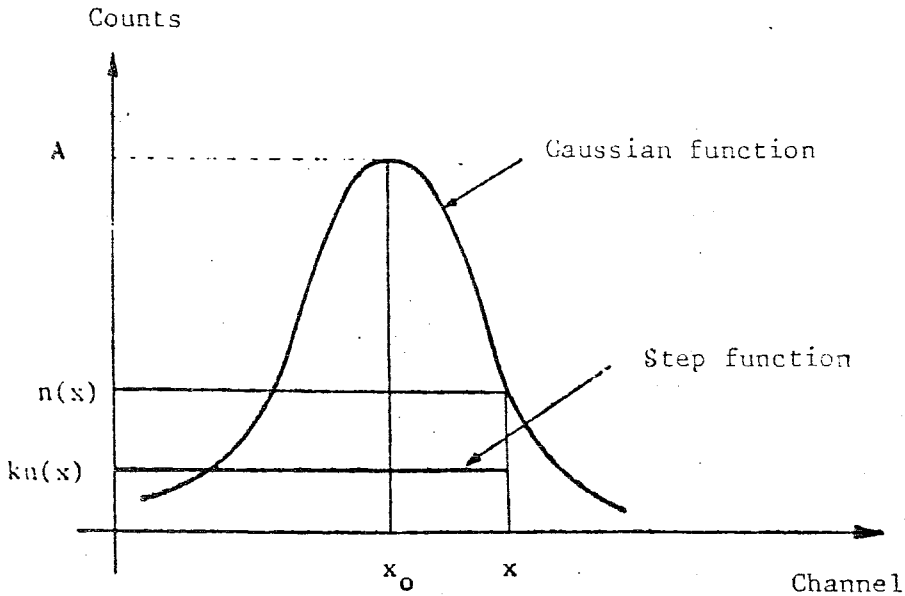


Fig.3.4. Schematical representation of step effect ⁽³⁾.

$$S(x) = A \int_x^{+\infty} k \exp \left| - \frac{1}{2\sigma_e^2} (\lambda - x_0)^2 \right| d\lambda \tag{3.24}$$

and evaluation of the integral gives;

$$S(x) = h \cdot \operatorname{erfc} \left(\frac{x - x_0}{\sigma_e} \right) \tag{3.25}$$

where

$$h = (2\pi)^{1/2} Ak\sigma_e \tag{3.26}$$

Here σ_e is taken to be equal to σ_g because the correlation between $S(x)$ and $D(x)$ must be minimum ⁽³⁾.

The Compton continuum is represented by a quadratic

polynomial.

$$C(x) = \sum_{i=1}^3 a_i x^{i-1} \quad (3.27)$$

Finally gathering all terms, the detector response function is obtained as

$$F(x) = \sum_{i=1}^3 a_i x^{i-1} + \sum_{j=1}^n \left\{ h_j \operatorname{erfc} \left(\frac{x-x_{oj}}{\sigma_g} \right) + A_{tj} \exp \left| B(x-x_{oj}) \right| \right. \\ \left. (1 - \exp \left| -\frac{1}{2} \left(\frac{x-x_{oj}}{\sigma_t} \right)^2 \right| \right) \delta + A_{gj} \exp \left| -\frac{1}{2} \left(\frac{x-x_{oj}}{\sigma_g} \right)^2 \right| \right\} \quad (3.28)$$

where n , is the number of photopeaks in a photopeak group h the amplitude of the step function, A_g the amplitude of the Gauss function and x_o is the peak channel position.

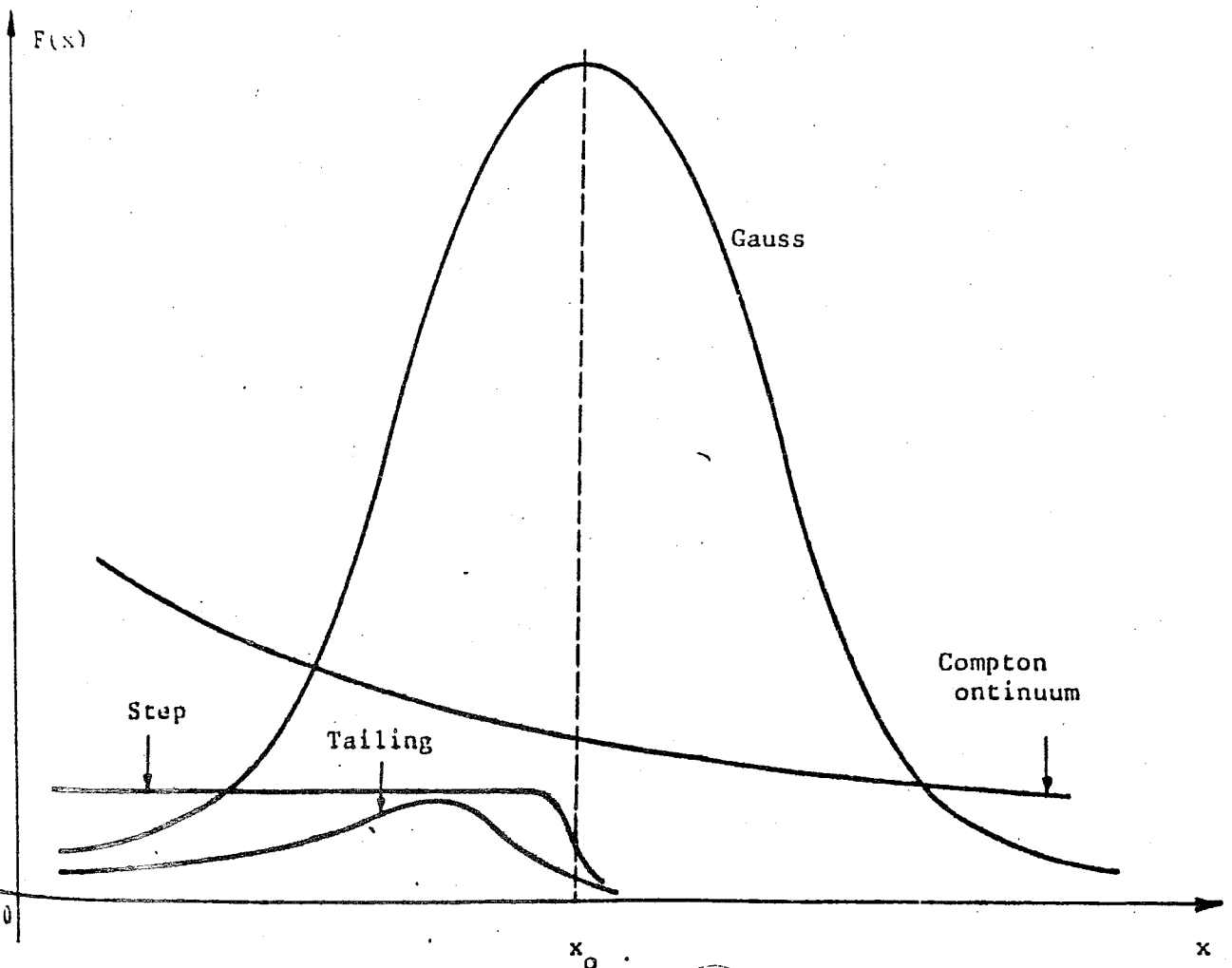


Fig.3.5. Schematic representation of the components of the photopeak function $F(x)$ for a singlet⁽³⁾.

The fitting of the function $F(x)$ given by eq. (3.28) to the experimental data points is done with the variable metric minimisation method (see Appendix A).

The peak areas are determined by calculating the area under the fitted function:

The area of the Gaussian is

$$A_G = A_g \int_{-\infty}^{+\infty} \exp \left[-\frac{1}{2} \left(\frac{x-x_0}{\sigma_g} \right)^2 \right] dx = (2\pi)^{1/2} A_g \sigma_g \quad (3.30)$$

and the area of the tailing function is given by

$$\begin{aligned} A_T &= \int_0^{Cx_0} A_t \exp \left[B(x-x_0) \right] \left\{ 1 - \exp \left[-\frac{1}{2} \left(\frac{x-Cx_0}{\sigma_t} \right)^2 \right] \right\} dx \\ &= \frac{A_t}{B} \exp(-Bx_0) \left[\exp(BCx_0) - 1 \right] + \\ &+ (2\pi)^{1/2} A_t \sigma_t \exp \left[\frac{1}{2} B^2 \sigma_t^2 + Bx_0(C-1) \right] \left[\operatorname{erf}(B\sigma_t) - \operatorname{erf} \left(\frac{Cx_0}{\sigma_t} + B\sigma_t \right) \right] \end{aligned} \quad (3.31)$$

Where the index j is omitted for clarity and $\operatorname{erf}(x)$ is defined in eq. (3.19).

The peak location which is an actual parameter of $F(x)$ is directly determined by the fitting process.

The goodness of fit is calculated by

$$\chi^2_V = \frac{1}{n-m} \sum_i \frac{1}{Y_i} \left[Y_i - F(x_i) \right]^2 \quad (3.32)$$

where Y_i are the experimental data points, n the number of channels in this fit and m the number of parameters in the fitting process.

In BUCAASA another test developed by Aarnio et al⁽²⁷⁾ the error correlation is also used:

$$R = \frac{1}{(n-m)} \sum_{i=1}^n \Delta_i \Delta_{i+1}, \quad (\Delta_{n+1} \stackrel{\text{def}}{=} \Delta_1) \quad (3.33)$$

where

$$\Delta_i = \frac{Y_i - F(x_i)}{\sqrt{F(x_i)}} \quad (3.34)$$

A good fit is indicated by $\chi^2_R < 10$ and $|R| \leq 1$.

The estimation of errors due to the parameters in the fit is done by employing the inverse of the Hessian matrix: The diagonal elements give the variances of the parameters whereas the off diagonal elements give the covariances (see Appendix B).

3.3. Energy and Efficiency Calibration

Experimental values of channels and corresponding energy and efficiency values obtained under identical conditions are supplied to the computer by the user.

In general the energy-channel relation can be represented by a parabolic polynomial^(3,22,26) and the energy efficiency relation by a function of the form;

$$F = pE^q \quad (3.35)$$

where p and q are constants for a given detector and source geometry, over the range 100 keV to several MeV⁽²²⁾.

The energy calibration function is given by

$$f(\underline{p}, x) = \sum_{i=1}^3 p_i x^{i-1} \quad (3.36)$$

where \underline{p} is the parameter vector, x is the channel number and $f(\underline{p}, x)$ is the corresponding photon energy. For the fitting process the linear least squares method is employed. The uncertainties in the determination of energy is mainly due to the spectrometer system therefore the uncertainties in

system therefore the uncertainties in channel may be taken to be equal to

$$\sigma_i^2 = \sigma^2 \cong S^2 = \frac{1}{M-(m+1)} \sum_{i=1}^M \{e_i - f(\underline{P}, x_i)\}^2 \quad (3.37)$$

here, $M-(m+1)$ is the degree of freedom related to fitting M data points to a polynomial of $(m+1)$ parameters e_i is the photopeak energy, $\sigma_i = \sigma$, is the standard deviation corresponding to photopeak energy e_i , and S^2 is the variance in the fitting process.

The errors in the determination of the energies is given by

$$\sigma_f(x_i) = \left(\sum_{\ell} \sum_k \frac{\partial f(\underline{P}, x_i)}{\partial P_{\ell}} \cdot \frac{\partial f(\underline{P}, x_i)}{\partial P_{\ell'}} \varepsilon_{\ell k} S^2 \right)^{1/2} \quad (3.38)$$

where $\underline{\varepsilon}$ is the error matrix calculated by taking $\sigma_i = 1$ (see Appendix B)

3.4. Nuclide Identification

The total number of known X and γ ray emissions include more than 48000 lines emitted by more than 2000 nuclides⁽²⁸⁾. In any practical analysis, the totality of these is impractical and therefore not required, specially selected reference libraries should be used in different applications. Such libraries should contain all nuclides which may appear in the spectra under analysis, and also a minimum of those which will not appear in any case⁽²⁹⁾.

Accordingly, different libraries have been developed for different applications using ZZ-GAMDAT-78⁽²⁸⁾ data collection as a data base.

There are basically two approaches to computer aided nuclide identification: a) Simple line matching, b) identification

with associated lines.

3.4.1. Simple Line Matching

Simple line matching is performed by comparing the calculated peak energies with the gamma-ray reference library one at a time.

The simple line matching is a tentative identification of possible peaks. Generally the computer codes accept a certain maximum energy difference between the identified peak energies and the gamma-ray reference library energies the value of which is supplied by the user.

The final result is obtained by inspecting the printout of the program. For an experienced worker this printout provides a fairly accurate and reliable method of identifying the component nuclides in the measured spectrum without the chore of manual computation.

3.4.2. Identification With Associated Lines

This method is based on the method suggested by Gunnink and Niday, however, the present implementation⁽²⁹⁾ has several improvements such as the tests to insure that only the right nuclides are accepted.

In this method a working matrix, which contains the branching intensities, is formed by comparing the computed peak energies in the analyzed spectrum with those in the reference library. If the computed energy of the first peak differs by less than a tolerance value, E_{tol} , from a line in the library, the program starts forming the first column of the working matrix. As the nuclide in the library may also have other gamma energies besides the first one, all those that lie in the comparison interval are compared with the measured peaks. For every library energy of this nuclide, the smallest difference between this energy and the fitting peak energies that determine the row of the working matrix where the branching intensity is written, is computed.

The process is then repeated for the next nuclide until all the peaks in the spectrum have been compared with the library. The resulting working matrix has the dimensions $N \times M$, where N is the number of fitted peaks in the spectrum and M the number of possible nuclides.

Along with the working matrix three vectors are formed. They contain the symbols of the possible nuclides, the confidence values for each nuclide, and the numbers which are used to write the accepted nuclides into the output matrices in the order of increasing proton number and atomic weight.

NUCLIDES

PHOTOPEAK ENERGIES	X		X				
		X					
					X		
		X					

Fig.3.6. The structure of the working matrix. Non zero elements of the matrix are marked with crosses (29).

The confidence value of a nuclide is an index computed to discriminate against probable nuclides. The initial value of the confidence index is 1. For each considered library gamma energy it is multiplied by the function.

$$f(\Delta E) = \exp \left[-(0.16/E_{tol}) (\Delta E)^2 \right] \quad (3.39)$$

where ΔE is the smallest computed difference between the library energy considered and the peaks in the spectrum. To account for small intensities a reference activity for each nuclide is computed. This reference activity is used to check whether such a small intensity should be seen in the spectrum or not.

After all the gamma energies of a nuclide that lie in

the interval of comparison is checked, the confidence value is multiplied by the function.

$$g(\Delta t) = \exp\left[-5.116856 \times 10^{-3} (\Delta t/T_{1/2})\right] \quad (3.40)$$

Where Δt is cooling time and $T_{1/2}$ is the half life of the nuclei. This assures the removal of nuclei with too short a half life to exist in the sample at the time of counting.

Finally, the confidence value is compared with a given limit. If it is smaller, the matrix column under consideration is cleared.

The above process is repeated for all nuclei and an interference matrix is formed, the unknown activities of the nuclides are determined by solving the matrix equation

$$\underline{\underline{B}} \underline{x} = \underline{D} \quad (3.41)$$

for the unknown activities \underline{x} ; $\underline{\underline{B}}$ is the interference matrix containing the branching intensities of the nuclides that were found to interfere with each other, and \underline{D} is a vector that contains the intensities of the peaks in the experimental spectrum that are assumed to be due to these nuclides. The equation is solved using the weighted linear least square technique. The weighing factors are the reciprocals of the errors of the calculated peak intensities. This takes into account the fact that stronger peaks can usually be calculated more accurately and therefore give better results than smaller peaks.

There are two acceptance criteria: none of the activities of the nuclides can be negative and none of the errors of the calculated activities more than 50 %. If one or both of these conditions are not fulfilled for some nuclide that nuclide is removed and the interference matrix is formed a new.

This process is repeated for all interference sets (29).

4. PROGRAM PACKAGE BUCAASA

The starting point of BUCAASA* is CAASA program developed by Ciftcioglu⁽³⁾, which was coded in FORTRAN-IV and ran on a PDP 11 microcomputer. The major shortcomings of CAASA were its lack of efficiency calibration and nuclide identification routines and to some extent the rather poor way of supplying initial guesses for the parameters in the fitting process.

The main aim in preparing the package was to make the programs user friendly-interactive- and more precise and accurate. For a general user although the principles behind the analysis are important, fast, automatic and easy to use programs are of greater value, for such programs are mainly used in routine work.

The package consists of four main programs, although it could be put into a single program format which was possible on CDC Cyber 170/815 system at Boğaziçi University where it was developed, however in order to make its adaptation to microcomputers easier it was decided to separate the self consistent parts. Though hierarchial in order, each program can be used separately and even for a mainframe computer considering the costs of occupying central memory area this division is highly beneficial and it allows the user to evaluate the results of each part and perform additional runs towards a more accurate analysis especially in academic work. For routine work, excepting cases of important multiplets even part two (BUCAASA/FIT) may not be used at all and a single consecutive run of parts one, three and four would be sufficient.

In deciding for the programming language to be employed FORTRAN 77 was chosen due to the familiarity of general users with earlier versions of FORTRAN language and its possibility of allowing structural programming thus leading to programs

* BUCAASA; Boğaziçi University Computer Aided Automatic Spectrum Analysis.

which are easily understood and can be maintained and modified with minimum cost. The present implementation has no extensions to the language meaning that it will run on any system which has a FORTRAN 77 compiler with no major modifications. However the fact that CDC Cyber 170/815 uses 60 bit words, hence its single precision is double precision for other systems must be taken into consideration, but this aspect is important only in part two: BUCAASA/FIT.

4.1. Organisation of BUCAASA

BUCAASA consists of four programs

a) BUCAASA/FIND: performs peak identification and calculates peak areas, and runs an estimate of some of the necessary parameters for the fitting process such as peak channel, right and left limits of peaks, FWHM and coefficients of the Compton polynomial.

b) BUCAASA/FIT: Performs the fitting of a function to the peak data points; the function can be a Gaussian, plus tailing or a Gaussian plus tailing plus a step function with a polynomial Compton background which are chosen by changing the values of a single parameter. As a result of this fitting, exact channel location of the peak and its area together with relevant error estimates are calculated.

c) BUCAASA/CALIBR: Performs the necessary energy and efficiency calibrations using the results of part II and calibration data supplied by the user.

d) BUCAASA/NUCLIDE: Through the associated lines technique⁽²⁹⁾ using purpose built libraries identifies the component isotopes and their activities.

The programs pass data to each other with standard FORTRAN 77 random access files. The usage of random access files permit individual runs for each photopeak group thus

leading to improvement in the results.

Each program needs very few input parameters which direct the flow of the program, i.e. the thoroughness of the analysis and which are supplied interactively. Although the programs can run batchwise, especially in BUCAASA/FIT, interactive usage helps to produce better results.

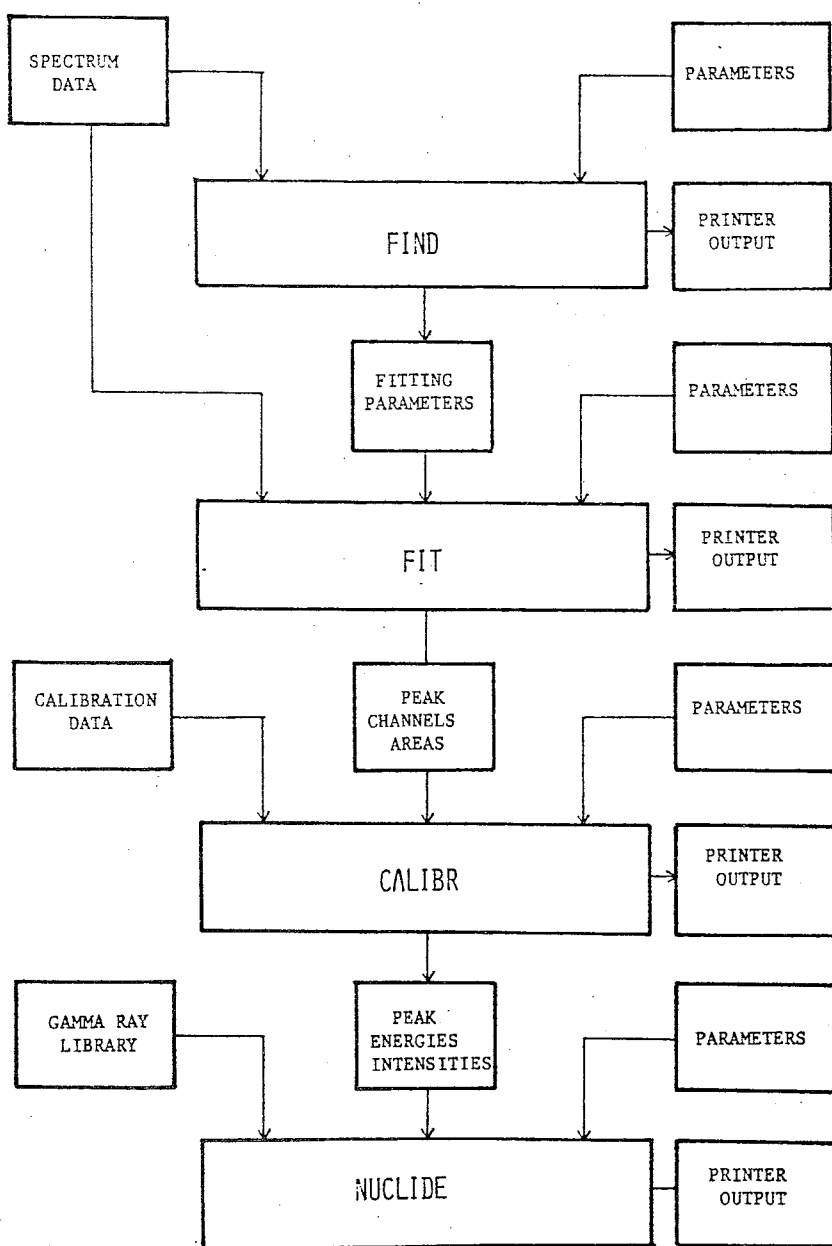


Fig.4.1. Schematical organization of BUCAASA with associated input and output files.

4.2. Program BUCAASA/FIND

BUCAASA/FIND consists of one main program and two subroutines.

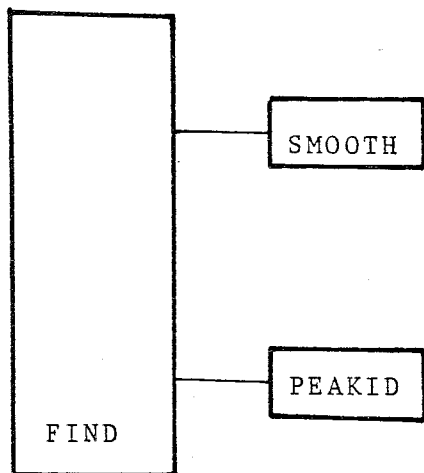


Fig.4.2. Subroutine structure of BUCAASA/FIND.

The main program controls input, output and communication with the subroutines, performs a tentative calculation of the peak areas by adding counts in the channels between the right and left limits of the peak and subtracts background which is computed by fitting a line through the right and left channels. A significance value for each peak is computed as

$$S = \frac{(A+2B)^{1/2}}{A} \times 100 \quad (4.1)$$

where A is the peak area and B is the background. Assuming that the peak can be represented by a Gaussian its area is given by

$$A_G = (2\pi)^{1/2} \sigma A \quad (4.2)$$

Therefore an initial guess for σ can be computed as

$$\sigma = \frac{A_G}{(2\pi)^{1/2} A} \quad (4.3)$$

Subroutine SMOOTH performs smoothing by the method of Savitzky and Golay (see subsection 3.1). Three, five, seven nine and eleven point smoothing is possible. Using the smoothed data the first derivative spectrum is calculated.

Subroutine PEAKID performs the peak identification using the first derivative spectrum (subsection 3.1.2). The right and left limits of the peaks, peak channels and multiplets are identified.

4.3. Program BUCAASA/FIT

BUCAASA/FIT consists of one main program, five subroutines and one function.

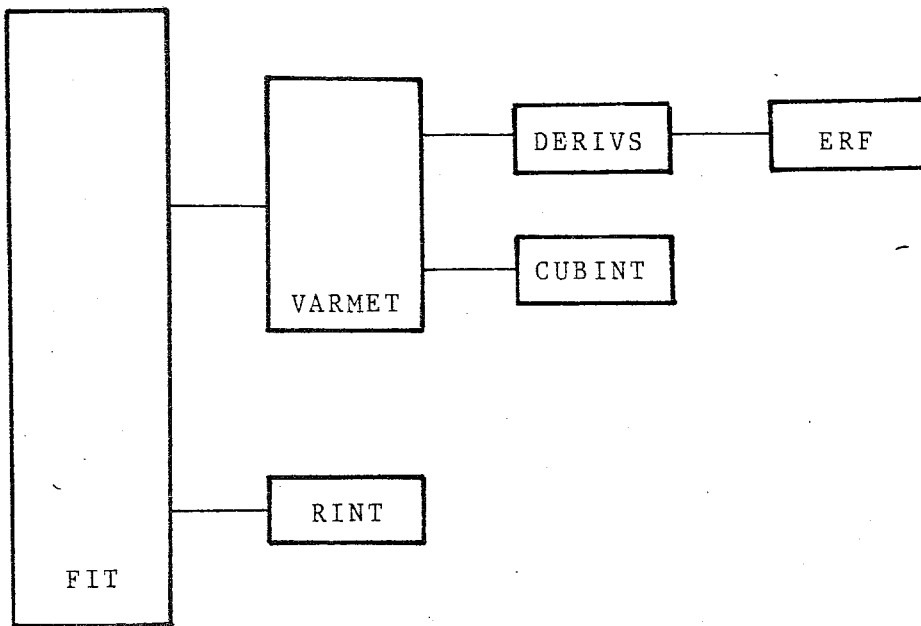


Fig.4.3. Subroutine structure of BUCAASA/FIT

Main program FIT controls input, output and performs the error estimation calculations (Appendix B). By assigning a value to the parameter IVAR the kind of fitting function can be chosen, the options being Gaussian plus polynomial background, Gaussian plus tailing and polynomial background, and Gaussian plus tailing plus the step function given by eq.(3.28) the necessary parameters are either supplied by the user or default and the values calculated by BUCAASA/FIT are used.

Subroutine VARMET is an implementation of the variable metric minimization method (Appendix A) for non linear least squares fitting. The iterations terminate when either 100 iterations have been completed or five consecutive values of

all parameters are found to be the same or all of the gradients are less than 10^{-11} or when one of the photopeak parameters become negative.

Subroutine DERIVS calculates the derivatives of the fitting function with respect to the parameters of the fit which are given by eqs.(A.35-43).

Subroutine CUBINT performs the cubic interpolation in order to calculate the optimum step length in the minimization (see Appendix A).

Subroutine RINT calculates the terms of the error equation for the tailing area (see Appendix B).

Subroutine ERF is used to compute the error function given by eq.(3.19).

Function ETS is used for to compensate underflow effects in the calculation of exponential functions.

4.4. Program BUCAASA/CALIBR

BUCAASA/CALIBR consists of one main program and four subroutines

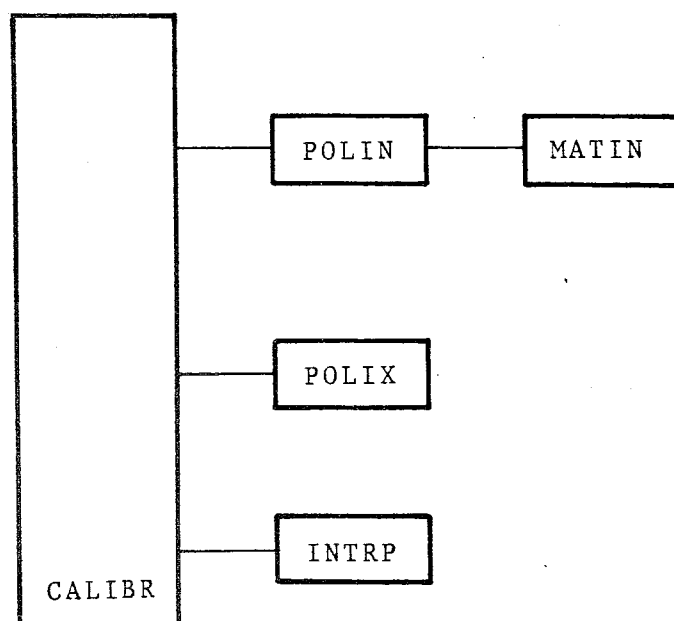


Fig.4.4. Subroutine structure of BUCAASA/CALIBR.

Main program CALIBR controls input, output and communication with the subroutines. Energy and efficiency calibration data are supplied by the user.

Subroutine POLIN performs the linear least squares fitting (see subsection 3.3).

Subroutine MATIN forms the inverse of the matrix whose elements are the coefficients of the resultant simultaneous linear equations from linear least squares fitting.

Subroutine POLIX calculates the energy and efficiency values using the coefficients determined by subroutine POLIN.

Subroutine INTRP interpolates logarithmically between efficiency calibration data points. This routine must be used only in cases where eq.(3.35) is not valid, i.e., for gamma energies less than 100 keV because an accurate error estimation is nearly impossible.

4.5. Program BUCAASA/NUCLIDE

BUCAASA/NUCLIDE Consists of one main program and eight subroutines

The main program controls only input output.

Subroutine IDENT performs the nuclide identification using the method of associated lines (subsection 3.4.2).

Subroutine LIBRAR reads in the gamma reference library for the identification routines.

Subroutine MATRIX forms the working matrix in the nuclide identification.

Subroutine CORR makes the time corrections to the activities calculated at the identification stage.

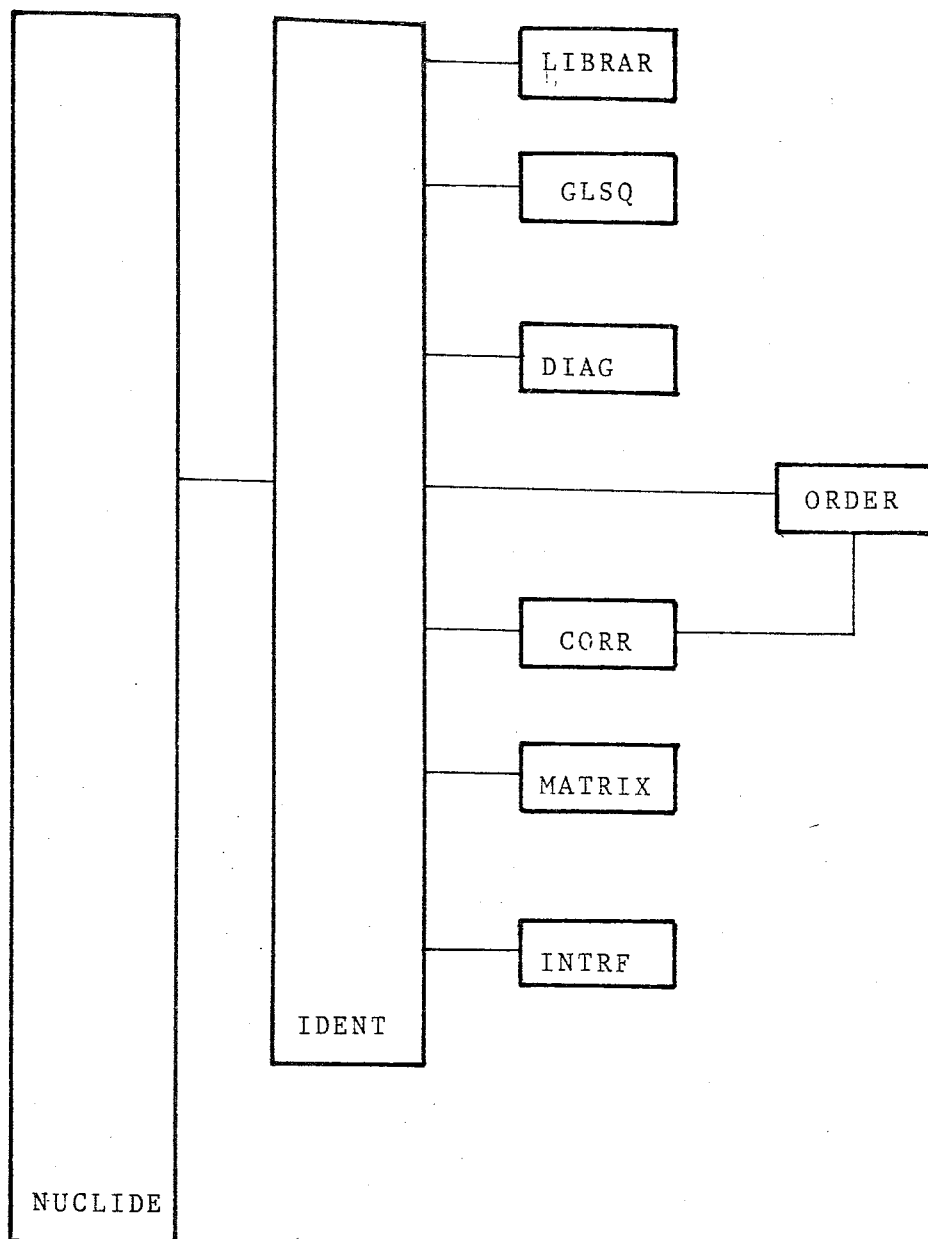


Fig.4.5. Subroutine structure of BUCAASA/NUCLIDE

Subroutine INTRF determines the interfering nuclides in the nuclide identification.

Subroutine GLSQ is a general linear least squares routine.

Subroutine DIAG determines the diagonal values of the inverse of the matrix produced from the GLSQ.

Subroutine ORDER arranges a number of arrays into the order of the ascending values of the first array.

5. DISCUSSIONS AND CONCLUSIONS

In 1976 as part of its Analytical Quality Control Services programme, the IAEA offered an intercomparison dealing with the evaluation of methods for processing Ge(Li) gamma-ray spectra⁽²⁴⁾. 212 sets of results from 163 laboratories in 34 Member States of the IAEA were received. The environment of 207 results was computers. From the evaluation of these results it was evident that no one particular method was overwhelmingly superior.

The information on methodology provided by the participants showed that many of them were using the same computer programs for spectrum evaluation. Four programs in particular were found to be relatively frequently used, namely SAMPO by 23 participants, GASPAN by 9 participants, GAMANAL by 8 participants and PHILIPOT by 7 participants. An intercomparison of these four programs showed that SAMPO was the best. However it was also found that success in evaluating these spectra was not so much dependent on the principle of the method used but more on the details of how this method was applied.

The major aim in preparing this package was supplying the analyst with a powerful and easy to use tool whose performance was not dependent on the user.

However, even from the beginning, i.e., peak identification routines, it was found that since gamma ray detection is a statistical phenomenon the criteria for identification were somewhat subjective; no method rejected the spurious peaks while identifying all the real ones however weak they may be and whatever their interferences are. Experienced human eye is still the best tool in identifying especially the multiple peaks.

In the fitting process, all the functions which are supposed to represent the experimental data as accurately as possible were determined to be valid only under special

experimental conditions. The functions are not easy to handle since nearly in every case they are non linear, and the non linear least squares methods used in fitting are always iterative processes, requiring initial guesses for the parameters in the fit. Optimization of those parameters requires tedious calibration runs until they are reasonably well determined for the system being used.

Taking into consideration the above stated facts the programs were designed to allow the user to choose the degree of thoroughness of the analysis he desires. A compromise was found to be necessary between accuracy and automatic use of the program.

In BUCAASA/FIND four parameters direct the peak identification process, by lowering their values, it is possible to detect even very weak peaks, however, the user can choose among them the peaks he considers to be significant for his work by adjusting the parameter PTEST. These are all subjective criteria but it must be stated that they are necessary in order to analyze exceptional spectra, e.g, peaks on high background, multiplets with a channel difference of less than three channels, etc. For routine work and well behaved spectra, i.e, spectra with low background and well defined peaks, they can be taken as constants.

In BUCAASA/FIT it is possible to use three different fitting functions all of them being a subset of eq. (3.28). Using eq. (3.28) in fitting is a tedious process since the initial guesses for the parameters have not been optimized due to lack of sufficient data. The main reason being our not being able to interface the counting system with the computer.

However, eq. (3.28) is one of the best functions representing the spectral data, for it was derived taking into consideration the physical events occurring through out the detection process. This is evident from the χ^2 parameters (see Table 5.3).

TABLE 5.1. Comparison of the results of the peak identification routines of BUCAASA and SAMPO80(30) for the IAEA G-2 program source no 2 spectrum(30)

Peak	Peak Channel		Notes
	BUCAASA/FIND	SAMPO80	
1	97.895	97.563	Multiplet
2	106.343	106.670	Multiplet
3	161.571	161.627	
4	246.203	246.201	
5	370.628	370.661	
6	414.249	414.223	
7	837.380	837.376	
8	917.378	917.376	
9	1078.138	1078.129	
10	1162.312	1162.301	
11	1546.830	1546.852	Annihilation peak
12	2526.858	2526.842	
13	3376.816	3376.819	

TABLE 5.2. Comparison of the results of peak fitting routines of BUCAASA* and SAMPO(30) for the IAEA G-2 program source no 2 spectrum(30)

Peak	Peak Channel		Peak Area		χ^2	
	BUCAASA	SAMPO80	BUCAASA	SAMPO80	BUCAASA	SAMPO80
5	370.658	370.661	5705474	5381146	425.9	1080.0
7	837.415	837.376	343154	352240	13.5	94.2
8	917.398	917.376	812008	813671	24.5	305.0
9	1078.145	1078.129	2306940	2317276	194.4	1760.0
10	1162.313	1162.301	308453	309687	12.7	194
11	1546.815	1546.852	156717	103390	21.1	6550
12	2526.870	2526.842	1637565	1633791	34.7	747
13	3376.860	3376.819	1225050	1222545	52.8	885

* Gaussian + Tailing + Parabolic compton continuum approximation is used.

In a non linear least squares fit the number of parameters that are used in the minimization must be kept few because sometimes the other parameters tend to compensate for the divergence of a parameter from its optimum value giving a low χ^2 value but leading to erroneous results. Considering this fact it is better not to use the step function since it does not give a considerable improvement (see Table 5.3). The parameter C which defines the shifting of the centroid of the tailing function is now thought to be constant for a given spectrometer system, however, again due to lack of sufficient data from different spectrometer systems and under different experimental conditions this points is still controversial and needs elaboration. Nevertheless it is evident from previous experience⁽³⁾ that its values is around 1.

For comparison purposes the gamma spectrum of the IAEA G-2 program source no 2 obtained by Koskelo et al⁽³⁰⁾ was analyzed. This data has several interesting features, i.e, it contains multiplets with intensity ratios less than 1:2 and all the peaks are situated on a very high background, thus providing an excellent challenge for any spectrum analysis program. The results of SAMPO80⁽³⁰⁾ are compared with BUCASA in Table 5.1.

It is evident that both programs are equally powerful. A later visual inspection showed that peaks no 3 and 4 were actually doublets which was confirmed by fitting. Both programs, BUCAASA and SAMPO80⁽³⁰⁾ overlooked this fact.

As a fitting function SAMPO80 uses a Gaussian with exponential tails on a quadratic background and the minimization of χ^2 is done by a linear least squares routine keeping the peak channels constant⁽³⁰⁾ whereas in BUCAASA. The variable metric minimization is used and the peak channels are allowed to vary. Although this sometimes causes the iteration to diverge, e.g, in the case of too far off initial parameters using e.q. (3.28) nearly in every case, better fits are obtained even with a pure Gaussian on a parabolic background (see Tables 5.2 and 5.3).

TABLE 5.3. Comparison of different fitting functions used by BUCAASA. Data obtained from the analysis of IAEA G2 program source no 2 spectrum(30)

Peak	Peak Channel			Peak Area			χ^2			χ^2_{N}		
	F1	F2	F3	F1	F2	F3	F1	F2	F3	F1	F2	F3
5	370.580	370.658	370.658	5253962	5705474	5950737	40975	425.9	5761.3	128.0	15.8	221.5
7	837.372	837.415	837.405	339917	343154	348099	42.9	13.5	18.9	3.0	1.9	3.2
8	917.364	917.398	917.376	792374	812008	806443	220.0	24.5	23.4	12.2	2.7	2.9
9	1078.109	1078.145	1078.125	2299111	2306940	2369293	2510.9	194.4	496.0	81.0	10.2	27.6
10	1162.292	1162.313	1162.315	302281	308453	311934	52.1	12.7	22.0	2.6	1.6	3.1
11	1546.809	1546.815	1546.823	149646	156717	165783	37.4	21.1	41.6	1.7	1.5	3.2
12	2526.837	2526.870	2526.844	1620984	1637565	1620374	1399.5	34.7	678.0	40.0	2.0	42.3
13	3376.782	3376.860	3376.857	1212251	1225050	1226269	1821.4	52.8	54.9	49.0	2.4	2.6

F1: Gaussian + Parabolic compton continuum

F2: Gaussian + Tailing + Parabolic compton continuum

F3: Gaussian + Tailing + Step + Parabolic compton continuum

For energy calibration in BUCAASA/CALIBR a linear least squares fit of a polynomial to the calibration data is used. Polynomials of order one and two give satisfactory results⁽³⁾ depending on the linearity of the spectrometer system. Again this provides estimates of the errors of the energy calibration. In SAMPO80 the errors are calculated by interpolating between the errors of each calibration point, however this can only give an estimate of the systematic error but not of the errors corresponding to the calibration process itself which is in SAMPO80 again an interpolation between calibration points. Nevertheless, considering that such errors are often less than the systematic error they can be neglected in routine work.

In nuclide identification an adapted version of SAMPOID is used which still seems to be the best code available.

The program package as it stands now is easy to implement on other main frame computers which have FORTRAN 77 compilers, however implementation on microcomputers requires overlaying. A user after a few runs will find it easy to use the package, but a thorough analysis using eq. (3.28) as the fitting function will present difficulties such as divergences but if time allows these problems can be overcome. Since after a few runs correct initial values for the parameters can be determined by analysing the gradients. It must be stated that most of the divergences occur as a result of hidden peaks which have been not identified by the peak search routines. In such a case careful visual inspection of the spectrum will yield the cause of the divergence. It must be stated that a blind faith in any computer program for gamma spectrum analysis will nearly in every case lead to erroneous results, because every criteria used in the analysis have a limited validity determined by the actual conditions of the analysis. Therefore computational programs are not sufficient, for a really accurate, precise and sensitive analysis and artificial intelligence techniques with pattern recognition capabilities simulating an experienced worker must be introduced into the field.

APPENDIX-A. THE VARIABLE METRIC MINIMIZATION METHOD

In this analysis, it is assumed that part of a spectrum can be represented by a function $F(x_i, \underline{p})$. x_i are the channel numbers and \underline{p} is the parameter vector. The fitting is based on the determination of parameters p_k through the least squares method such that sum of the squares of the deviation of $F(x_i, p_k)$ function from the data is a minimum.

$$R^2 = \sum w_i [y_i - F(x_i, \underline{p})]^2 \quad (\text{A.1})$$

gives the weighted sum of the squares of the deviation thus

$$\frac{\partial R^2}{\partial p_k} = 0 \quad (\text{A.2})$$

must be satisfied.

R^2 is a measure of the goodness of fit. If in eq. (A.1) $w_i = 1/\sigma_i^2$ is considered where σ_i^2 is the variance of the datum at channel x_i then the statistical variation of R^2 is described by the Chi-Square distribution. For this reason eq. (A.1) can be rewritten as

$$\chi^2(x, \underline{p}) = \sum_i \frac{1}{\sigma_i^2} [y_i - F(x_i, \underline{p})]^2 \quad (\text{A.3})$$

where χ^2 is the independent variable of the Chi-Square distribution. And thus eq. (A.2) is reduced to

$$\frac{\partial \chi^2}{\partial p_k} = -2 \sum_i \frac{1}{\sigma_i^2} [\bar{y}_i - F(x_i, \underline{p})] \frac{\partial F(x_i, \underline{p})}{\partial p_k} = 0 \quad (\text{A.4})$$

and from eq. (A.2)

$$\sum_i \frac{1}{\sigma_i^2} y_i \frac{\partial F(x_i, \underline{p})}{\partial p_k} = \sum_i \frac{1}{\sigma_i^2} F(x_i, \underline{p}) \frac{\partial F(x_i, \underline{p})}{\partial p_k} \quad (\text{A.5})$$

Considering the Taylor expansion of a general function $f(\underline{x}, \underline{p})$ neglecting the third and the higher order terms

$$f(\underline{x}, \underline{p} + \Delta \underline{p}) = f(\underline{x}, \underline{p}) + \sum_j \frac{\partial f(\underline{x}, \underline{p})}{\partial p_j} \Delta p_j + \frac{1}{2} \sum_j \sum_k \frac{\sigma^2 f(\underline{x}, \underline{p})}{\sigma p_j \sigma p_k} \Delta p_j \Delta p_k \quad (\text{A.6})$$

or in short

$$\Delta f(\underline{x}, \underline{p}) = f(\underline{x}, \underline{p} + \Delta \underline{p}) - f(\underline{x}, \underline{p}) = \sum_j a_j \Delta p_j + \frac{1}{2} \sum_{jk} G_{jk} \Delta p_j \Delta p_k \quad (\text{A.7})$$

can be written. Here \underline{p} is the parameter vector. Taking the derivatives with respect to Δp_j

$$\underline{g} = \underline{a} + \underline{G} \Delta \underline{p} \quad (\text{A.8})$$

is obtained. Here \underline{g} , is the gradient vector at the point defined by the vector \underline{p} in the parameter space, \underline{a} is the derivative vector at the point of Taylor expansion and \underline{G} is the Hessian matrix whose elements are defined by

$$G_{jk} = \frac{\partial^2 f(\underline{x}, \underline{p})}{\partial p_j \partial p_k} \quad (\text{A.9})$$

Multiplying both sides of eq. (A.7) with $-\underline{G}^{-1}$

$$-\underline{G}^{-1} \underline{g} = -\underline{G}^{-1} \underline{a} - \Delta \underline{p} \quad (\text{A.10})$$

can be written.

Assuming that \underline{G} is constant around the minimum and considering $\underline{g} = 0$ at the minimum

$$\underline{a} + \underline{G} \Delta \underline{p}_0 = 0 \quad (\text{A.11})$$

is obtained from eq. (A.8).

Here $\Delta \underline{p}_0$ is the increment in $\Delta \underline{p}$ necessary to reach the

minimum. Multiplying both sides of eq. (A.10) with \underline{G}^{-1} and substituting the values obtained, namely $\underline{G}^{-1}\underline{a}$ in eq. (A.9)

$$\Delta \underline{p}_0 - \Delta \underline{p} = -\underline{G}^{-1} \underline{g} \quad (\text{A.12})$$

is found.

Since the Hessian matrix is in general not constant $\Delta \underline{p}_0$ cannot be readily calculated from eq. (A.11). For this reason an arbitrary positive definite and symmetrical matrix \underline{H} is used. This matrix is used in eq. (A.11) instead of \underline{G}^{-1} and \underline{G}^{-1} is formed with iteration in order to satisfy this equation.

The step vector $\Delta \underline{s}_i$ belonging to i^{th} iteration from (eq. A.11) is

$$\Delta \underline{s}_i = -\underline{H}_i \underline{g}_i \quad (\text{A.13})$$

At the end of each iteration \underline{H}_i is changed suitably while maintaining its positive-definiteness. Since \underline{g}_i is in the direction of steepest ascent and \underline{H}_i is positive definite and

$$\Delta \underline{s}_i^T \underline{g}_i = \underline{g}_i^T \underline{H}_i \underline{g}_i \quad (\text{A.14})$$

is always positive definite, $\Delta \underline{s}_i$ will be in the direction of the minimum. Taking \underline{H} as the identity matrix in the initial step forces the initial step to be in the direction of the steepest descent.

Iteration process can be described as follows:

Let us assume that at the i^{th} step the point in the parameter space is represented by \underline{p}_i the gradient vector at this point is \underline{g}_i and \underline{H} is \underline{H}_i .

(a) As the function approaches the minimum on the path $\underline{p}_i + \lambda_i \Delta \underline{s}_i$ where $\Delta \underline{s}_i = -\underline{H}_i \underline{g}_i$ a value α_i is calculated such that $f(x, \underline{p}_i + \lambda_i \Delta \underline{s}_i)$ with respect to λ is a minimum. For

$\lambda_i = \alpha_i f(x, \underline{p}_i + \alpha_i \Delta \underline{s}_i)$ is a minimum. Since the direction of $\Delta \underline{s}_i$ is towards the minimum α_i is always positive.

(b) Defining

$$\underline{\sigma}_i = \alpha_i \Delta \underline{s}_i \quad (\text{A.15})$$

the new values of the parameters

$$\underline{p}_{i+1} = \underline{p}_i + \underline{\sigma}_i \quad (\text{A.16})$$

are calculated.

(c) Using \underline{p}_{i+1} , $f(x, \underline{p}_{i+1})$ and \underline{g}_{i+1} are calculated

(d) Taking

$$\underline{Y}_i = \underline{g}_{i+1} - \underline{g}_i \quad (\text{A.17})$$

$$\underline{A}_i = \frac{\underline{\sigma}_i \underline{\sigma}_i^T}{\underline{\sigma}_i^T \underline{Y}_i} \quad (\text{A.18})$$

$$\underline{B}_i = \frac{\underline{H}_i \underline{Y}_i \underline{Y}_i^T \underline{H}_i}{\underline{Y}_i^T \underline{H}_i \underline{Y}_i} \quad (\text{A.19})$$

The H matrix is changed as

$$\underline{H}_{i+1} = \underline{H}_i + \underline{A}_i + \underline{B}_i \quad (\text{A.20})$$

where \underline{H}_{i+1} is still positive definite⁽³⁾.

(e) Making $i = i+1$, the steps a through d are repeated until the minimum is reached.

The minimization is terminated if all the components in the next step change by less than 10^{-11} , or if five succeeding values of χ^2 are the same, or if 100 iterations have been completed.

The variable metric minimization is carried in program BUCAASA/FIT by subroutine VARMET.

The value of $\lambda_{\min} = \alpha_i$ in step (a) is calculated through cubic interpolation:

Assuming that the variation of $f_i(x, \lambda)$ is a cubic function

$$f_i(x, \lambda) = a\lambda^3 + b\lambda^2 + c\lambda + d \quad (\text{A.21})$$

can be written here $a, b, c,$ and d are constants.

$$\frac{\partial f_i(x, \lambda)}{\partial \lambda} = 3a\lambda^2 + 2b\lambda + c \quad (\text{A.22})$$

taking $\partial f_i / \partial \lambda = 0$

$$\lambda_{\min} = \alpha_i = \frac{-b \pm \sqrt{b^2 - 3ac}}{3a} \quad (\text{A.23})$$

and

$$\left. \frac{f_i(x, \lambda)}{\partial \lambda} \right|_{\lambda = 0} = c = g_0 \quad (\text{A.24})$$

$$\left. \frac{\partial f_i(x, \lambda)}{\partial \lambda} \right|_{\lambda = \lambda_k} = 3a\lambda_k^2 + 2b\lambda_k + c = g_1 \quad (\text{A.25})$$

is obtained.

Here g_0 and g_1 are the derivatives at M and N in fig A.1. If h_0 and h_1 are the values of $f(x_i, \lambda)$ at points M and N respectively.

$$f_i(x, 0) = d = h_0 \quad (\text{A.26})$$

$$f_i(x, \lambda_k) = a\lambda_k^3 + b\lambda_k^2 + c\lambda_k + d = h_1 \quad (\text{A.27})$$

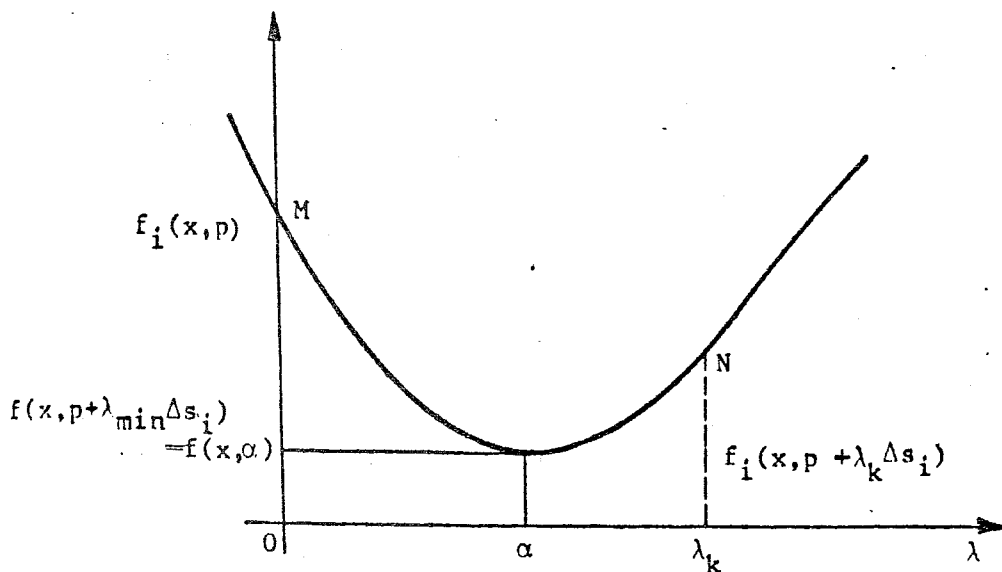


Fig. A.1. The schematic representation of $f_i(x, p + \lambda \Delta s_i)$ for the cubic interpolation.

can be written.

From eqs. (A.23), (A.24), (A.25) and (A.26)

$$a = \frac{1}{\lambda_k^2} \left[\frac{2(h_0 - h_1)}{k} + g_0 + g_1 \right] \quad (\text{A.28})$$

$$b = \frac{3(h_1 - h_0)}{\lambda_k^2} - \frac{2g_0 + g_1}{\lambda_k} \quad (\text{A.29})$$

can be found.

Taking

$$Z = 3 \frac{h_0 - h_1}{\lambda_k} + g_0 + g_1 \quad (\text{A.30})$$

and

$$W = (Z^2 - g_0 g_1)^{1/2} \quad (\text{A.31})$$

$$\alpha = \alpha_k = \lambda_k \left(1 - \frac{Z + g_1 - w}{g_0 + g_1 + 2Z} \right) \quad (\text{A.32})$$

is obtained.

The cubic interpolation is implemented in BUCAASA/FIT under the subroutine name CUBINT.

Defining

$$F_D(x, \underline{p}) = A_t \exp \left[B(x-x_0) \right] \left\{ 1 - \exp \left[-\frac{1}{2} \left(\frac{x-x_0}{t} \right)^2 \right] \right\} \delta \quad (\text{A.33})$$

from

$$-\frac{\partial \chi^2}{\partial p_k} = 2 \sum_i \left\{ \frac{1}{\sigma_i} \left[(y_i - F(x_i, \underline{p})) \right] \frac{\partial F(x_i, \underline{p})}{\partial p_k} \right\} \quad (\text{A.34})$$

$F(x_i, \underline{p})$ being given by eq. (3.28), the derivatives are readily calculated as

$$\frac{\partial F(x, \underline{p})}{\partial a_k} = x^{k-1} \quad (\text{A.35})$$

$$\frac{\partial F(x, \underline{p})}{\partial h} = \operatorname{erfc} \left(\frac{x-x_0}{\sigma_g} \right) \quad (\text{A.36})$$

$$\frac{\partial F(x, \underline{p})}{\partial A_t} = \frac{F_D(x, \underline{p})}{A_t} \quad (\text{A.37})$$

$$\frac{\partial F(x, \underline{p})}{\partial A_g} = \exp \left[-\frac{1}{2} \left(\frac{x-x_0}{\sigma_g} \right)^2 \right] \quad (\text{A.38})$$

$$\frac{\partial F(\underline{x}, \underline{p})}{\partial x_o} = \left[\frac{h}{\sigma_g \sqrt{2\pi}} + A_g \frac{x-x_o}{\sigma_g^2} \right] \exp \left[-\frac{1}{2} \left(\frac{x-x_o}{\sigma_g} \right)^2 \right] -$$

$$- \left\{ B F_D(\underline{x}, \underline{p}) - \frac{C}{\sigma_t^2} (x-Cx_o) \left[F_D(\underline{x}, \underline{p}) - A_t \exp(B(x-x_o)) \right] \right\} \delta \quad (\text{A.39})$$

$$\frac{\partial F(\underline{x}, \underline{p})}{\partial B} = F_D(\underline{x}, \underline{p}) (x-x_o) \quad (\text{A.40})$$

$$\frac{\partial F(\underline{x}, \underline{p})}{\partial C} = \frac{x_o}{\sigma_t} (x-Cx_o) \left\{ F_D(\underline{x}, \underline{p}) - A_t \exp \left[B(x-x_o) \right] \right\} \delta \quad (\text{A.41})$$

$$\frac{\partial F(\underline{x}, \underline{p})}{\partial \sigma_t} = \frac{(x-Cx_o)}{\sigma_t^3} \left\{ F_D(\underline{x}, \underline{p}) - A_t \left[\exp B(x-x_o) \right] \right\} \delta \quad (\text{A.42})$$

$$\frac{\partial F(\underline{x}, \underline{p})}{\partial \sigma_g} = \left[\frac{h}{\sigma_g^2 \sqrt{2\pi}} (x-x_o) + A_g \frac{(x-x_o)}{\sigma_g^3} \right] \exp \left[-\frac{1}{2} \left(\frac{x-x_o}{\sigma_g} \right)^2 \right]$$

$$\quad (\text{A.43})$$

Where the index j has been omitted for clarity.

APPENDIX-B. ERROR ESTIMATION IN FITTING

B.1. Error Estimates of the Parameters in Fitting

A function $F(x_i, \underline{p})$ which is linear with respect to the parameters given by the vector \underline{p} can be written as

$$F(x_i, \underline{p}) = \sum_j p_j P_j(x_i) \quad (\text{B.1})$$

where $P_j(x_i)$ are any functions of the independent variables x_i .

The variances in determining the parameters p_j are given by the standard formulation as

$$\sigma_{p_j}^2 = \sum_i \sum_{i'} \sigma_{ii'} \frac{\partial p_j}{\partial y_i} \frac{\partial p_j}{\partial y_{i'}} \quad (\text{B.2})$$

here, $\sigma_{ii'}$, in general represents the variances and covariances of the data points and for $i = i'$ variances are given by

$$\sigma_i^2 = \sigma_{ii'} \quad (\text{B.3})$$

In eq. (B.2) y_i and $y_{i'}$ represent the data points. Since in optimizing the parameters of the photopeak function $F(x, \underline{p})$, the data points are used, the indeterminacies of the parameters will be a function of the standard deviations of every data point.

Since in this study it is assumed that a high resolution spectrometer system (Ge(Li) based) is used, consequently it is assumed that there is no correlation among the data points. For this reason from eq. (B.2) and (B.3)

$$\sigma_{p_j}^2 = \sum_i \left[\sigma_i^2 \left(\frac{\partial p_j}{\partial y_i} \right)^2 \right] \quad (\text{B.4})$$

can be written.

From eq. (B.1) the derivatives of $F(x_i, \underline{p})$ with respect to p_j can be readily found as

$$\frac{\partial F(x_i, \underline{p})}{\partial p_j} = P_j(x_i) \quad (\text{B.5})$$

By substituting eq. (B.5) in eq. (A.5)

$$\sum_i \frac{1}{\sigma_i^2} y_i P_k(x_i) = \sum_i \frac{1}{\sigma_i^2} P_k(x_i) \sum_j p_j P_j(x_i) \quad (\text{B.6})$$

is obtained. Defining

$$\beta_k = \sum_i \frac{1}{\sigma_i^2} y_i P_k(x_i) \quad (\text{B.7})$$

and

$$\alpha_{kj} = \sum_i \frac{1}{\sigma_i^2} P_k(x_i) P_j(x_i) = \frac{1}{2} \frac{\partial^2 \chi^2(x, \underline{p})}{\partial p_k \partial p_j} \quad (\text{B.8})$$

eq. (B.6) can be written as

$$\underline{\beta} = \underline{\alpha} \underline{p} \quad (\text{B.9})$$

or

$$\underline{p} = \underline{\alpha}^{-1} \underline{\beta} \quad (\text{B.10})$$

and by defining

$$\underline{\epsilon} = \underline{\alpha}^{-1} \quad (\text{B.11})$$

$$\underline{p} = \underline{\epsilon} \underline{\beta} \quad (\text{B.12})$$

or

$$p_j = \sum_k \epsilon_{jk} \beta_k = \sum_k \epsilon_{jk} \sum_i \frac{1}{\sigma_i} y_i p_k(x_i) \quad (\text{B.13})$$

Thus for the derivative in eq. (B.4)

$$\frac{\partial p_j}{\partial y_i} = \sum_k \epsilon_{jk} \frac{1}{\sigma_i} p_k(x_i) \quad (\text{B.14})$$

can be written.

And eq. (B.4) is transformed to

$$\begin{aligned} \sigma_{pj}^2 &= \sum_i \sigma_i^2 \left(\frac{\partial p_j}{\partial y_i} \right)^2 = \sum_k \sum_l \{ \epsilon_{jk} \epsilon_{jl} \sum_i \left[\frac{1}{\sigma_i} p_k(x_i) p_l(x_i) \right] \} \\ &= \sum_k \sum_l \epsilon_{jk} \epsilon_{jl} \alpha_{kl} = \epsilon_{jj} \end{aligned}$$

Thus ϵ can be defined as the Error Matrix.

Similarly for the covariances

$$\sigma_{pj} \sigma_{pk} = \epsilon_{jk} \quad (\text{B.16})$$

is obtained.

Using eq. (B.15) the indeterminacies in the parameters calculated with the linear least squares method can be estimated. If we consider the parabolic expansion of $\chi^2(x, \underline{p})$, it can be shown that $\Delta p_k = (\epsilon_{kk})^{1/2} = \sigma p_k$ in one of the parameters causes to increase $\chi^2(x, \underline{p})$ by 1 or in other words,

$$\chi_{\nu+1}^2(x, p_1, p_2, \dots, p_k + (\epsilon_{kk})^{1/2}, \dots, p_n) = \chi^2(x, p_1, p_2, \dots, p_k, \dots, p_n) + 1 \quad (\text{B.17})$$

Here ν represents the degree of freedom. If we consider

$\nu = n - m$ here n is the number of data points and m is the number of parameters found by the optimization process. The mean value of χ^2 the independent variable of the Chi-Square distribution is equal to ν . And an increase of 1 in the degrees of freedom forces the mean value of χ^2 to increase by 1. Since eq. (B.17) satisfies this condition the definitions in eq. (B.15) and (B.16) can be used for a non linear least squares optimization process.

In the iteration process in the variable metric minimisation process the matrix \underline{H}_i approaches to \underline{H}_m the inverse Hessian Matrix which is by definition the second derivative matrix.

$$\underline{H}_m = \left\| \left\| \frac{\partial^2 F(x, p)}{\partial p_j \partial p_k} \right\| \right\|^{-1} = \underline{V} \quad (\text{B.18})$$

Using eqs. (B.8), (B.11) and (B.18)

$$\underline{\varepsilon} = \alpha^{-1} = 2 \underline{V} \quad (\text{B.19})$$

can be written. An exact analysis of the statistical errors in a non linear function is nearly impossible since function used represents the data only approximately. Therefore eq. (B.19) has a limited validity since it does not take into consideration the deviations from the best function to represent the data.

In the situations where the function is approximate χ^2 is generally greater than one and the deviation is greater than that given by eq. (B.15) and is a function of χ^2 . Considering this fact instead of eq. (B.19)

$$\varepsilon \cong \chi^2 \nu \underline{V} = \underline{V} \quad (\text{B.20})$$

can be used as an approximation. Here \underline{V} is generally called the variance-covariance matrix.

The standard deviation of every parameter σ_{p_j} is given by

$$\sigma_{p_j} = (v_{jj})^{1/2} = (\chi^2 v_{jj})^{1/2} \quad (\text{B.21})$$

and the overall standard deviation of function $f(\underline{p})$ is given by

$$\sigma_f = \left(\sum_j \sum_k \frac{\partial f(\underline{p})}{\partial p_j} \frac{\partial f(\underline{p})}{\partial p_k} v_{jk} \chi^2 v \right)^{1/2} \quad (\text{B.22})$$

B.2. Error Estimates for Areas

The standard deviations of the areas given by eq. (3.30) and (3.31) are calculated as follows:

In general the standard deviation of a function

$$y = f(u, v, \dots) \quad (\text{B.23})$$

is given by

$$\sigma_y^2 = \sigma_u^2 \left(\frac{\partial y}{\partial u} \right)^2 + \sigma_v^2 \left(\frac{\partial y}{\partial v} \right)^2 + 2 \sigma_{uv} \left(\frac{\partial y}{\partial u} \right) \left(\frac{\partial y}{\partial v} \right) + \dots \quad (\text{B.24})$$

Where σ_u^2 , σ_v^2 , ..., are the variances and σ_{uv} are the covariances.

The standard deviation of the area of the Gaussian function given by eq. (3.30) is calculated by considering eq. (B.24) as

$$\sigma_{A_G}^2 = \left(\frac{\partial A_G}{\partial A_g} \right)^2 \sigma_{A_g}^2 + \left(\frac{\partial A_G}{\partial \sigma_g} \right)^2 \sigma_g^2 + 2 \left(\frac{\partial A_G}{\partial A_g} \right) \left(\frac{\partial A_G}{\partial \sigma_g} \right) \sigma_{A_g} \sigma_g \quad (\text{B.25})$$

And in similar manner the standard deviation of the area of the tailing function can be computed from

$$\begin{aligned}
\sigma_{A_T}^2 &= \left(\frac{\partial A_T}{\partial A_t}\right)^2 \sigma_{A_t} + \left(\frac{\partial A_T}{\partial B}\right)^2 \sigma_B^2 + \left(\frac{\partial A_T}{\partial C}\right)^2 \sigma_C^2 + \left(\frac{\partial A_T}{\partial x_o}\right)^2 \sigma_{x_o}^2 + \\
&+ \left(\frac{\partial A_T}{\partial \sigma_t}\right)^2 \sigma_{\sigma_t}^2 + 2\left(\frac{\partial A_T}{\partial A_t}\right)\left(\frac{\partial A_T}{\partial B}\right) \sigma_{A_t B} + 2\left(\frac{\partial A_T}{\partial A_t}\right)\left(\frac{\partial A_T}{\partial C}\right) \sigma_{A_t C} + \\
&+ 2\left(\frac{\partial A_T}{\partial A_t}\right)\left(\frac{\partial A_T}{\partial x_o}\right) \sigma_{A_t x_o} + 2\left(\frac{\partial A_T}{\partial A_t}\right)\left(\frac{\partial A_T}{\partial \sigma_t}\right) \sigma_{A_t \sigma_t} + \\
&+ 2\left(\frac{\partial A_T}{\partial B}\right)\left(\frac{\partial A_T}{\partial C}\right) \sigma_{BC} + 2\left(\frac{\partial A_T}{\partial B}\right)\left(\frac{\partial A_T}{\partial x_o}\right) \sigma_{Bx_o} + \\
&+ 2\left(\frac{\partial A_T}{\partial B}\right)\left(\frac{\partial A_T}{\partial \sigma_t}\right) \sigma_{B\sigma_t} + 2\left(\frac{\partial A_T}{\partial C}\right)\left(\frac{\partial A_T}{\partial x_o}\right) \sigma_{Cx_o} + \\
&+ 2\left(\frac{\partial A_T}{\partial C}\right)\left(\frac{\partial A_T}{\partial \sigma_t}\right) \sigma_{C\sigma_t} + 2\left(\frac{\partial A_T}{\partial x_o}\right)\left(\frac{\partial A_T}{\partial \sigma_t}\right) \sigma_{x_o \sigma_t} \quad (B.26)
\end{aligned}$$

All the variances and covariances in eqs. (B.25) and (B.26) are given by the matrix \underline{v} in eq. (B.20).

The derivatives in eqs. (B.25) and (B.26) are as follows

$$\frac{\partial A_G}{\partial A_g} = (2\pi)^{1/2} \sigma_g \quad (B.27)$$

$$\frac{\partial A_G}{\partial \sigma_g} = (2\pi)^{1/2} A_g \quad (B.28)$$

$$\begin{aligned}
\frac{\partial A_T}{\partial A_t} &= \frac{1}{B} \left(\exp(-Bx_o) \left[\exp(BCx_o) - 1 \right] + (2\pi)^{1/2} \sigma_t \exp \left[\frac{1}{2} B^2 \sigma_t^2 + Bx_o(C-1) \right] \right) \\
&\times \left[\operatorname{erf}(B\sigma_t) - \operatorname{erf} \left(\frac{Cx_o}{\sigma_t} + B\sigma_t \right) \right] \quad (B.29)
\end{aligned}$$

$$\begin{aligned} \frac{\partial A_T}{\partial B} = & -\frac{A_t}{B} \exp(-Bx_o) \left[\exp(B(x_o)-1) + A_T \left[B\sigma_t^2 + x_o(C-1) \right] \right] \\ & + A_t \sigma_t^2 \exp(-Bx_o) \left[1 - \exp\left(-\frac{1}{2} \frac{C^2 x_o^2}{\sigma_t^2}\right) \right] + A_t x_o \frac{C}{B} \exp(-Bx_o) \end{aligned} \quad (B.30)$$

$$\frac{\partial A_T}{\partial C} = A_t x_o \exp(-Bx_o) + A_T B x_o - A_t x_o \exp\left(-Bx_o - \frac{1}{2} \frac{C^2 x_o^2}{\sigma_t^2}\right) \quad (B.31)$$

$$\begin{aligned} \frac{\partial A_T}{\partial \sigma_t} = & (1+B^2 \sigma_t^2) \frac{1}{\sigma_t} \left[A_T + \frac{A_t}{B} \exp(-Bx_o) \right] - \frac{A_t}{B \sigma_t} \exp\left[Bx_o(C-1)\right] \\ & - A_t \sigma_t \left(B - \frac{Cx_o}{\sigma_t^2}\right) \exp\left(-\frac{1}{2} \frac{C^2 x_o^2}{\sigma_t^2} - Bx_o\right) \end{aligned} \quad (B.32)$$

$$\frac{\partial A_T}{\partial x_o} = B(C-1) A_T + CA_t \exp(-Bx_o) \left[1 - \exp\left(-\frac{1}{2} \frac{C^2 x_o^2}{\sigma_t^2}\right) \right] \quad (B.33)$$

In eq. (B.25-33) the index j has been omitted for clarity.

APPENDIX-C. USERS' GUIDE FOR BUCAASA

In order to make the programs more user friendly the number of subjective parameters supplied by the user have been kept to a minimum, however some parameters are still necessary to provide a flexibility in controlling the flow of the programs.

All the data are inputted interactively, excepting those that are read from files and there are no format restrictions for input, i.e. free format is used.

C.1. Input Data for BUCAASA/FIND

Record 1. JOB (Job heading less than 50 alphanumeric characters)

Record 2. ATGE, ATLT, FAC, ADEL, ATEST, PTEST

(The first four are peak search parameters, all of them can be taken as 1. PTEST is the significance test parameter for the peak found by the routine, it can take any value in the range 0-100).

Record 3. INIT, IFIN, ISMT, DISK, ISTORE, ISWO

(INIT: Initial channel of the spectrum to be considered in the analysis

IFIN: Last channel of the spectrum to be considered in the analysis

ISMT: Smoothing parameter

2*ISMT+3 point smoothing is performed

ISMT: 5 no smoothing

IDISK: 1 Spectrum will be input manually

0 Spectrum will be read in from a random access file

ISTORE: 1 The results will be stored in a random access file for use by BUCAASA/FIT

0 The results will not be stored

ISWO: 1 Results of smoothing will be printed out

0 Results of smoothing not be printed

If IDISK=0

Record | 4-(IFIN-INIT+1) | Spectrum data

If IDISK=1

Record 4. NAME (Less Than 8 alphanumeric characters)
The name of the random access file which contains the spectrum data. RECL must be equal to 2.

If ISTORE=1

Record 5 or (IFIN-INIT). NAME2 (less Than 8 alphanumeric characters)

The name of the random access file which will contain the results of peak identification process. It will later be used by BUCAASA/FIT.

C.2. Input Data for BUCAASA/FIT

Record 1. JOB (Job heading less than 50 alphanumeric characters)

Record 2. INUM IGUES IDISK ISAVE II IVAR IRPT ISET

INUM: The number of the peak

IGUES: 1 Initial parameters will be read in from R.A.F. prepared by BUCAASA/FIND
0 Input manual

IDISK: 0 Spectrum data will be input manually
1 Spectrum data will be read in from a R.A.F.

ISAVE: 0 The results of the analysis will not be stored
1 The results of the analysis will be stored in a R.A.F. for use by BUCAASA/CALIBR

II Degree of the Compton polynomial -1 Must be between 1 and 3.

IVAR: 1 Amplitude of the Gaussian is variable (Gaussian + Compton Fitting)
2 Amplitude + centroid are variable (Gaussian + Compton Fitting)
3 Amplitude + centroid + FWHM are variable (Gaussian + Compton Fitting)
4 Gaussian + Tailing + Compton Fitting
5 Gaussian + Tailing + Step + Compton Fitting

IRPT: 0 Do not repeat analysis
1 Repeat fitting by taking IVAR=IVAR+1 (IVAR must be less than 5)

ISET: 0 Stop execution after fitting
 1 Read data for another fitting
 -1 Used for sequential fitting for a whole peak
 set valid only if IGUES=1. In this case INUM
 must be equal to 2.

IF IDISK=1

Record 3. NAM2 (less than 8 alphanumeric characters)
 The name of the R.A.F. which contains the
 spectrum data. RECL must be equal to 2.

IF ISAVE=1

Record 4. NAM3 (less than 8 alphanumeric characters)
 The name of the R.A.F. which will contain the
 results of the fitting process. It will later
 be used by BUCAASA/CALIBR

IF IGUES=1

Record 5. NAM (less than 8 alphanumeric characters)
 The R.A.F. created by BUCAASA/FIND

IF IGUESS=0

Record 5. INIT, IFIN, MUL
 INIT Left channel of the peak region
 IFIN Right channel of the peak region
 MUL: The number of peaks in the peak region
 (Multiplicity parameter)

Record 6. SIG, (XJ(J), J=1, MUL)

SIG: FWHM/2.335: Width parameter

XJ(J): Approximate peak channel for each peak.

Record 7. (AI(I), I=1, IP)

IP: Number of parameters in fit

AI(I): I=1, II Coefficients of the Compton polynomial
 (If IVAR=3 AI(I), I=II+1, II+MUL coefficients of the
 step function)

 AI(I), I=II+MUL+1, IP Heights of the
 Gaussians

For $IVAR \leq 4$

AI(I), I=II+1, IP Heights of the Gaussians

IF $IVAR \geq 4$

Record 8. AT, BT, CT, SIGT

Tailing function parameters

IF IDISK=0

Record |9-(IFIN-INIT+1)| Spectrum data

C.3. Input Data for BUCAASA/CALIBR

Record 1. JOB (less than 50 alphanumeric characters)
Job heading.

Record 2. NP, MP, SYSER

NP: Number of energy calibration points

MP: Order of the polynomial used for calibration

SYSER: Systematic error for energy calibration

Record |3-(3+NP)| Energy calibration data

(Peak channels and corresponding energies in keV)

Record(NP+4). LP, SYSEF, EFIN

LP: Number of efficiency calibration points

SYSEF: Systematic error for efficiency calibration

EFIN: 1 Interpolate between calibration data points

0 Fit a line

IF EFIN=1

Record(NP+5)-(NP+LP+5). Efficiency calibration data

Energies in keV, efficiencies and corresponding errors in percent

IF EFIN=0

Record(NP+5)-(NP+LP+5) Efficiency calibration data

Energies in keV and efficiencies.

Record(NP+LP+6). NAM (less than 8 alphanumeric characters) R.A.F. which contains the results of BUCAASA/FIT.

Record(NP+LP+7)NAM2 (less than 8 alphanumeric characters) The name of the sequential, formatted file which will contain the results of energy and efficiency calibration to be used by BUCAASA/NUCLIDE.

C.4. Input Data for BUCAASA/NUCLIDE .

Record 1. JOB (less than 50 alphanumeric characters)
Job heading

Record 2. TCO, TEX, TWA, TLIVE, ETOL

TCO: Counting time in minutes

TEX: Irradiation time in minutes

TWA: Cooling time in minutes

TLIVE: Live time of detection in seconds

ETOL: Energy tolerance used in gamma line identification in keV

Record 3. INF (less than 8 alphanumeric characters)
The name of the sequential, formatted file created by BUCAASA/CALIBR

Record 4. LIBF (less than 8 alphanumeric characters)
The sequential formatted file which contains the gamma library, e.g. half lives, energies, etc.

The format of the gamma library LIBF is as follows

Record 1. String 'UNK' read into UNK

Record 2. BLNK. Any string of 8 characters which marks the beginning of the library. This same string

must also mark the end of the library.

Record 3. LIB, BNR

Library name and number FORMAT(A8,2X,E10.0)

Record 4. ISO, THA, IHA, NGA, APR, ANE, CRO, THR

(A8, 2X, E 10.0, A1, 7X, I2, 4E10.0, 62X)

ISO: Nuclide's name (e.g. ZN-65)

THA: Its half life

IHA: Unit of half life |M(inute), H(our), D(ay), Y(ear)|

NGA: Number of gammalines

APR: Number of protons

ANE: Number of neutrons

CRO: Cross section for thermal neutron capture

THR: Threshold cross section

The following lines of FORMAT(8E10.0) contain pairs of peak energies (keV) and branching ratio (per cent).

APPENDIX-D. IMPLEMENTATION GUIDE FOR BUCAASA

BUCAASA as a whole is coded in ANSI FORTRAN 77 programming language. There are two exceptions to the standard.

- a) The PROGRAM statement which is compulsory for the FTN5 compiler of CDC Cyber 170/815 and can be omitted in other systems, contains several file informations.
- b) Non standard functions TIME and DATE can be omitted
 TIME supplies the current time
 DATE supplies the current date
 Both of them are character functions and return a string 10 characters long.

D.1. The File Structure of BUCAASA

Since the package consists of four main programs it was found necessary to use files for data communication between consecutive programs. A description of the files is given in Tables D.1-D.5.

TABLE D.1. Files used by BUCAASA/FIND

File #	Name*	Type	Notes
5	-	Sequential	Terminal input file
6	-	Sequential	Terminal output file
11	-	Sequential	Printer file
15	NAME2	Random Access (RECL=50)	Transfer file; contains results of peak identification
16	NAME	Random Access (RECL=2)	Spectrum file

* Only user supplied names are given

TABLE D.2. Files used by BUCAASA/FIT

File #	Name	Type	Notes
5	-	Sequential	Terminal input file
6	-	Sequential	Terminal output file
11	-	Sequential	Printer file
15	NAM	Random Access (RECL=50)	Transfer file, contains the results of peak identification
16	NAM2	Random Access (RECL=2)	Spectrum file
17	NAM3	Random Access (RECL=30)	Transfer file, contains results of fitting

TABLE D.3. Files used by BUCAASA/CALIBR

File #	Name	Type	Notes
5	-	Sequential	Terminal input file
6	-	Sequential	Terminal output file
11	-	Sequential	Printer file
15	NAM2	Sequential Formatted	Transfer file, contains the results of calibration
17	NAM	Random Access (RECL=30)	Transfer file, contains results of fitting

TABLE D.4. Files used by BUCAASA/NUCLIDE

File #	Name	Type	Notes
5	-	Sequential	Terminal input file
6	-	Sequential	Terminal output file
11	-	Sequential	Printout file
15	INF	Sequential FMT	Transfer file, contains the results of calibration
17	LIBF	Sequential FMT	Gamma library file

SDATA(NCHAN) Smoothed spectrum
 SIG(NPEAK) Width parameter
 SM(NCHAN) Standard deviation of counts in each
 channel
 TDATA(NPEAK) Background subtracted counts in each
 channel.

D.2.2. Subroutine SMOOTH

DATA(NCHAN) Spectrum
 DDATA(NCHAN) First derivative spectrum
 IFIN See appendix C
 INIT
 IO 2*IO+1 point smoothing is performed
 ISMT See appendix C
 MCOE(5) Normalization constants for smoothing
 NDEN(5) Normalization constants for first deriva-
 tives
 NMCOE(6,5) Convolution coefficients for smoothing
 and first derivative
 SDATA(NCHAN) Smoothed spectrum
 SM(NCHAN) Standard deviation spectrum.

D.2.3. Subroutine PEAKID

ADEL
 ADL
 ATEN
 ATES parameters for peak search
 ATEST
 ATGE
 ATLT
 DATA(NCHAN) Spectrum
 DDATA(NCHAN) First derivative spectrum
 IPKN(NPEAK) Multiplicity parameter for each peak
 JFIT(NPEAK)
 JMUL(NPEAK)
 MAX(NPEAK) Right channel of the peak
 MIN(NPEAK) Left channel of the peak

PEAK(NPEAK) Centroid of the peak
 PR(20) Centroid of the peak (temporary storage)
 SDATA(NCHAN) Smoothed data
 SM(NCHAN) Standard deviation spectrum.

D.2.4. Program FIT

AF(15) Parameters in fitting
 AI(15)
 AG(5) Area of Gaussians
 AIC(5) Tailing height parameter
 AIX Parameter used in compensating for step
 HX function
 AT Ag/At
 BT
 CT Parameters of the tailing function
 SIGT
 EAF Error matrix
 ERRC Error correlation parameter
 F(50) Values of the fitted function
 IC Number of parameters in fit
 IDISK
 IFIN
 IGUES
 IT
 INIT
 INUM See Appendix C
 IRPT
 ISAVE
 ISET
 ISTOP
 IVAR
 NAM
 NAM2 See Appendix C
 NAM3
 NP Number of channels in fit

NPK Number of peaks to be fitted
 RD(5) $\partial AT_j / \partial P_k$ (see Appendix B)
 SIG Peak width parameter
 VARI(5) Variance of peak area
 W(50) Weighting constants
 X(50) Channel numbers
 XJ(5) Gaussian centroid channels
 Y(50) Spectrum data

D.2.5. Subroutine VARMET

AF(15) Parameters in fit
 AI(15)
 AIC(5) Tailing height parameter
 AT Ag/At
 BT
 CT Parameters of the tailing function
 SIGT
 CHIF χ_v^2
 CSQ1 χ^2
 CSQ2
 EAF(15,15) Error matrix
 EPs Convergence test parameter
 ETAA Step length
 F(50) Values of the fitted function
 GA(15)
 GB(15) Gradient vectors
 GC(15)
 H(15,15) Hessian matrix
 IC Number of parameters in fit
 IKNT Number of iterations
 IRPT See Appendix C
 IVAR
 MUL Multiplicity parameter for peak groups
 SIG Peak width parameter

XFA
 XFB χ^2
 XFD
 Y(50) Spectrum

D.2.6. Subroutine DERIVS

EXPF(50) Values of the gaussian function
 FMODG(50) F_D (see Appendix A)
 NP Number of channels
 G Gradients

D.2.7. Subroutine CUBINT

A
 GAMMA
 G1
 G2 See Appendix A
 W
 X1
 X2

D.2.8. Subroutine RINT

RD(5,15) $\partial AT_j / \partial P_k$ (See Appendix B)
 RIN(5) Tailing area

D.2.9. Program CALIBR

ACE(50) Energy calibration data (energy values in KeV)
 RCEP(50) Energy calibration data (Channel values)
 AREA(150) Peak areas
 EAREA(150) Errors in peak area determination
 EEF(150) Efficiency errors %
 EENGY(150) Calculated energyg erros
 EFIN See Appendix C
 EFL2(150) Calibrated Efficiency values
 ENGY(150) Calibrated energy value
 EPK(150) Errors in peak channel determination

LP See Appendix C
 MP
 NP
 MUL Multiplicity parameter
 mX Number of peaks
 SYSEF See Appendix C
 SYSER

D.2.10. Subroutine POLIN

N : Order of the fitting polynomial + 1
 M L Number of calibration points
 YC: The fitted values
 S : Variance

D.2.11. Subroutine MATIN

A : The matrix to be inverted
 B : Inverse of A

D.2.12. Subroutine POLIX

C(10) Co-efficients of the polynomial
 YD(150) Value of the fitted function
 YE(L50) Corresponding errors

D.2.13. Subroutine INTRP

XX(N) Calibration data
 YY(N)
 Y(M) interpolated values
 YE((M) interpolated errors

D.2.14. Program NUCLIDE

ETOL
 INF
 LIBF
 TCO See Appendix C
 TEX
 TLIVE
 TWA

D.2.15. Subroutine CORR

A(80,30) The associated lines matrix

ACOL2(30) Ordering numbers

ACOL5(30) Saturation activities

ASAT

COL(30) Names of the isotopes

CONF(30) Confidence values

EFER(30) Efficiency error

EFFSUM(30) Intensity of peaks

ENER(30) Energy of peaks

ETOL Energy tolerance

FITCH(30) Peak centroid

HALF(30) Halflives of isotopes

ITUN(30) Names of the isotopes

NUMF Number of peaks

TCO

TEX See Appendix C

TLIVE

TWA

D.2.16. Subroutine DIAG

N: Number of diagonal elements of the matrix

A(80,30) The matrix whose diagonal values of its inverse are to be determined.

D.2.17. Subroutine GLSQ

A(80,30): Coefficient matrix of simultaneous linear equations

X(30) : Interference coefficients

D.2.18. Subroutine IDENT

A(80,30) The associated lines matrix

ACOL2(30) Ordering numbers

ACOL5(30) Saturation activities

ANEU: Number of neutrons of the isotope

APRO: Number of protons of the isotope
 B(80,30): Interference matrix
 CONF(30) Confidence values
 EREF(30) Gamma energies of the isotopes
 EFER(100) Efficiency errors
 EFFSUM(100) Intensity of the peaks
 ENERG(100) Energy of the peaks
 ETOL: Energy tolerance
 FITCH(100) Centroid of the peaks
 GREF(30) Branching intensities of the isotopes
 HALF(30) Half lives of the isotopes
 ITUNN(30) symbols of the isotopes

 TCO
 TEX See Appendix C
 TLIVE
 TWA

 THAR: Half life of the isotope
 X(30): Interference coefficients.

D.2.19. Subroutine INTRF

A(80,30): Associated lines matrix
 NUMF: Number of peaks

D.2.20. Subroutine LIBRAR

ANE: Number of neutrons of the isotope
 APR: Number of protons of the isotope
 ENE(30): Energies of the gamma lines
 IHA: Symbol of the unit of half life
 LINES: Total number of gamma lines of the isotopes in
 the library
 NGA: Number of gamma lines of an isotope in the
 library
 NDISO: Total number of isotopes in the library
 PCE(30): Branching intensities of the isotopes

 THA Half life of the isotope
 THH

D.2.21. Subroutine MATRIX

A(80,30) Associated lines matrix
ACOL2(30) Ordering numbers
ACOL5(30) Saturation activities
COL(30) Names of the isotopes
CONF(30) Confidence values
EFER(100) Efficiency errors
EFFSUM(100) Intensities of the peaks
ENERG(100) Energies of the peaks
ETOL: Energy tolerance parameter
FITCH(100) Centroid of the peaks
GREF(30) Branching ratios of the gamma lines of an
isotope
HALF(30) Half lives of the isotopes
ITUNN(30) Names of the isotopes
NUMF: Number of peaks

D.2.22. Subroutine ORDER

S(30)
T(30)
W(30)
Z(30) Vectors to be ordered
Y(30)
X(30)

SNEW
TNEW
WNEW New values to be entered into the vectors
ZNEW
XNEW

APPENDIX-E. LISTING OF BUCAASA

FIN5,I=NEFIND,L=L,B=B.

```

1 PROGRAM FIND(INPUT,OUTPUT,CUF,TAPE5=INPUT,TAPE6=OUTPUT,TAPE11=OUF)
2 *****
3 * PROGRAM BUCASA/FIND *****
4 * AUTHOR: DR. OZER CIFTCIOGLU, ITU (1979) *
5 * REVISED AND DEVELOPED BY : LEVENT AKIN, BU (1984) *
6 *****
7 PARAMETER(NPEAK=100,NCHAN=4096)
8 DIMENSION AREAP(NPEAK),BGDP(NPEAK)
9 DIMENSION DATA(NCHAN),SDATA(NCHAN),DDATA(NCHAN),SM(NCHAN)
10 DIMENSION PCERR(NPEAK),TDATA(NCHAN),BDATA(NCHAN),A(NPEAK,10)
11 DIMENSION H1(NPEAK),H2(NPEAK),MIN(NPEAK),MAX(NPEAK),JFIT(NPEAK)
12 DIMENSION PEAK(NPEAK,10),IPKN(NPEAK),SIG(NPEAK)
13 COMMON ATGE,ATLT,FAC,ADEL,ATEST
14 CHARACTER*6 NAME,NAME2
15 CHARACTER*10 TIME,DATE,GUN,SAAT
16 CHARACTER*50 JOB
17 DATA ON/2.302585141/
18 GUN=DATE()
19 SAAT=TIME()
20 WRITE(6,*)'JOB ?'
21 READ(5,4) JOB
22 WRITE(6,*)'ATGE ATLT FAC ADEL ATEST PTEST'
23 READ(5,*) ATGE,ATLT,FAC,ADEL,ATEST,PTEST
24 WRITE(6,*)'INIT IFIN ISMT IDISK ISOR ISKO'
25 READ(5,*) INIT,IFIN,ISMT,IDISK,ISOR,ISKO
26 WRITE(11,3) GUN,SAAT,JOB,INIT,IFIN,ATGE,ATLT,FAC,ADEL,ATEST,PTEST
27 DG 101 I=1,NCHAN
28 DATA(I)=0.0
29 DDATA(I)=0.0
30 SDATA(I)=0.0
31 SM(I)=0.0
32 IF(IDISK.EQ.0) THEN
33 WRITE(11,*)' SPECTRUM INPUT MANUALLY'
34 WRITE(6,*)'PLEASE ENTER SPECTRUM DATA'
35 DO 200 I=INIT,IFIN
36 READ(5,*)DATA(I)
37 ELSE
38 WRITE(6,*)'NAME OF THE SPECTRUM FILE?'
39 READ(5,2)NAME
40 OPEN(UNIT=16,FILE=NAME,ACCESS='DIRECT',FORM='UNFORMATTED',
41 * RECL=2)
42 DO 210 I=INIT,IFIN
43 READ(16,REC=I)DATA(I)
44 WRITE(11,*)' SPECTRUM INPUT FROM FILE ',NAME
45 ENDIF
46 CALL SMOOTH(INIT,IFIN,ISMT,DATA,SDATA,DDATA,SM,NCHAN)
47 IF(ISWO.EQ.1) THEN
48 WRITE(11,15)
49 DO 122 I=INIT,IFIN
50 WRITE(11,14) I,DATA(I),SDATA(I),DDATA(I),SM(I)
51 ENDIF
52 CALL PEAKID(INIT,IFIN,K,ISMT,DATA,SDATA,DDATA,SM,NCHAN,NPEAK,H1,
53 H2,MIN,MAX,JFIT,IPKN,PEAK)
54 IF(K.LE.0) THEN
55 WRITE(11,11)

```

```

56 STOP
57 ENDIF
58 DO 320 N=1,K
59   NPIN=MIN(N)+1
60   NMAX=MAX(N)-1
61   AREA=0.0
62   BGD=0.0
63   AA=MAX(N)-MIN(N)
64   DC 310 L=NHIN,NMAX
65   BDATA(L)=EXP((H2(N)-H1(N))/AN*(L-MIN(N))+H1(N))*ON)
66   TDATA(L)=DATA(L)-BDATA(L)
67   IF(TDATA(L).LT.0.0) TDATA(L)=0.0
68   AREA=AREA+TDATA(L)
69   BGD=BGD+BDATA(L)
70   AREAP(N)=AREA
71   BGD(P(N))=BGD
72   PCERR(N)=SQRT((AREA+BGD)*100./AREA)
73   H1(N)=EXP(H1(N)*ON)
74   H2(N)=EXP(H2(N)*ON)
75   A(N,1)=H1(N)
76   A(N,2)=(H1(N)-H2(N))/(MIN(N)-MAX(N))
77   A(N,3)=-A(N,2)*0.01
78   DC 315 L=1,JFIT(N)
79   LL=L+3
80   KK=INT(PEAK(N,L)+0.5)-2
81   A(N,LL)=0.0
82   DO 314 I=KK+1, KK+3
83   CC=1.0
84   DO 312 J=KK+1, KK+3
85   IF(I.EQ.J) GO TO 312
86   CC=CC*(PEAK(N,L)-J)/(I-J)
87   CC=CC*CC
88   CONTINUE
89   A(N,LL)=A(N,LL)+TDATA(I)*CC
90   SIG(N)=AREAP(N)/(A(N,4)*2.5066283)
91   NP=0
92   YY=0.0
93   EY=0.0
94   E=0.0
95   E2=0.0
96   DC 325 N=1,K
97   IF(PCERR(N).LE.PTEST.AND.JFIT(N).EQ.1) THEN
98     NM=NM+1
99     YY=YY+SIG(N)
100    EY=EY+SIG(N)*PEAK(N,1)
101    E=E+PEAK(N,1)
102    E2=E2+PEAK(N,1)**2
103  ENDIF
104 CONTINUE
105 IF(NM.GT.1) THEN
106   P=(YY*E2-EY*E)/(NM*E2-E*E)
107   O=(NM*EY-E*YY)/(NM*E2-E*E)
108   DO 326 N=1,K
109     IF(PCERR(N).LE.PTEST)SIG(N)=P+O*PEAK(N,1)
110  ENDIF
111  IF(ISTOR.GE.1) THEN
112

```

```

113 WRITE(6,*)'NAME OF THE INTERMEDIATE FILE'
114 RFAD(5,2)NAME2
115 OPEN(UNIT=15,FILE=NAME2,ACCESS='DIRECT',RECL=50)
116 LN=1
117 DO 340 N=1,K
118 IF(PCERR(N).LE.PTEST) THEN
119   LN=LN+1
120   WRITE(15,REC=LN)LN,MIN(N),MAX(N),JFIT(N),(PEAK(N,L),L=1,
121   * JFIT(N)),(A(N,L),L=1,JFIT(N)+3),SIG(N)
122   ENDIF
123   CONTINUE
124   WRITE(15,REC=1)LN
125   ENDIF
126   WRITE(11,9)
127   LN=0
128   DO 350 N=1,K
129   IF(PCERR(N).LE.PTEST) THEN
130     LN=LN+1
131     WRITE(11,10)LN,MIN(N),MAX(N),AREAP(N),BGDP(N),PCERR(N),SIG(N),
132     (PEAK(N,L),L=1,JFIT(N))
133     ELSE
134     WRITE(11,17)MIN(N),MAX(N),AREAP(N),BGDP(N),PCERR(N),SIG(N),
135     (PEAK(N,L),L=1,JFIT(N))
136     ENDIF
137     CONTINUE
138     WRITE(11,12) LN
139     STOP
140 *****
141 2 FCRMAT(A6)
142 4 FCRMAT(A50)
143 3 FCRMAT(1H1,10(*,*), 'BUCAASA/FIND REV. 2.1',2A10,10(*,*)//
144 &' JOB: ',A50/' PEAK SEARCH BETWEEN',I5,' AND',I5,' CHANNELS',/
145 &' ATGE=',F5.2,' ATLT=',F5.2,' FAC=',F5.2,' ADEL=',F5.2,
146 &' ATEST=',F5.2,' PTEST=',F5.2//)
147 15 FCRMAT(//2X,' SMOOTHED DATA AND FIRST DERIVATIVES'//2X,
148 *'CH,NO',8X,'DATA',11X,'SDATA',11X,'DDATA',11X,'STD.DEV',)
149 FCRMAT(16,2X,E14.6,2X,E14.6,4X,E14.6,4X,E14.6,4X,E14.6)
150 11 FCRMAT(//10X,'** NO PEAKS WERE DETECTED **')
151 9 FCRMAT(120,'** PEAKS FOUND **'//,
152 &7X,'MIN.CHN',1X,'MAX.CHN',2X,'PEAK AREA',2X,
153 &'COMP.CONT',3X,'STD.DEV',2X,'SIGMA',4X,'PEAK CHANNELS'//)
154 FCRMAT(1X,13,2(4X,14),2(4X,F8.0),4X,F5.1,4X,F5.3,5(4X,F8.3))
155 12 FCRMAT(//10X,'TOTAL NUMBER OF DETECTED PHOTOPEAK GROUPS',14)
156 FCRMAT(4X,2(4X,14),2(4X,F8.0),4X,F5.1,4X,F5.3,5(4X,F8.3))
157 *****
158 END

```

```

--VAR IABLE MAP--(LO=4)
--NAME--ADDRESS--BLOCK-----PROPERTIES-----TYPE-----SIZE-----
A 62222B // REAL 1000 ATGE 0B //
ADEL 3B // REAL ATLT 1B //
AN 67473B REAL BDATA 52222B
AREA 67471B REAL RGD 67472B
AREAP 1546B REAL BGDP 1712B
ATEST 4B // REAL CC 67502B

```

```

1 SUBROUTINE SMOOTH(INIT,IFIN,ISMT,DATA,SDATA,DDATA,SM,NCHAN)
2 DIMENSION NMCOE(6,5),MCOE(5),NDEN(5)
3 DIMENSION DATA(NCHAN),SDATA(NCHAN),DDATA(NCHAN),SM(NCHAN)
4 DATA NMCOE,MCOE,NDEN/2,1,4*0,17,12,-3,3*0,17,6,3,-2,2*0,179,135,30,
5 *55,15,0,1,43,120,60,-10,-45,18,4,35,21,2*429,2,10,28,60,110/
6 IF(ISMT.GT.4) GO TO 400
7 IC=ISMT+1 GO TO 400
8 INIT=INIT+10
9 IFIN=IFIN-10
10 DO 200 I=INIT,IFIN
11 SCATA(I)=DATA(I)*NMCOE(1,IO)
12 DO 210 K=1,IO
13 L=I-K
14 M=I+K
15 SCATA(I)=SDATA(I)+(DATA(L)+DATA(M))*NMCOE(K+1,IO)
16 SCATA(I)=SDATA(I)/MCOE(IO)
17 IF(DATA(I).LT.4.) GO TO 212
18 IF(DATA(I)-SDATA(I).GT.DATA(I)) SDATA(I)=DATA(I)
19 IF(SDATA(I).LT.1.) SDATA(I)=1.
20 SM(I)=SQRT(SDATA(I))
21 INIT=INIT+10
22 IFIN=IFIN-10
23 DO 300 I=INIT,IFIN
24 DCATA(I)=0.0
25 DC 310 K=1,IO
26 L=I-K
27 M=I+K
28 DCATA(I)=DDATA(I)+K*(SDATA(M)-SDATA(L))
29 DCATA(I)=DDATA(I)/NDEN(IO)
30 RETURN
31 DO 400 IO
32 I=INIT,IFIN
33 IF(SDATA(I).LT.1.) SDATA(I)=1.
34 SM(I)=SQRT(SDATA(I))
35 INIT=INIT+2
36 IFIN=IFIN-2
37 DG 460 I=INIT,IFIN
38 DCATA(I)=0.0
39 DO 430 K=1,2
40 L=I-K
41 M=I+K
42 DCATA(I)=DDATA(I)+K*(SDATA(M)-SDATA(L))
43 DCATA(I)=DDATA(I)/NDEN(2)
44 RETURN
45 END

```

--VARIABLE MAP--(LO=A)

--NAME--	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE	--NAME--	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
DATA	4	DUMMY-ARG		REAL		IO	3778	3	DUMMY-ARG	INTEGER	
DDATA	6	DUMMY-ARG		REAL		ISMT				INTEGER	
I	400B			INTEGER		K	402B			INTEGER	
IFIN	2	DUMMY-ARG		INTEGER		L	404B			INTEGER	
INIT	1	DUMMY-ARG		INTEGER		M	405B			INTEGER	

```
1 SUBROUTINE PEAKID(I,I,IFF,JPK,ISMT,DATA,SDATA,DDATA,SM,NCHAN,NPEAK  
2 *,HI,H2,MIN,MAX,JFIT,IPKN,PEAK)  
3 DIMENSION INT1(20),INT2(20),FOOT(20),PK(20),JMUL(10)  
4 DIMENSION DATA(NCHAN),SDATA(NCHAN),DDATA(NCHAN),SM(NCHAN)  
5 DIMENSION H1(NPEAK),H2(NPEAK),MIN(NPEAK),MAX(NPEAK),JFIT(NPEAK),  
6 *IPKN(NPEAK),PEAK(NPEAK,10)  
7 COMMON ATGE,ATLT,FAC,ADEL,ATEST  
8 DATA J,IFST,IFNL,ON/1,0,0,2,302585141/  
9 IST=II  
10 IFT=I  
11 IF(DATA(IST).GE.1000.) THEN  
12 IF(DATA(IST).GE.3000.) THEN  
13 ATEN=FAC*SQRT(DATA(IST)*2.E-4)  
14 ELSE  
15 ATEN=ATGE  
16 ENDIF  
17 ELSE  
18 ATEN=ATLT  
19 ENDIF  
20 IF(ISMT.LE.1.OR.ISMT.GT.4) THEN  
21 ADL=1.  
22 ELSE  
23 SMP=0.25*(ISMT-1)  
24 ADL=1.+SMP  
25 ATEN=ATEN*(1.-SMP)  
26 ENDIF  
27 ADL=ADL*ADEL  
28 NCL=ADL  
29 ND2=ADL+ADL  
30 ND4=ADL+ADL+ADL+ADL  
31 NC5=ND4+ADL  
32 ATE=ATEN#0.4*ATEST  
33 ICAUT=0  
34 IRT=0  
35 JMUL(IFST)=1  
36 DC 305 N=IST,IFF  
37 DO=ATEN*SM(N)  
38 IF(DDATA(N).GT.00) GO TO 310  
39 CONTINUE  
40 J=J-1  
41 JPK=J  
42 IF(J) 800,900,800  
43 IF(IFST.LE.1) THEN  
44 MIN(J)=N-1  
45 MET=MIN(J)  
46 ELSE  
47 IF(ABS(DDATA(N+1)).LE.DC) THEN  
48 IFT=IFT-1  
49 MAX(J)=IST-1  
50 GO TO 600  
51 ENDIF  
52 ENDIF  
53 IRC=0  
54 DEFI=0.0  
55 NND=N+ND2
```

```

56 DO 370 M=NND,IFF
57 DO=ATEN*SM(M)
58 IF(DDATA(M).LE.DO) THEN
59   ICAUT=ICAUT+1
60   IF(DDATA(M).LT.0.0) GO TO 400
61   IF(IRT.EQ.0) THEN
62     IF(ICAUT.NE.ND2) THEN
63       JMUL(IFT)=JMUL(IFT)+1
64       IRT=1
65     ELSE
66       GO TO 370
67     ENDIF
68   IF(ICAUT.GE.ND4) THEN
69     IST=M
70     IF(IFT.EQ.1) GO TO 100
71     IFT=IFT-1
72     GO TO 600
73   ENDIF
74 ELSE
75   DERI=DDATA(M-1)
76   IF(ABS(DDATA(M) -DERI).LE.DO) THEN
77     IRG=IRG+1
78     IF(IRG.EQ.ND4) JMUL(IFT)=JMUL(IFT)+1
79   ENDIF
80   ICAUT=0
81 ENDIF
82 CONTINUE
83 GO TO 750
84 PM=M-1
85 DELM=DDATA(M-1)/(DDATA(M-1)-DDATA(M))
86 PK(IFT)=PM*DELM
87 MM=M*NDL
88 IIT=0
89 IRG=0
90 DERI=0.0
91 DO 450 L=MM,IFF
92 DON=--ATEN*SM(L)
93 IF(DDATA(L).GT.DON) GO TO 505
94 DERI=DDATA(L-1)
95 DMJN=SM(L)*ATES
96 IF(ABS(DDATA(L) -DERI).GT.DMIN) THEN
97   IIT=0
98   IF(ABS(DDATA(L) -DERI).LE.-DON) THEN
99     IRG=IRG+1
100    IF(IRG.EQ.ND4) JMUL(IFT)=JMUL(IFT)+1
101  ELSE
102    IRG=0
103  ENDIF
104 ELSE
105   IF(IIT.LT.ND2) THEN
106     IIT=IIT+1
107   ELSE
108     MEF=L-IIT-1
109     IF(DATA(MEF).GT.DATA(MEF).OR.DDATA(MEF).GE.0.0) GO TO 500
110     JMUL(IFT)=JMUL(IFT)+1
111     WRITE(11,5) MEF
112

```

```

113 IIT=0
114 ENDIF
115 CONTINUE
116 IFNL=1
117 JPK=J
118 GO TO 800
119 L=L-IIT-1
120 INT1(IFL)=L
121 IIT=0
122 LL=L
123 LL=LL+1
124 IF(LL-IFL) 515,520,795
125 LDEL=LL-L
126 IF(LDEL.GE.ND5) GO TO 530
127 DO=ATEN*SM(LL)
128 IF(ABS(DDATA(LL)).LE.DO) GO TO 510
129 DMIN=SM(LL)*ATES
130 DERI=DDATA(LL-1)
131 IF(ABS(DDATA(LL)-DERI).LT.DMIN) GO TO 510
132 INT2(IFL)=LL-1
133 IF(DDATA(LL-1).LT.20.) THEN
134 SUM=0.0
135 DO 540 IL=INT1(IFL),INT2(IFL)
136 SUM=SUM+ALOG10(DATA(IL))
137 FOOT(IFL)=SUM/LDEL
138 ELSE
139 FOOT(IFL)=ALOG10(DATA(L))
140 ENDIF
141 IF(LDEL.GT.ND2) GO TO 600
142 IF(DDATA(LL).GE.0.0) THEN
143 IFT=IFT+1
144 PK(IFL)=0.0
145 IST=LL
146 GO TO 300
147 ENDIF
148 MM=LL
149 JMUL(IFL)=JMUL(IFL)+1
150 WRITE(11,5) MM
151 GO TO 405
152 FIF=FOOT(IFL)
153 IF(MIN(J).GT.II) THEN
154 LPT=1
155 LST=MIN(J)
156 IF(DATA(LST).LE.20.) THEN
157 SUM=ALOG10(DATA(LST))
158 LRV=LST-LPT
159 IF(LRV.LT.II) GO TO 635
160 DO=ATEN*SM(LRV)
161 IF(ABS(DDATA(LRV)).GE.DO) GO TO 635
162 SUM=SUM+ALOG10(DATA(LRV))
163 LPT=LPT+1
164 IF(LPT-ND5) 620,635,635
165 FTI=SUM/LPT
166 ELSE
167 FTI=ALOG10(DATA(LST))
168 ENDIF
169
450 ENDIF
500 GO TO 800
505 L=L-IIT-1
510 INT1(IFL)=L
515 LL=L
510 LL=LL+1
515 IF(LL-IFL) 515,520,795
520 LDEL=LL-L
520 IF(LDEL.GE.ND5) GO TO 530
520 DO=ATEN*SM(LL)
520 IF(ABS(DDATA(LL)).LE.DO) GO TO 510
530 DMIN=SM(LL)*ATES
530 DERI=DDATA(LL-1)
530 IF(ABS(DDATA(LL)-DERI).LT.DMIN) GO TO 510
530 INT2(IFL)=LL-1
530 IF(DDATA(LL-1).LT.20.) THEN
530 SUM=0.0
540 DO 540 IL=INT1(IFL),INT2(IFL)
540 SUM=SUM+ALOG10(DATA(IL))
540 FOOT(IFL)=SUM/LDEL
540 ELSE
540 FOOT(IFL)=ALOG10(DATA(L))
540 ENDIF
540 IF(LDEL.GT.ND2) GO TO 600
540 IF(DDATA(LL).GE.0.0) THEN
540 IFT=IFT+1
540 PK(IFL)=0.0
540 IST=LL
540 GO TO 300
540 ENDIF
540 MM=LL
540 JMUL(IFL)=JMUL(IFL)+1
540 WRITE(11,5) MM
540 GO TO 405
540 FIF=FOOT(IFL)
540 IF(MIN(J).GT.II) THEN
540 LPT=1
540 LST=MIN(J)
540 IF(DATA(LST).LE.20.) THEN
540 SUM=ALOG10(DATA(LST))
540 LRV=LST-LPT
540 IF(LRV.LT.II) GO TO 635
540 DO=ATEN*SM(LRV)
540 IF(ABS(DDATA(LRV)).GE.DO) GO TO 635
540 SUM=SUM+ALOG10(DATA(LRV))
540 LPT=LPT+1
540 IF(LPT-ND5) 620,635,635
540 FTI=SUM/LPT
540 ELSE
540 FTI=ALOG10(DATA(LST))
540 ENDIF
540
600 GO TO 405
620 SUM=ALOG10(DATA(LST))
620 LRV=LST-LPT
620 IF(LRV.LT.II) GO TO 635
620 DO=ATEN*SM(LRV)
620 IF(ABS(DDATA(LRV)).GE.DO) GO TO 635
620 SUM=SUM+ALOG10(DATA(LRV))
620 LPT=LPT+1
620 IF(LPT-ND5) 620,635,635
620 FTI=SUM/LPT
620 ELSE
620 FTI=ALOG10(DATA(LST))
620 ENDIF
620
630 SUM=ALOG10(DATA(LST))
630 LRV=LST-LPT
630 IF(LRV.LT.II) GO TO 635
630 DO=ATEN*SM(LRV)
630 IF(ABS(DDATA(LRV)).GE.DO) GO TO 635
630 SUM=SUM+ALOG10(DATA(LRV))
630 LPT=LPT+1
630 IF(LPT-ND5) 620,635,635
630 FTI=SUM/LPT
630 ELSE
630 FTI=ALOG10(DATA(LST))
630 ENDIF
630
635 SUM=ALOG10(DATA(LST))
635 LRV=LST-LPT
635 IF(LRV.LT.II) GO TO 635
635 DO=ATEN*SM(LRV)
635 IF(ABS(DDATA(LRV)).GE.DO) GO TO 635
635 SUM=SUM+ALOG10(DATA(LRV))
635 LPT=LPT+1
635 IF(LPT-ND5) 620,635,635
635 FTI=SUM/LPT
635 ELSE
635 FTI=ALOG10(DATA(LST))
635 ENDIF
635

```

```

170 ELSE
171   MIN(J)=II
172   IFST=1
173   FTI=ALOGIO(DATA(II))
174   ENDIF
175   IF(IFT.LE.1) THEN
176     HI(J)=FTI
177     H2(J)=FOOT(IFT)
178     PEAK(J,1)=PK(1)
179     IPKN(J)=1
180     MAX(J)=INT1(IFT)
181     IST=MAX(J)+1
182     IPEK=PEAK(J,1)+0.5
183     IF(MAX(J)-IPEK.GT.ND2) THEN
184       JPK=J
185       JFIT(J)=JMUL(J)-1
186       MULT=JFIT(J)+1
187       JFIT(J)=IPKN(J)
188       J=J+1
189     ENDIF
190   ELSE
191     PIN=MIN(J)
192     PFI=INT1(IFT)
193     HI(J)=FTI
194     IO=0
195     I=1
196     JFIT(J)=-1
197     SLP=(FIF-FTI)/(PFI-PIN)
198     PIM=INT1(I)
199     FCI=FTI+SLP*(PIM-PIN)
200     KI=I-IO
201     PEAK(J,KI)=PK(I)
202     DO=ATEN*SM(INT1(I))
203     EFCM=EXP(FOOT(I)*ON)-EXP(FCI*ON)
204     JFIT(J)=JFIT(J)+JMUL(I)
205     IF(EFCM.LE.DO) THEN
206       MAX(J)=INT1(I)
207       H2(J)=FOOT(I)
208       IPKN(J)=I-IO
209       IO=I
210       MULT=JFIT(J)+1
211       JFIT(J)=IPKN(J)
212       J=J+1
213     MIN(J)=INT2(I)
214     HI(J)=FOOT(I)
215     JFIT(J)=-1
216   ENDIF
217 I=I+1
218 IF(I-IFT) 705,725,725
219 MAX(J)=INT1(IFT)
220 H2(J)=FOOT(IFT)
221 IPEK=INT2(IFT-1)
222 IF(MAX(J)-IPEK.GT.ND2) THEN
223   JPK=J
224   PEAK(J,I-IO)=PK(I)
225   IPKN(J)=IFT-IO
226   JFIT(J)=JFIT(J)+JMUL(IFT)

```



```
1 PROGRAM FIT(INPUT,OUTPUT,YAZ,TAPE6=OUTPUT,TAPE5=INPUT,TAPE11=YAZ)
2 *****
3 PROGRAM BUCASA/FI
4 *
5 * AUTHOR: DR. OZER CIFTIOGLU, ITU (1979)
6 * REVISED AND DEVELOPED BY: LEVENT AKIN, BU (1984)
7 * *****
8 DIMENSION AREA(5),EII(5),EAREA(5),VARI(5),EAFSR(15),EAREAG(5),
9 EBI(9),AG(5)
10 COMMON AI(15),AF(15),EAF(15,15),AIC(5),RD(5,15),RIN(5)
11 COMMON X(50),Y(50),W(50),F(50),WRES(50),BGDI(50),XJ(6)
12 COMMON II,IP,IC,NP,MUL,SIG,IVAR,IRPT,ISTOP,IN
13 COMMON AT,BT,CT,SIGT
14 EXTERNAL ERF
15 LOGICAL JXST
16 CHARACTER*7 NAM,NAM2,NAM3
17 CHARACTER*10 TIME,DATE,GUN,SAAT
18 CHARACTER*50 JOB
19 GUN=DATE()
20 SAAT=TIME()
21 WRITE(11,1200) GUN,SAAT
22 FORMAT(1H,6('*'),' BUCASA/FIT REV: 3.0 ',2A10,6('*'))
23 PRINT*,'NAME OF JOB?'
24 READ(5,1100) JOB
25 FORMAT(A50)
26 WRITE(11,1110) JOB
27 FORMAT(' JOB : ',A50)
28 100 CONTINUE
29 PRINT*,'INUM IGUES IDISK ISAVE II IVAR IRPT ISET'
30 READ*,INUM,IGUES,IDISK,ISAVE,II,IVAR,IRPT,ISET
31 ISTOP=0
32 IF(IDISK.EQ.1) THEN
33 PRINT*,'NAME OF THE SPECTRUM FILE?'
34 READ(*,2) NAM2
35 INQUIRE(FILE=NAM2,EXIST=JXST)
36 IF(.NOT.JXST) THEN
37 PRINT*,'THERE IS NO SUCH FILE'
38 GO TO 256
39 ENDIF
40 WRITE(11,*)'SPECTRAL DATA READ IN FROM FILE',NAM2
41 ENDIF
42 IF(ISAVE.EQ.1) THEN
43 PRINT*,'NAME OF THE OUTPUT FILE?'
44 READ(*,2)NAM3
45 OPEN(17,FILE=NAM3,ACCESS='DIRECT',RECL=30)
46 WRITE(11,*)'OUTPUT FILE IS ',NAM3
47 ENDIF
48 IF(IGUES) 215,240,215
49 PRINT*,'NAME OF THE INPUT FILE?'
50 READ(5,1000) NAM
51 FORMAT(A7)
52 INQUIRE(FILE=NAM,EXIST=JXST)
53 IF(.NOT.JXST) THEN
54 PRINT*,'THERE IS NO SUCH FILE'
55 GO TO 215
56 ENDIF
```

```

56 WRITE(I1,*) 'INITIAL VALUES READ IN FROM FILE ',NAM
57 OPEN(15,FILE=NAM,ACCESS='DIRECT',RECL=50)
58 IF(ISET.EQ.-1) THEN
59 READ(15,REC=1)NPK
60 IF(ISAVE.EQ.1.AND.ISET.EQ.-1)WRITE(I7,REC=1)NPK
61 ENDIF
62 READ(15,REC=INUM) NNN,INIT,IFIN,MUL,(XJ(J),J=1,MUL),
63 *(BBI(J),J=1,MUL+3),SIG
64 ISTOP=0
65 DO 211 I=1,II
66 AI(I)=8BI(I)
67 IN=II
68 IF(IVAR.GT.4) THEN
69 IN=II+MUL
70 IP=II+MUL+MUL
71 AIX=.15
72 HX=.85
73 AI(1)=AI(1)+AI(2)*(IFIN-INIT)*(1.0-AIX)
74 DO 212 I=1,MUL
75 K=II+I
76 AI(K)=(AIX-1.0)*AI(2)*(IFIN-INIT)*HX
77 AI(2)=AI(2)*AIX
78 J=II+MUL+1
79 ELSE
80 J=II+1
81 IP=II+MUL
82 ENDOF
83 IF(IVAR.GT.3) THEN
84 AT=0.1
85 BT=0.5
86 CT=1.0
87 SIGT=1.75
88 ENDOF
89 K=3
90 DO 213 I=J,IP
91 K=K+1
92 AI(I)=BBI(K)
93 IF(IVAR.GT.3) THEN
94 DO 50 J=1,MUL
95 L=IN+J
96 AIC(J)=AT*AI(L)
97 ENDOF
98 GO TO 250
99 PRINT*, 'INIT IFIN MUL'
100 READ*,INIT,IFIN,MUL
101 PRINT*, 'SIG,(XJ(J),J=1,MUL,*)'
102 READ*,SIG,(XJ(J),J=1,MUL)
103 IP=II+MUL
104 IN=II
105 IF(IVAR.GT.4) THEN
106 IN=IN+MUL
107 IP=IP+MUL
108 ENDOF
109 PRINT*, '(AI(I),I=1,IP,)'
110 READ*,(AI(I),I=1,IP)
111 IF(IVAR.GT.3) THEN
112 PRINT*, 'ENTER AT BT CT SIGT'

```

```

113 READ*,AT,BT,CT,SIGT
114 DO 249 J=1,MUL
115 L=IN+J
116 AIC(J)=AT*AI(L)
117 ENDF
118
119 WRITE(11,4)INUM,INIT,IFIN,MUL,II,IVAR,IRPT,IGUES
120 *,IDISK,ISAVE,ISET
121 4 FORMAT(' INUM INIT IFIN MUL II IVAR IRPT IGUES',
122 *, IDISK ISAVE ISET '/ 9I5,2X,2I5)
123 NP=IFIN-INIT+1
124 IF(IDISK.EQ.0) THEN
125 PRINT*, 'PLEASE ENTER SPECTRUM DATA'
126 DO 255 I=1,NP
127 READ*,Y(I)
128 ELSE
129 OPEN(16,FILE=NAM2,ACCESS='DIRECT',RECL=2)
130 DO 257 I=1,NP
131 K=I+INIT-1
132 READ(16,REC=K) Y(I)
133 ENDF
134 DO 300 I=1,NP
135 X(I)=I
136 W(I)=1./Y(I)
137 DO 360 J=1,MUL
138 XJ(J)=XJ(J)-INIT+1
139 IF(IVAR.LE.0) GO TO 950
140 GC TO (410,420,440,450,450),IVAR
141 IC=IP
142 GO TO 550
143 IC=IP*MUL
144 IPL=IP+1
145 K=I-IPL+1
146 AI(I)=XJ(K)
147 GO TO 550
148 IC=IP*MUL+1
149 IPL=IP+1
150 IP2=IC-1
151 DO 500 I=IPL,IP2
152 K=I-IPL+1
153 AI(I)=XJ(K)
154 AI(IC)=SIG
155 GO TO 550
156 IC=IP*MUL*2+4
157 IPL=IP+1
158 IP2=IP*MUL
159 DO 510 I=IPL,IP2
160 K=I-IPL+1
161 AI(I)=XJ(K)
162 IP3=IP2+1
163 IP4=IP2*MUL
164 DO 520 I=IP3,IP4
165 K=I-IP3+1
166 AI(I)=AIC(K)
167 AI(IC-3)=BT
168 AI(IC-2)=CT
169 AI(IC-1)=SIGT

```

```

170 AI(IC)=SIG
171 WRITE(11,1500) (AI(I),I=1,II)
172 FORMAT(1X,'INITIAL PARAMETERS:'/20('-'')/
173 *,'COMPTON CONTINUUM',F6.3, A0=F10.1, A1=F8.2,
174 *,' A2=',F8.2)
175 IF(IVAR.EQ.4)THEN
176   IF(IVAR.EQ.5)WRITE(11,1600) (J,AI(II+J),J=1,MUL)
177   FORMAT(/,'STEP FUNCTION'/5(1X,:'H',II,:' ',F8.2))
178   WRITE(11,1700) (J,AI(IN+J),J=1,MUL)
179   FORMAT(/,'PEAK HEIGHTS (GAUSS)'/5(1X,:'AG',II,:' ',F11.1))
180   WRITE(11,1800) (J,AI(IN+2*MUL+J),J=1,MUL)
181   FGRMAT(/,'TAILING HEIGHTS'/5(1X,:'AT',II,:' ',F10.1))
182   WRITE(11,1900) (J,AI(IN+MUL+J),J=1,MUL)
183   FORMAT(/,'PEAK CHANNELS'/5(1X,:'XO',II,:' ',F9.3))
184   WRITE(11,2000) (AI(II),I=IC-3,IC)
185   FORMAT(/,'B=',F6.3, 'C=',F6.3, 'SIGMAT=',F6.3, 'SIGMAG=',F6.3)
186   ELSE
187     WRITE(11,1700) (J,AI(II+J),J=1,MUL)
188     WRITE(11,1900) (J,AI(II+MUL+J),J=1,MUL)
189     WRITE(11,2800) AI(IC)
190     FORMAT(/,'SIGHAG=',F6.3)
191     ENDIF
192   CALL VARMET
193   IF(ISTOP.LE.0) GO TO 580
194   GO TO 900
195 580 IF(IVAR.LT.4) GO TO 590
196   DO 586 I=1,IC
197   EAFSR(I)=SQRT(EAF(I,I))
198 586 WRITE(11,2100) (AF(I),EAFSR(I),I=1,II)
199 2100 FCRMAT(/,'FINAL PARAMETERS:'/18('-'')/,'COMPTON CONTINUUM',/
200   &,' A0=',F11.1, '+/-' ,F7.1, A1=F8.2, '+/-' ,F6.1, A2=,
201   &,' F6.2, '+/-' ,F6.1)
202   IF(IVAR.EQ.5)WRITE(11,2200) (J,AF(II+J),EAFSR(II+J),J=1,MUL)
203   FCRMAT(/,'STEP FUNCTION'/5(1X,:'H',II,:' ',F8.2, '+/-' ,F6.1))
204 2200 WRITE(11,2300) (J,AF(IN+J),EAFSR(IN+J),J=1,MUL)
205 2300 FORMAT(/,'PEAK HEIGHTS (GAUSS)'/5(1X,:'AG',II,:' ',F11.1,
206   &,' '+/-' ,F7.1))
207   WRITE(11,2400) (J,AF(IN+2*MUL+J),EAFSR(IN+2*MUL+J),
208   &,' J=1,MUL)
209 2400 FORMAT(/,'TAILING HEIGHTS'/5(1X,:'AT',II,:' ',F10.1, '+/-' ,
210   &,' F6.1))
211   WRITE(11,2500) (AF(I),EAFSR(I),I=IC-3,IC),AF(IC)*2.35482
212 2500 FORMAT(/,'B=',F6.3, '+/-' ,F5.3, 'C=',F6.3, '+/-' ,F5.3,
213   &,' SIGMAT=',F6.3, '+/-' ,F5.3, 'SIGMAG=',F6.3, '+/-' ,F5.3,
214   &,' FWHM=',F6.3)
215   GO TO 595
216 590 WRITE(11,2100) (AF(I),EAF(I),I=1,II)
217   WRITE(11,2300) (J,AF(II+J),EAF(II+J),J=1,MUL)
218 2180 WRITE(11,2900) AF(IC),EAF(IC),AF(IC)*2.25482
219 2900 FORMAT(/,'SIGMAG=',F6.3, '+/-' ,F5.3, 'FWHM=',F6.3)
220 595 ERRC=0.0
221 D1=(Y(NP)-F(NP))/SQRT(ABS(F(NP)))
222 DO 630 I=1,NP
223   D0=01
224   D1=(Y(I)-F(I))/SQRT(ABS(F(I)))
225   ERRC=ERRC+D0*D1
226   ERRC=ERRC/(NP-IC)

```

```

227 DO 700 J=1,MUL
228 IF(IVAR.GT.3) GO TO 688
229 K=J+II
230 AREA(J)=AF(K)*(2.5066282*SIG)
231 IF(IVAR.GT.2) GO TO 680
232 EAREA(J)=EAF(K,K)/AF(K)*100.
233 XJ(J)=XJ(J)+INIT-1
234 GO TO 700
235 EAF(K,K)=EAF(K,K)/AF(K)
236 EAF(IC,IC)=EAF(IC,IC)/AF(IC)
237 EAREA(J)=SORT(EAF(K,K)**2+EAF(IC,IC)**2)*100.
238 GO TO 699
239 K=J+IN
240 EAREAG(J)=SQRT(EAF(K,K)/AF(K)**2+EAF(IC,IC)/AF(IC)**2)+
241 E2*EAF(IC,K)/AF(K)*AF(IC)
242 AREA(J)=AF(K)*2.5066282*SIG
243 CALL RINT
244 AG(J)=AREA(J)
245 AREA(J)=AREA(J)+RIN(J)
246 RC(J,1)=2.5066282*SIG
247 RC(J,IC)=AF(K)*2.5066282
248 II=II+J
249 IPJ=IP+J
250 IICJ=IP+MUL+J
251 VARI(J)=RD(J,1)*(RD(J,1)*EAF(II,J,II)+2*RD(J,2)*EAF(II,J,IPJ)+
252 E2*RD(J,3)*EAF(II,J,IICJ)+2*RD(J,IC-3)*EAF(II,J,IC-3)+
253 E2*RD(J,IC-2)*EAF(II,J,IC-2)+2*RD(J,IC-1)*EAF(II,J,IC-1)+
254 E2*RD(J,IC)*EAF(II,J,IC))+RD(J,2)*(RD(J,2)*EAF(IP,J,IPJ)+
255 E2*RD(J,3)*EAF(IP,J,IICJ)+2*RD(J,IC-3)*EAF(IP,J,IC-3)+
256 E2*RD(J,IC-2)*EAF(IP,J,IC-2)+2*RD(J,IC-1)*EAF(IP,J,IC-1)+
257 E2*RD(J,IC)*EAF(IP,J,IC))+RD(J,3)*(RD(J,3)*EAF(IICJ,IC)+
258 E2*RD(J,IC-3)*EAF(IICJ,IC-3)+2*RD(J,IC-2)*EAF(IICJ,IC-2)+
259 E2*RD(J,IC)*EAF(IICJ,IC))
260 DC 693 I=IC-3,IC
261 DO 693 N=IC-3,IC
262 VARI(J)=VARI(J)+RD(J,I)*RD(J,N)*EAF(I,N)
263 EII(J)=(SORT(ABS(VARI(J)))/AREA(J))*100.
264 EAREA(J)=EII(J)
265 XJ(J)=XJ(J)+INIT-1
266 CONTINUE
267 IF(IVAR.GE.4) THEN
268 WRITE(11,2700) (J,XJ(J),EAFSR(IN+MUL+J),RIN(J),AG(J),
269 EAREA(J),EAREA(J),J=1,MUL)
270 FORMAT(/5X,'PEAK CHNL',16X,'TAILING AREA',4X,
271 E,'GAUSS AREA',4X,'TOTAL AREA',4X,'% ERROR'/
272 E5(1X,':',12,2X,F8.3,' +/-',4X,F5.3,4X,F9.1,4X,F11.1,4X,
273 E'F11.1,4X,F7.3/))
274 ELSE
275 WRITE(11,3000) (J,XJ(J),EAF(II+MUL+J,II+MUL+J),AREA(J),
276 EAREA(J),J=1,MUL)
277 EAREA(J),J=1,MUL)
278 FORMAT(/5X,'PEAK CHNL',19X,'AREA',4X,'% ERROR'/
279 E5(1X,':',12,2X,F8.3,' +/-',F5.3,4X,F11.1,4X,F7.3/))
280 ENDIF
281 IF(ISAVE.EQ.1) WRITE(17,REC=INUM)MUL,(XJ(J),EAF(J,J),AREA(J),
282 EAREA(J),J=1,MUL)
283 WRITE(11,631) ERR
284 FORMAT(/15X,'ERR.CORR=',1PE14.7//)

```

```

284 IF(IVAR.EQ.5.OR.IRPT.EQ.0)GO TO 900
285 DO 730 J=1,MUL
286 XJ(J)=XJ(J)-INIT+1
287 IVAR=IVAR+1
288 WRITE(11,14)
289 FORMAT(' THE INITIAL VALUES ARE OBTAINED FROM THE PREVIOUS FIT ')
290 WRITE(11,15) INUM,IVAR,IRPT,ISET
291 FORMAT(1X,' INUM IVAR IRPT ISET '/1X,4I5)
292 DO 770 I=1,II
293 AI(I)=AF(I)
294 IF(IVAR.EQ.4) THEN
295 AT=0.11
296 BT=0.3
297 CT=1.1
298 SIGT=5.0
299 IN=II
300 DO 775 J=1,MUL
301 AIC(J)=AT*AI(II+J)
302 IP=II*MUL
303 ENDIF
304 IF(IVAR.EQ.5)THEN
305 IN=II*MUL
306 JP=II*MUL*MUL
307 DO 780 I=II+1,II+MUL
308 AI(I)=1.
309 ENDIF
310 GO TO(410,420,440,450,450),IVAR
311 IF(ISET) 952,920,910
312 IF(ISET-1) 920,200,100
313 WRITE(11,16)
314 FORMAT(' PLEASE CHECK THE INITIAL VALUES ')
315 FCMAT(A7)
316 STOP
317 INUM=INUM+1
318 IF(INUM.LE.NPK) GO TO 220
319 STOP
320 END
    
```

---VARIABLE MAP---(L0=A)

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
AF	17B	//		REAL	15
AG	3612B	//	EAREA	REAL	5
AI	0B	//	EAREAG	REAL	5
AIC	377B	//	EII	REAL	5
AIX	3647B	//	ERRC	REAL	5
AREA	3531B	//	F	REAL	50
AT	1220B	//	GUN	REAL	5
BB1	3601B	//	HX	REAL	9
6GD	1116B	//	I	REAL	50
BT	1221B	//	IC	REAL	9
CT	1222B	//	IDISK	REAL	50
DO	3715B	//	IFIN	REAL	50
DI	3713B	//	IGUES	REAL	50
EAF	36B	//	II	REAL	225
EAFSR	3555B	//	IICJ	REAL	15
			IJJ	REAL	15
			EAREA	REAL	3543B
			EAREAG	REAL	3574B
			EII	REAL	3536B
			ERRC	REAL	3712B
			F	REAL	752B
			GUN	REAL	3623B
			HX	REAL	3650B
			I	REAL	3645B
			IC	REAL	1210B
			IDISK	REAL	3634B
			IFIN	REAL	3642B
			IGUES	REAL	3633B
			II	REAL	1206B
			IICJ	REAL	3721B
			IJJ	REAL	3717B

00=-LUNG/-OIFAKG=-COMMON/-FIXED,CJ= USER/-FIXED,DB=-TB/-SB/-SL/ ER/-TD/-PMD/-ST,PL=5000
FTN5,I=AD,L=L,B=ADB.

```

1 SUBROUTINE VARMET
2 DIMENSION XA(15),XB(15),GA(15),GB(15),GC(15),S(15),SMA(15),
3 *H(15,15)
4 COMMON AI(15),AF(15),EAF(15,15),AIC(5),RD(5,15),RIN(5)
5 COMMON X(50),Y(50),W(50),F(50),WRES(50),BGD(50),XJ(6)
6 COMMON II,IP,IC,NP,MUL,SIG,IVAR,IRPT,ISTOP,IN
7 COMMON AT,BT,CT,SIGT
8 EPS=1.E-11
9 IXX=1
10 STEP=0.01
11 DO 20 I=1,IC
12 XA(I)=AI(I)
13 IKNT=0
14 IT=0
15 DO 40 I=1,IC
16 DO 40 J=1,IC
17 H(I,J)=0.0
18 DO 50 I=1,IC
19 H(I,I)=1.0
20 CALL DERIVS(XA,XFA,GA)
21 IF(IXX.EQ.1)WRITE(11,1) XFA
22 FGRMAT(1X,'INITIAL CHISQR=',E14.6/1X,' GRADIENTS')
23 WRITE(11,2) (GA(I),I=1,IC)
24 FORMAT(1X,5E14.6)
25 IKNT=IKNT+1
26 CSOL=XFA
27 GPA=0.0
28 DO 80 I=1,IC
29 S(I)=0.0
30 DG 70 J=1,IC
31 S(I)=S(I)-H(I,J)*GA(J)
32 GPA=GPA+GA(I)*S(I)
33 IF(GPA.GE.0.0) GO TO 30
34 ETAA=-(XFA+XFA)/GPA
35 IF(ETAA.GT.1.0) ETAA=1.0
36 DO 100 I=1,IC
37 SMA(I)=ETAA*S(I)
38 XB(I)=XA(I)+SMA(I)
39 GO TO (200,115,117,119,119),IVAR
40 KI=IP+1
41 DO 116 I=K1,IC
42 J=I-K1+1
43 XJ(J)=XB(I)
44 GC TO 200
45 KI=IP+1
46 K2=IC-1
47 DO 118 I=K1,K2
48 J=I-K1+1
49 XJ(J)=XB(I)
50 SIC=XB(IC)
51 GO TO 200
52 KI=IP+1
53 K2=IP+MUL
54 DO 121 I=K1,K2
55 J=I-K1+1

```

```

56 121 XJ(J)=XB(I)
57 K3=K2+1
58 K4=K2+MUL
59 DO 122 I=K3,K4
60 K=I-K3+1
61 AJC(K)=XB(I)
62 BT=XB(IC-3)
63 CT=XB(IC-2)
64 SIGT=XB(IC-1)
65 SIG=XB(IC)
66 GAMMA=ETAA
67 CALL DERIVS(XB,XFB,GB)
68 GPB=0.0
69 DO 210 I=1,IC
70 GPB=GPB+GB(I)*S(I)
71 IF(XFB.GE.XFA.OR.GPB.GE.0.0) GO TO 220
72 ETAA=ETAA+ETAA
73 GO TO 90
74 220 IIT=0
75 XFD=XFA
76 CALL CUBINT(XFA,XFB,GAMMA,GPA,GPB,ALPHA)
77 IF(ALPHA.LE.C.0) GO TO 510
78 DO 240 I=1,IC
79 SMA(I)=ALPHA*S(I)
80 XB(I)=XA(I)+SMA(I)
81 GO TO (300,151,153,162,162),IVAR
82 K1=IP+1
83 DO 152 I=K1,IC
84 XJ(I-K1+1)=XB(I)
85 GO TO 300
86 K1=IP+1
87 K2=IC-1
88 DO 154 I=K1,K2
89 XJ(I-K1+1)=XB(I)
90 SIG=XB(IC)
91 GO TO 300
92 K1=IP+1
93 K2=IP+MUL
94 DO 163 I=K1,K2
95 XJ(I-K1+1)=XB(I)
96 K3=K2+1
97 K4=K2+MUL
98 DO 164 I=K3,K4
99 AIC(I-K3+1)=XB(I)
100 BT=XB(IC-3)
101 CT=XB(IC-2)
102 SIGT=XB(IC-1)
103 SIG=XB(IC)
104 CALL DERIVS(XB,XFB,GB)
105 CSO2=XFB
106 GPB=0.0
107 DO 310 I=1,IC
108 GPB=GPB+GB(I)*S(I)
109 IF(XFB.LE.EPS) GO TO 540
110 IF(GPB.LT.0.0.OR.ABS((XFD-XFB)/XFD).LT.0.001) GO TO 320
111 IIT=IIT+1
112 IF(IIT.GE.5) GO TO 320

```

```

113 GAMMA=ALPHA
114 XFD=XFB
115 GO TO 230
116 SIGY=0.0
117 DO 330 I=1,IC
118 GC(I)=GB(I)-GA(I)
119 SIGY=SIGY+GC(I)*SMA(I)
120 IF(SIGY.EQ.0.0) THEN
121 SIG=SIG+STEP
122 AI(IC)=SIG
123 WRITE(11,4) SIG
124 GO TO 10
125 ENDIF
126 SIGHY=0.0
127 DO 350 I=1,IC
128 S(I)=0.0
129 DO 340 J=1,IC
130 S(I)=S(I)+H(I,J)*GC(J)
131 SIGHY=SIGHY+GC(I)*S(I)
132 DO 360 I=1,IC
133 DO 360 J=1,IC
134 H(I,J)=H(I,J)+SMA(I)*SMA(J)/SIGY-S(I)*S(J)/SIGHY
135 IF(ABS((CSOL-CSO2)/CSO1).GT.0.001) GO TO 370
136 II=II+1
137 IF(II-4) 380,380,540
138 IT=0
139 IF(IKNT.GT.100) GO TO 520
140 ISS=0
141 DO 390 I=1,IC
142 GA(I)=GB(I)
143 IF(ABS(GB(I)).LE.EPS) ISS=ISS+1
144 XA(I)=XB(I)
145 IF(ISS.EQ.IC) GO TO 540
146 XFA=XFB
147 K=II+I*MUL
148 DO 400 I=K,IC
149 IF(XA(I).LT.0.0) GO TO 500
150 CONTINUE
151 GO TO 60
152 WRITE(11,5)
153 WRITE(11,2) (XA(I),I=1,IC)
154 ISTOP=1
155 RETURN
156 WRITE(11,6)
157 DO 530 I=1,IC
158 AF(I)=XB(I)
159 IRPT=0
160 RETURN
161 DO 550 I=1,IC
162 XA(I)=XB(I)
163 AF(I)=XB(I)
164 WRITE(11,7) IKNT
165 WRITE(11,2) (GB(I),I=1,IC)
166 CHIF=CSO2/(NP-IC)
167 IF(IVAR.LE.3) THEN
168 DO 560 I=1,IC
169 EAF(I,I)=SORT(CHIF*H(I,I))

```

320

330

340

350

360

370

380

390

400

500

510

520

530

540

550

560


```

1  SUBROUTINE DERIVS(XX,CHISO,G)
2  DIMENSION EXPF(50,5),XX(15),G(15),FMODG(50,5),ZE(50,5)
3  COMMON AI(15),AF(15),EAF(15,15),AIC(5),RD(5,15),RIN(5)
4  COMMON X(50),Y(50),H(50),F(50),WRES(50),BGD(50),XJ(6)
5  COMMON II,IP,IC,NP,MUL,SIG,IVAR,IRPT,ISTOP,IN
6  COMMON AT,BT,CT,SIGT
7  IF(IVAR.LE.3) GO TO 1001
8  DG 1006 J=1,MUL
9  DC 1006 I=1,NP
10 IF(X(I).LE.CT*XJ(J)) GO TO 1004
11 FMODG(I,J)=0.
12 ZE(I,J)=0.0
13 GO TO 1006
14 FMODG(I,J)=ETS(BT*(X(I)-XJ(J)))*(1.-ETS(-(X(I)-CT*XJ(J))**2
15 /(.2*.SIGT*SIGT)))
16 ZE(I,J)=1.0
17 EXPF(I,J)=ETS(-(X(I)-XJ(J))**2/(2*SIG**2))
18 GO TO 1008
19 DO 1002 J=1,MUL
20 DO 1002 I=1,NP
21 FMODG(I,J)=0.0
22 EXPF(I,J)=ETS(-(X(I)-XJ(J))**2/(2*SIG**2))
23 CHISO=0.0
24 DG 1020 I=1,NP
25 F(I)=0.0
26 DO 1010 K=1,II
27 F(I)=F(I)+XX(K)*(X(I)**(K-1))
28 IF(IVAR.LE.4) GO TO 1011
29 DO 1013 J=1,MUL
30 K=II+J
31 ATF=(X(I)-XJ(J))/SIG
32 CALL ERF(ATF,ARF)
33 F(I)=F(I)+XX(K)*(0.5-ARF)
34 DG 1014 J=1,MUL
35 L=IN+J
36 F(I)=F(I)+XX(L)*EXPF(I,J)+AIC(J)*FMODG(I,J)
37 GO TO 1016
38 DO 1015 J=1,MUL
39 L=II+J
40 F(I)=F(I)+XX(L)*EXPF(I,J)+AIC(J)*FMODG(I,J)
41 WRES(I)=W(I)*(F(I)-Y(I))
42 CHISO=CHISO+W(I)*(F(I)-Y(I))**2
43 DG 1025 K=1,II
44 G(K)=0.0
45 DG 1025 I=1,NP
46 G(K)=G(K)+2*WRES(I)*(X(I)**(K-1))
47 IF(IVAR.LE.4) GO TO 1026
48 DC 1028 J=1,MUL
49 L=II+J
50 G(L)=0.0
51 DC 1028 I=1,NP
52 ATF=(X(I)-XJ(J))/SIG
53 CALL ERF(ATF,ARF)
54 G(L)=G(L)+WRES(I)*(1.0-2.*ARF)
55 DC 1029 J=1,MUL

```

```

56 L=IN+J
57 G(L)=0.0
58 DC 1029 I=1,NP
59 G(L)=G(L)+2*WRES(I)*EXPF(I,J)
60 GO TO 1031
61 1026 DO 1030 J=1,MUL
62 L=II+J
63 G(L)=0.0
64 DC 1030 I=1,NP
65 G(L)=G(L)+2*WRES(I)*EXPF(I,J)
66 1031 IF(IVAR-3) 1035,1035,1060
67 1035 IF(IVAR-2) 1050,1040,1040
68 1040 DO 1045 J=1,MUL
69 L=II+J
70 K=IP+J
71 G(K)=0.0
72 DO 1045 I=1,NP
73 G(K)=G(K)+2*WRES(I)*XX(L)*EXPF(I,J)*((X(I)-X(J(J)))/SIG**2)
74 IF(IVAR.NE.3) GO TO 1050
75 G(IC)=0.0
76 DO 1047 I=1,NP
77 DO 1047 J=1,MUL
78 L=II+J
79 1047 G(IC)=G(IC)+2*WRES(I)*XX(L)*EXPF(I,J)*((X(I)-X(J(J)))*2/SIG**3)
80 GO TO 100
81 1060 DO 1065 J=1,MUL
82 IM=II+J
83 L=IN+J
84 K=IP+J
85 G(K)=0.0
86 DO 1065 I=1,NP
87 G(K)=G(K)+2*WRES(I)*XX(L)*EXPF(I,J)*((X(I)-X(J(J)))/SIG**2)+
88 &AIC(J)*ZE(I,J)*((-BT)*FMODG(I,J)+CT*((X(I)-CT*X(J(J)))/(SIG**2))*
89 &(FMODG(I,J)-ETS*(BT*(X(I)-X(J(J))))))
90 IF(IVAR.EQ.5)G(K)=G(K)+2*WRES(I)*EXPF(I,J)*XX(IM)/SIG/2.506628274
91 1065 CCNTINUE
92 DO 1075 J=1,MUL
93 M=IP+MUL+J
94 G(M)=0.0
95 DO 1075 I=1,NP
96 G(M)=G(M)+2*WRES(I)*FMODG(I,J)
97 G(IC-3)=0.0
98 DO 1077 I=1,NP
99 DO 1077 J=1,MUL
100 G(IC-3)=G(IC-3)+2*WRES(I)*AIC(J)*((X(I)-X(J(J)))*FMODG(I,J)
101 G(IC-2)=0.0
102 DO 1082 I=1,NP
103 DO 1082 J=1,MUL
104 G(IC-2)=G(IC-2)+2*WRES(I)*AIC(J)*((1./SIGT**2)*((X(I)-CT*X(J(J)))*
105 &(FMODG(I,J)-ETS*(BT*(X(I)-X(J(J)))))*ZE(I,J)*XJ(J)
106 G(IC-1)=0.0
107 DO 1085 I=1,NP
108 DO 1085 J=1,MUL
109 G(IC-1)=G(IC-1)+2*WRES(I)*AIC(J)*((X(I)-CT*X(J(J)))*2)*
110 &(1./SIGT**3)*((FMODG(I,J)-ETS*(BT*(X(I)-X(J(J)))))*ZE(I,J)
111 G(IC)=0.0
112 DO 1087 I=1,NP

```

```

113 DO 1087 J=1, MUL
114 L=IN+J
115 IM=II+J
116 G(IC)=G(IC)+2*WRES(I)*XX(L)*EXP(I,J)*((X(I)-XJ(J))**2/SIG**3)
117 IF(IVAR.EQ.5)G(IC)=G(IC)+2*WRES(I)*EXP(I,J)*XX(IH)/SIG**2/2.506628274
118 6*(X(I)-XJ(J))
119 1087 CONTINUE
120 100 RETURN
121 END
    
```

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE	NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
AF	178	//		REAL	15	IRPT	1215B	//		INTEGER	75
AI	08	//		REAL	15	ISTOP	1216B	//		INTEGER	5
AIC	377B	//		REAL	5	IVAR	1214B	//		INTEGER	
ARF	3001B	//		REAL		J	2766B			INTEGER	
AT	1220B	//		REAL		K	2775B			INTEGER	
ATF	3000B	//		REAL		L	3003B			INTEGER	
BGD	1116B	//		REAL	50	M	3025B			INTEGER	
BT	1221B	//		REAL		MUL	1212B	//		INTEGER	
CHI SQ	2	DUMMY-ARG		REAL		NP	1211B	//		INTEGER	
CT	1222B	//		REAL		RD	404B	//		REAL	
EAF	36B	//		REAL	225	RIN	517B	//		REAL	5
EXP	1410B	//		REAL	250	SIG	1213B	//		REAL	
F	752B	//		REAL	50	SIGT	1223B	//		REAL	
FMDG	2002B	//		REAL	250	W	670B	//		REAL	
G	3	DUMMY-ARG		REAL	15	WRES	1034B	//		REAL	50
I	2770B	//		INTEGER		X	524B	//		REAL	50
IC	1210B	//		INTEGER		XJ	1200B	//		REAL	6
II	1206B	//		INTEGER		XX	1	DUMMY-ARG		REAL	15
IM	3022B	//		INTEGER		Y	606B	//		REAL	50
IN	1217B	//		INTEGER		ZE	2374B	//		REAL	250
IP	1207B	//		INTEGER							

NAME	TYPE	ARGS	CLASS
EKF	REAL	2	SUBROUTINE
ETS		1	FUNCTION

STATEMENT LABELS	ADDRESS	BLOCK	PROPERTIES	DEF	TYPE	SIZE	NAME	ADDRESS	BLOCK	PROPERTIES	DEF
100	1361B			120	1013	INACTIVE		1031	547B		66
1001	1118			19	1014	INACTIVE		1035	INACTIVE		67
1002	INACTIVE		DO-TERM	22	1015	INACTIVE		1040	INACTIVE		68
1003	#NO REFS*			8	1016	314B		1045	INACTIVE	DO-TERM	73
1004	40B			14	1020	INACTIVE		1047	INACTIVE	DO-TERM	79
1005	#NO REFS*			11	1025	INACTIVE		1050	700B		80
1006	66B			17	1026	506B		1060	701B		81
1008	151B		DO-TERM	23	1028	INACTIVE		1065	INACTIVE	DO-TERM	91
1010	INACTIVE		DO-TERM	27	1029	INACTIVE		1075	INACTIVE	DO-TERM	96
1011	266B			38	1030	INACTIVE		1077	INACTIVE	DO-TERM	100

```

1 SUBROUTINE CUBINT(X1,X2,GAMMA,G1,G2,A)
2 Z=3.0*((X1-X2)/GAMMA)+G2+G1
3 W=Z#Z-G2*G1
4 IF(W.GE.0) THEN
5   W=SQRT(W)
6   A=GAMMA*(1.0-((G2+W-Z)/(G2-G1+W+W)))
7 ELSE
8   WRITE(11,10)
9   A=0.0
10  ENDIF
11  RETURN
12 10. FORMAT(1X,' W IS COMPLEX , EXECUTION ENDS...')
13  END
  
```

---VARIABLE MAP---(LO=A)

---NAME---	---ADDRESS---	---BLOCK---	---PROPERTIES---	---TYPE---	---SIZE---
A	6	DUMMY-ARG		REAL	
GAMMA	3	DUMMY-ARG		REAL	
G1	4	DUMMY-ARG		REAL	
G2	5	DUMMY-ARG		REAL	
W	66B			REAL	
X1	1	DUMMY-ARG		REAL	
X2	2	DUMMY-ARG		REAL	
Z	65B			REAL	

---PROCEDURES---(LO=A)

---NAME---	---TYPE---	---ARGS---	---CLASS---
SORT	GENERIC	1	INTRINSIC

---STATEMENT LABELS---(LO=A)

---LABEL---	---ADDRESS---	---PROPERTIES---	---DEF---
10	52B	FORMAT	12

---ENTRY POINTS---(LO=A)

---NAME---	---ADDRESS---	---ARGS---
CUBINT	5B	6

---I/O UNITS---(LO=A)

---NAME---	---PROPERTIES---
TAPE11	FMT/SEQ

```

1 SUBROUTINE RINT
2 COMMON AI(15),AF(15),EAF(15,15),AIC(5),RD(5,15),RIN(5)
3 COMMON X(50),Y(50),W(50),F(50),WRES(50),BGD(50),XJ(6)
4 COMMON II,IP,IC,NP,MUL,SIG,IVAR,IRPT,ISTOP,IN
5 COMMON AT,BT,CT,SIGT
6 DO 10 J=1,MUL
7   ARG1=BT*SIGT
8   ARG2=(CT*XJ(J)/SIGT)+BT*SIGT
9   CALL ERF(ARG1,RES1)
10  CALL ERF(ARG2,RES2)
11  RIN(J)=(AIC(J)/BT)*EXP(-BT*XJ(J))*(EXP(BT*CT*XJ(J))-1.)+
12  &SQR(2.*3.1415926)*AIC(J)*SIGT*EXP(0.5*(BT*SIGT)**2)+BT*XJ(J)*
13  &(CT-1.)*(RES1-RES2)
14  RD(J,3)=RIN(J)/AIC(J)
15  RD(J,2)=(AIC(J)/BT)*BT*(CT-1.)*EXP(BT*XJ(J))*(CT-1.)+BT*
16  &EXP(-BT*XJ(J))+BT*(CT-1)*(RIN(J)-(AIC(J)/BT)*EXP(-BT*
17  &XJ(J))*(EXP(BT*CT*XJ(J))-1.))-AIC(J)*CT*EXP(-BT*XJ(J))-0.5*(CT*
18  &XJ(J)/SIGT)**2)
19  RD(J,IC-3)=-AIC(J)/BT**2)*EXP(-BT*XJ(J))*(EXP(BT*CT*XJ(J))-1.)+
20  &(AIC(J)/BT)*EXP(-BT*XJ(J))*(XJ(J))*(CT-1.)*EXP(BT*XJ(J)*CT)+
21  &XJ(J)+(BT*(SIGT**2)+XJ(J))*(CT-1.)*(RIN(J)-(AIC(J)/BT)*EXP(-BT*
22  &XJ(J))*(EXP(BT*CT*XJ(J))-1.))+AIC(J)*(SIGT**2)*EXP(BT*XJ(J)*
23  &(CT-1.))-AIC(J)*SIGT**2)*EXP(-0.5*(CT*XJ(J)/SIGT)**2)-BT*XJ(J))
24  RD(J,IC-2)=RIN(J)*BT*XJ(J)+AIC(J)*XJ(J)*EXP(-BT*XJ(J))
25  &(1.-EXP(-0.5*(CT*XJ(J)/SIGT)**2))
26  RE(J,IC-1)=(1+(BT*SIGT)**2)*(1./SIGT)*(RIN(J)-(AIC(J)/BT)*EXP
27  &(-BT*XJ(J))*(EXP(BT*CT*XJ(J))-1.))+AIC(J)*BT*SIGT*EXP(BT*XJ(J)
28  &*(CT-1.))-AIC(J)*SIGT*(BT-(CT*XJ(J)/SIGT)**2))*EXP(-0.5*(CT*
29  &XJ(J)/SIGT)**2)-BT*XJ(J))
30  RETURN
31  END

```

--VARIABLE	MAP--(LO=A)	--ADDRESS--BLOCK--	PROPERTIES	TYPE	SIZE	NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
AF	178	//	REAL		15	ISTOP	12168	//	INTEGER		
AI	08	//	REAL		15	IVAR	12148	//	INTEGER		
AIC	3778	//	REAL		5	J	4538		INTEGER		
ARG1	4558		REAL			MUL	12128	//	INTEGER		
ARG2	4568		REAL			NP	12118	//	INTEGER		
AT	12208	//	REAL			RD	4048	//	REAL		75
BGD	11168	//	REAL		50	RES1	4578		REAL		
BT	12218	//	REAL			RES2	4608		REAL		
CT	12228	//	REAL			RIN	5178	//	REAL		5
EAF	368	//	REAL		225	SIG	12138	//	REAL		
F	7528	//	REAL		50	SIGT	12238	//	REAL		
IC	12108	//	INTEGER			W	6708	//	REAL		50
II	12068	//	INTEGER			WRES	10348	//	REAL		50
IN	12178	//	INTEGER			X	5248	//	REAL		50
IP	12078	//	INTEGER			XJ	12008	//	REAL		6
IRPT	12158	//	INTEGER			Y	6068	//	REAL		50

```

1 SUBROUTINE ERF(Z,RES)
2 ZE=ABS(Z*0.70710678)
3 DE=(0.8540765+ZE*(0.30781819+ZE*(0.063832389-ZE*
4 80.00018240507)))/(1.0+ZE*(0.65097426+ZE*(0.22948482+ZE*
5 80.034030182)))
6 TE=1.7724539+ZE*(2.0-DE)
7 QU=EXP(-ZE**2)*TE/(1.7724539*(ZE*TE+1.0))
8 C=-0.5
9 IF(Z.LT.0.0) C=0.5
10 RES=(QU-1.0)*C
11 RETURN
12 END
  
```

--VARIABLE MAP--(LO=A)

--NAME--	--ADDRESS--	--BLOCK--	--PROPERTIES--	--TYPE--	--SIZE--
C	102B			REAL	
DE	77B			REAL	
QU	101B			REAL	
RES	2	DUMMY-ARG		REAL	
TE	100B			REAL	
Z	1	DUMMY-ARG		REAL	
ZE	76B			REAL	

--PROCEDURES--(LO=A)

--NAME--	--TYPE--	--ARGS--	--CLASS--
ABS	GENERIC	1	INTRINSIC
EXP	GENERIC	1	INTRINSIC

--ENTRY POINTS--(LO=A)

--NAME--	--ADDRESS--	--ARGS--
ERF	5B	2

--STATISTICS--

PROGRAM-UNIT LENGTH 1058 = 69
 SCM STORAGE USED 61700B = 25536
 COMPILE TIME 0.192 SECONDS

```

1 FUNCTION ETS(X)
2 IF(X.LE.-675.0) THEN
3   ETS=0.0
4 ELSE
5   ETS=EXP(X)
6 ENDIF
7 RETURN
8 END

```

```

---VARIABLE MAP---(LO=A)
-NAME-----ADDRESS---BLOCK-----PROPERTIES-----TYPE-----SIZE

```

```

ETS      279      REAL
X         1      DUMMY-ARG      REAL

```

```

---PROCEDURES---(LO=A)
-NAME-----TYPE-----ARGS-----CLASS-----

```

```

EXP      GENERIC      1      INTRINSIC

```

```

---ENTRY POINTS---(LO=A)
-NAME-----ADDRESS-----ARGS-----

```

```

ETS      60      1

```

```

---STATISTICS---

```

```

PROGRAM-UNIT LENGTH      328 = 26
SCM STORAGE USED        617008 = 25536
COMPILE TIME            0.073 SECONDS
12.05.22.UCLP, AA, P04 , 1.194KLNS.

```

```

1 PROGRAM CALIBR ( INPUT,OUTPUT,CIK,TAPE5=INPUT,TAPE6=OUTPUT,
2 6TAPE11=CIK)
3 *****
4 * PROGRAM BUCAASA/CALIBR
5 * AUTHOR : DR. OZER CIFTCIOGLU, ITU (1979)
6 * REVISED AND DEVELOPED BY: LEVENT AKIN, BU (1984)
7 * *****
8 * DIMENSION PK(150),ENY(150),EENGY(150),EN(15),EF(15),ENL(15),
9 * EFL(15),EFL2(150),AREA(150),EAREA(150),EPA(150),EEF(150),ERL(150)
10 * DIMENSION RCCP(50),ACE(50),W(50),C(50),CE(10),XI(10,10),WE(50)
11 CHARACTER*7 NAM,NAM2
12 CHARACTER*10 TIME,DATE,GUN,SAAT
13 CHARACTER*50 JOB
14 LOGICAL JXST
15 GUN=DATE()
16 SAAT=TIME()
17 WRITE(6,*) 'NAME OF JOB?'
18 READ(5,75)JOB
19 FORMAT(A50)
20 WRITE(11,80) GUN,SAAT, JOB
21 FGMAT(1H1,6(' '),BUCAASA/CALIBR REV 3.1 ',2A10,6(' ')) /
22 85X, JOB: ',A50)
23 WRITE(6,*)'NP,MP,SYSER'
24 READ(5,*)NP,MP,SYSER
25 WRITE(6,*)'ENTER CALIBRATION DATA'
26 WRITE(6,*)'CHANNEL ENERGY'
27 DO 10 I=1,NP
28 READ(5,*) RCCP(I),ACE(I)
29 W(I)=1.
30 WRITE(11,3)
31 FORMAT(10X,'ENERGY CALIBRATION DATA'/17X,'CHANNEL',6X,
32 8,'ENERGY(KEV)')
33 DO 15 I=1,NP
34 WRITE(11,4) I,RCCP(I),ACE(I)
35 FORMAT(10X,I2,5X,F8.3,5X,F8.3)
36 WRITE(6,*)'LP,SYSEF,EFIN'
37 READ(5,*) LP,SYSEF,EFIN
38 IF(EFIN.EQ.1) THEN
39 WRITE(6,*)'ENERGY EFFICIENCY EFF-ERR'
40 DO 24 I=1,LP
41 READ(5,*) EN(I),EF(I),ENL(I)
42 WRITE(11,1)
43 FORMAT(//10X,'EFFICIENCY CALIBRATION DATA'/14X,'ENERGY(KEV)',
44 85X,'EFFICIENCY',10X,'EFF-ERR')
45 DO 22 I=1,LP
46 WRITE(11,2) I,EN(I),EF(I),ENL(I)
47 FORMAT(10X,I2,5X,F8.3,5X,1PE14.7,3X,1PE14.7)
48 ELSE
49 WRITE(6,*)'ENTER CALIBRATION DATA'
50 WRITE(6,*)'ENERGY EFFICIENCY'
51 DO 25 I=1,LP
52 READ(5,*) EN(I),EF(I)
53 ENL(I)=ALOG(EN(I))
54 EFL(I)=ALOG(EF(I))
55 WE(I)=1.

```

```

56 WRITE(11,5)
57 FORMAT(/,10X,'EFFICIENCY CALIBRATION DATA',14X,'ENERGY(KEV)',
58 5X,'EFFICIENCY',/)
59 DO 17 I=1,LP
60 WRITE(11,6) I,EN(I),EF(I)
61 FORMAT(10X,12,5X,F8.3,5X,1PE14.7)
62 ENDIF
63 WRITE(6,*)'NAME OF THE FIT FILE?'
64 READ(5,82)NAM
65 FORMAT(A7)
66 INQUIRE(FILE=NAM,EXIST=JXST)
67 IF(.NOT.JXST) THEN
68 WRITE(6,*)'THERE IS NO SUCH FILE !'
69 GO TO 55
70 ENDIF
71 OPEN(17,FILE=NAM,ACCESS='DIRECT',RECL=30)
72 WRITE(11,*)'DATA INPUT FROM FILE ',NAM
73 WRITE(6,*)'NAME OF THE TRANSFER FILE?'
74 READ(5,82)NAM2
75 OPEN(15,FILE=NAM2)
76 READ(17,REC=1)NX
77 MX=1
78 DO 68 I=2,NX+1
79 READ(17,REC=I)MUL,(PK(J),EPK(J),AREA(J),EAREA(J),
80 6J=MX,MX+MUL-1)
81 MX=MX+MUL
82 CALL POLIN(NP,MP,RCCP,ACE,M,C,ENGY,XI,ES,CE)
83 M=MP+1
84 IF(MP.LE.0) STOP
85 CALL POLIX(M,MX,PK,C,XI,ENGY,EENGY,ES,1)
86 DC 32 I=1,MX
87 EENGY(I)=SORT((EENGY(I)*ENGY(I)+0.01)**2+SYSEF**2+
88 6((EPK(I)/PK(I)*ENGY(I))**2)
89 IF(EFIN.EQ.1) THEN
90 CALL INTRP(EN,EF,ENL,ENGY,EFL2,EEF,EAREA,LP,MX,SYSEF)
91 GO TO 100
92 ENDIF
93 CALL POLIN(LP,1,ENL,EFL,WE,C,EFL2,XI,ES,CE)
94 DO 99 I=1,MX
95 ERL(I)=ALOG(ENGY(I))
96 CALL POLIX(2,MX,ERL,C,XI,EFL2,EEF,ES,2)
97 DO 60 I=1,MX
98 EFL2(I)=EXP(EFL2(I))
99 EEF(I)=SORT((EFL2(I)*EXP(EEF(I))+0.01)**2+SYSEF**2)
100 CONTINUE
101 WRITE(11,7)
102 WRITE(15,84) MX
103 84 FORMAT(I3)
104 7 FORMAT(/,5X,'CALIBRATION RESULTS',/,' PEAK# CHANNEL ERROR-CHN'
105 *,' ENERGY(KEV) ERROR(KEV) AREA EPROR(%) INTENSITY',
106 *,' ERROR(2)')
107 DO 78 I=1,MX
108 WRITE(11,8)I,PK(I),EPK(I),ENGY(I),EENGY(I),AREA(I),EAREA(I),
109 6AREA(I)/EFL2(I),EEF(I)
110 8 FORMAT(1X,I3,3X,F8.3,3X,F5.3,3X,F9.3,8X,F5.3,3X,E11.4,3X,F7.3,
111 63X,E11.4,3X,F7.3)
112 WRITE(15,85)PK(I),ENGY(I),AREA(I)/EFL2(I),EEF(I)

```

113 FORMAT(4E14.7)
 114 CONTINUE
 115 STOP
 116 END

--VARIABLE MAP--(L0=A)

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE	NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
ACE	4217B			REAL	50	JOB	4711B			CHAR*50	
AREA	2557B			REAL	150	JXST	4716B			LOGICAL	
C	4363B			REAL	50	LP	4725B			INTEGER	
CE	4445B			REAL	10	M	4743B			INTEGER	
EAREA	3005B			REAL	150	MP	4720B			INTEGER	
EEF	3461B			REAL	150	MUL	4737B			INTEGER	
EENGY	2007B			REAL	150	MX	4735B			INTEGER	
EF	2254B			REAL	15	NAM	4705B			CHAR*7	
EFIN	4727B			REAL		NAM2	4706B			CHAR*7	
EFL	2312B			REAL	15	NP	4717B			INTEGER	
EFL2	2331B			REAL	150	NX	4734B			INTEGER	
EN	2235B			REAL	15	PK	1333B			REAL	150
ENGY	1561B			REAL	150	RCCP	4135B			REAL	50
ENL	2273B			REAL	15	SAAT	4710B			CHAR*10	
EPK	3233B			REAL	150	SYSEF	4726B			REAL	
EKL	3707B			REAL	150	YSER	4721B			REAL	
ES	4742B			REAL		W	4301B			REAL	50
GUV	4707B			CHAR*10		WE	4623B			REAL	50
I	4722B			INTEGER		XI	4457B			REAL	100
J	4740B			INTEGER							

--PROCEDURES--(L0=A)

NAME	TYPE	ARGS	CLASS	NAME	TYPE	ARGS	CLASS
ALJG	REAL	1	INTRINSIC	POLIN		10	SUBROUTINE
DATE	CHAR*10	0	FUNCTION	POLIX		9	SUBROUTINE
EXP	GENERIC	1	INTRINSIC	SQRT		1	INTRINSIC
INTRP		10	SUBROUTINE	TIME		0	FUNCTION

--STATEMENT LABELS--(L0=A)

LABEL	ADDRESS	PROPERTIES	DEF	LABEL	ADDRESS	PROPERTIES	DEF
1	672B	FORMAT	43	15	INACTIVE	DO-TERM	34
2	704B	FORMAT	47	17	INACTIVE	DO-TERM	60
3	656B	FORMAT	31	22	INACTIVE	DO-TERM	46
4	666B	FORMAT	35	24	INACTIVE	DO-TERM	41
5	711B	FORMAT	57	25	INACTIVE	DO-TERM	55
6	722B	FORMAT	61	32	INACTIVE	DO-TERM	87
7	732B	FORMAT	104	55	271B		64
8	751B	FORMAT	110	60	INACTIVE	DO-TERM	100
10	INACTIVE	DO-TERM	29	68	INACTIVE	DO-TERM	81
				75	644B	FORMAT	19
				78	INACTIVE	DO-TERM	114
				80	646B	FORMAT	21
				82	726B	FORMAT	65
				84	730B	FORMAT	103
				85	762B	FORMAT	113
				99	INACTIVE	DO-TERM	95
				100	504B		101

```

1  SUBROUTINE POLIN(M,N,X,Y,H,A,YC,D,S,EC)
2  DIMENSION X(100),Y(100),YC(100),W(100),XC(20),YX(10),A(10),B(10)
3  DIMENSION C(10,10),D(10,10),EC(100)
4  MPI=M+1
5  M2=M+M
6  DO 20 K=1,M2
7  XC(K)=0.0
8  DO 15 I=1,N
9  XC(K)=XC(K)+(W(I)*(X(I)**K))
10 CONTINUE
11 YX1=0.0
12 WI=0.0
13 DO 22 I=1,N
14 WI=WI+W(I)
15 YX1=YX1+W(I)*Y(I)
16 DO 30 K=1,M
17 YX(K)=0.0
18 DO 25 I=1,N
19 YX(K)=YX(K)+(W(I)*(Y(I)*(X(I)**K)))
20 CONTINUE
21 DO 40 I=1,MPI
22 DO 35 J=1,MPI
23 IPJM2=I+J-2
24 IF(IPJM2.EQ.0) THEN
25 C(I,J)=WI
26 ELSE
27 C(I,J)=XC(IPJM2)
28 ENDIF
29 CONTINUE
30 CONTINUE
31 B(I)=YX1
32 DO 45 I=2,MPI
33 B(I)=YX(I-1)
34 CALL MATIN(C,D,MPI)
35 IF(MPI.LE.0) THEN
36 M=0
37 RETURN
38 ENDIF
39 DO 55 I=1,MPI
40 A(I)=0.0
41 DO 54 J=1,MPI
42 A(I)=A(I)+D(I,J)*B(J)
43 CONTINUE
44 DO 60 I=1,N
45 YC(I)=0.0
46 DO 60 J=1,MPI
47 YC(I)=YC(I)+(A(J)*(X(I)**(J-1)))
48 DI=N-MPI
49 S=0
50 SDEV=0.0
51 DO 70 I=1,N
52 DEV=Y(I)-YC(I)
53 S=S+W(I)*(DEV**2)
54 SDEV=SDEV+DEV
55 S=S/01

```



```

1 SUBROUTINE INTRP(XX,YY,YYE,X,Y,YE,EA,N,M,SYS)
2 DIMENSION XX(N),YY(N),YYE(N),X(M),Y(M),YE(M),EA(M)
3 DO 10 J=1,M
4 DG 10 I=1,N-1
5 IF(X(J).GT.XX(I).AND.X(J).LE.XX(I+1))THEN
6 Y(J)=EXP((ALOG(X(J))*ALOG(YY(I))/YY(I+1))+
7     ALOG(XX(I))*ALOG(YY(I+1))-ALOG(XX(I+1))*ALOG(YY(I))))/
8     ALOG(XX(I)/XX(I+1))
9 YE(J)=EXP((ALOG(X(J))*ALOG(YYE(I))/YYE(I+1))+
10    ALOG(XX(I))*ALOG(YYE(I+1))-ALOG(XX(I+1))*ALOG(YYE(I))))/
11    ALOG(XX(I)/XX(I+1))
12 ENDDIF
13 YE(J)=SORT(YE(J)**2+EA(J)**2+SYS**2)
14 CONTINUE
15 RETURN
16 END

```

--VARIABLE MAP--(LO=A)

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE	NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
EA	7	DUMMY-ARG		REAL	ADJ-ARY	X	4	DUMMY-ARG		REAL	ADJ-ARY
I	2358			INTEGER		XX	1	DUMMY-ARG		REAL	ADJ-ARY
J	2338			INTEGER		Y	5	DUMMY-ARG		REAL	ADJ-ARY
M	9	DUMMY-ARG		INTEGER		YE	6	DUMMY-ARG		REAL	ADJ-ARY
N	8	DUMMY-ARG		INTEGER		YY	2	DUMMY-ARG		REAL	ADJ-ARY
SYS	10	DUMMY-ARG		REAL		YYE	3	DUMMY-ARG		REAL	ADJ-ARY

--PROCEDURES--(LO=A)

NAME	TYPE	ARGS	CLASS
ALDG	REAL	1	INTRINSIC
EXP	GENERIC	1	INTRINSIC
SORT	GENERIC	1	INTRINSIC

--STATEMENT LABELS--(LO=A)

-LABEL-ADDRESS-----PROPERTIES-----DEF

10 INACTIVE DO-TERM 14

--ENTRY POINTS--(LO=A)

-NAME-ADDRESS-ARGS----

INTRP 58 10

00=-LUNG/-UT,ARG=-COMMON/-FIXED,CS= USER/-ID/-PMD/-ST,PL=5000
FIN5,I=CC,L=LICAL,B=CALIBR.

```

1  SUBROUTINE MATIN(A,B,N)
2  DIMENSION A(10,10),S(10,10)
3  DATA EPS/1.E-10/
4  DO 6 I=1,N
5  DO 6 J=1,N
6  B(I,J)=0.0
7  DO 7 I=1,N
8  B(I,I)=1.0
9  DEL=1.
10 DO 45 K=1,N
11 IF (K.GE.N) GO TO 30
12 IMAX=K
13 AMAX=ABS(A(K,K))
14 KPI=K+1
15 DO 20 I=KPI,N
16 IF(AMAX.LT.ABS(A(I,K))) THEN
17   IMAX=I
18   AMAX=ABS(A(I,K))
19 ENDIF
20 CONTINUE
21 IF(IMAX.EQ.K) GO TO 30
22 DO 29 J=1,N
23 ATMP=A(IMAX,J)
24 A(IMAX,J)=A(K,J)
25 A(K,J)=ATMP
26 BTMP=B(IMAX,J)
27 B(IMAX,J)=B(K,J)
28 B(K,J)=BTMP
29 DEL=-DEL
30 CONTINUE
31 IF(ABS(A(K,K)).LE.EPS) GO TO 93
32 DEL=A(K,K)*DEL
33 DIV=A(K,K)
34 DO 38 J=1,N
35 A(K,J)=A(K,J)/DIV
36 B(K,J)=B(K,J)/DIV
37 DO 43 I=1,N
38 AMULT=A(I,K)
39 IF(I.EQ.K) GO TO 43
40 DO 42 J=1,N
41 A(I,J)=A(I,J)-AMULT*A(K,J)
42 B(I,J)=B(I,J)-AMULT*B(K,J)
43 CONTINUE
44 CONTINUE
45 RETURN
46 WRITE(6,*) 'SINGULAR MATRIX EXECUTION ENDS'
47 N=0
48 RETURN
49 END

```

COMMON7=FIXED,CS=USER/=-FIXED,DB=-1B/-SB/-SL/ ER/-ID/-PMD/-ST,PL=5000
 FTN5,I=CC,L=LCAL,B=CALIBR.

```

1  SUBROUTINE POLIX(M,K,XD,C,XI,YD,YE,S,IPIS)
2  DIMENSION XD(150),YD(150),C(10),XI(10,10),YE(150),G(20)
3  MM=M
4  IF(IPIS.EQ.2)C(1)=EXP(C(1))
5  DO 10 I=1,K
6  YD(I)=0.0
7  DO 10 J=1,MM
8  YD(I)=YD(I)+C(J)*(XD(I)**(J-1))
9  YE(I)=0.0
10 DO 20 J=1,MM
11 G(J)=XD(I)**(J-1)
12 DO 30 L=1,MM
13 DO 30 N=1,MM
14 YE(I)=YE(I)+G(L)*XI(L,N)*G(N)
15 DO 40 I=1,K
16 YE(I)=SQRT(YE(I)*S)*100/YD(I)
17 RETURN
18 END
19

```

--VARIABLE MAP--(LO=A)

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE	NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
C	4	DUMMY-ARG		REAL	10	MM	224B			INTEGER	
G	2008			REAL	20	N	235B			INTEGER	
I	225B			INTEGER		S	8			REAL	150
IPIS	9	DUMMY-ARG		INTEGER		XD	3		DUMMY-ARG	REAL	100
J	227B			INTEGER		XI	5		DUMMY-ARG	REAL	150
K	2	DUMMY-ARG		INTEGER		YD	6		DUMMY-ARG	REAL	150
L	233B			INTEGER		YE	7		DUMMY-ARG	REAL	150
N	1	DUMMY-ARG		INTEGER							

--PROCEDURES--(LO=A)

NAME	TYPE	ARGS	CLASS
EXP	GENERIC	1	INTRINSIC
SORT	GENERIC	1	INTRINSIC

--STATEMENT LABELS--(LO=A)

LABEL	ADDRESS	PROPERTIES	DEF
10	INACTIVE	DO-TERM	8
20	INACTIVE	DO-TERM	12
30	INACTIVE	DO-TERM	15
40	INACTIVE	DO-TERM	17

FTND,I=IDEN,L=LID,B=NUCLIDE

```

1  PROGRAM NUCLIDE(INPUT,OUTPUT,CIK,TAPE6=OUTPUT,TAPE5=INPUT,
2  TAPE11=CIK)
3  *****
4  * PROGRAM BUCASA/NUCLIDE (SAMPO80 PART III) *****
5  * AUTHOR : KOSKELO ET AL. (1982) *
6  * REVISED AND ADAPTED BY : LEVENT AKIN, 3U (1984) *
7  *****
8  CHARACTER*7 INF,LIBF
9  CHARACTER*50 JOB
10 CHARACTER*10 TIME,DATE,GUN,SAAT
11 LOGICAL JXST
12 COMMON/TIMES/TCO,TWA,TEX,TLIVE,ETOL
13 GUN=DATE(1)
14 SAAT=TIME(1)
15 WRITE(6,*)'NAME OF JOB '
16 READ(5,10)JOB
17 WRITE(11,30) GUN,SAAT,JOB
18 WRITE(6,*) 'TCO TEX TWA TLIVE ETOL '
19 READ(5,*)TCO,TEX,TWA,TLIVE,ETOL
20 IF(TCO.LE.0.0) TCO=1.0
21 IF(TEX.LE.0.0) TEX=1.0
22 IF(TWA.LE.0.0) TWA=1.0
23 WRITE(11,40)TCO,TWA,TEX,TLIVE,ETOL
24 100 WRITE(6,*)'NAME OF THE INPUT FILE?'
25 READ(5,10)INF
26 INQUIRE(FILE=INF,EXIST=JXST)
27 IF(.NOT.JXST) THEN
28 WRITE(6,*)'NO SUCH FILE'
29 GO TO 100
30 ENDF
31 OPEN(14,FILE=INF,RECL=80)
32 WRITE(6,*)'NAME OF THE LIBRARY FILE?'
33 READ(5,10)LIBF
34 INQUIRE(FILE=LIBF,EXIST=JXST)
35 IF(.NOT.JXST) THEN
36 WRITE(6,*)'NO SUCH FILE'
37 GO TO 200
38 ENDF
39 OPEN(2,FILE=LIBF)
40 CALL IDENT
41 STDP
42 10 FORMAT(A7)
43 20 FORMAT(A50)
44 30 FORMAT(IH1,1X,10(' '),BUCAASA/NUCLIDE REV 1.0,'ZAL0,
45 &10(' ')/'JOB : ',A50/)
46 40 FORMAT(1X,COUNT, TIME= ',F11.2,'(MIN)', ' WAIT. TIME= ',
47 &F11.2,'(MIN)', ' EXSPSR. TIME= ',F11.2,' (MIN)',
48 &'LIVE C. TIME= ',F11.2,'(SEC)'/1X,'EN. TOL= ',F4.2,'(KEY)')
49 END

```

FTNS,I=IDEM,L=LID,B=NUCLIDE. COMMON/FIXED,UCS=USER7-FIXED,UB=-1B/-3B/-SL/ ER/-ID/-PM0/-ST,PL=5000

```

1  SUBROUTINE CORR(JB,JA,AL2,NUMF,JG,ICHEC)
2  CHARACTER*8 COL,ITUNN
3  COMMON/FITIN/FITCH(100),ENERG(100),EFFSUM(100),EFER(100)
4  COMMON/COR/B(80,30),ROH(30),X(30),IL(30),CONF(30),
5  EHALF(30),ACOL5(30),XINT(30),XCONF(30),XER(30),
6  EACOL2(30),ACOL3(30)
7  COMMON/TIMES/TCO,TWA,TEX,TLIVE,ETOL
8  COMMON/INTF/A(80,30),JFL(30),KFL(30)
9  COMMON COL(30),ITUNN(30)
10  DO 183 K=1,JB
11  KK=KFL(K)
12  IF(JA,NE,1)GO TO 1801
13  JJ=JFL(1)
14  IF(EFER(JJ),GT,50.0,DR.EFFSUM(JJ),LE,0.0)GO TO 176
15  ERROR=EFER(JJ)
16  GC TO 1198
17  1801 ERROR=100.*SQRT(B(K,K))/X(K)
18  CCOR=(1.-EXP(-AL2*TCO/HALF(KK)))/(AL2*TCO/HALF(KK))
19  TCHECK=365.*24.*60.
20  IF(HALF(KK),GT,TCHECK) CCOR=1.
21  WCOR=EXP(-AL2*TWA/HALF(KK))
22  WTEST=AL2*TWA/HALF(KK)
23  IF(WTEST,GT,0.0001) GO TO 591
24  KERR=1.
25  WCOR=0.
26  DO 6311 IND=1,5
27  KERR=KERR*FLOAT(IND)
28  WCOR=WCOR+(-WTEST)**IND/KERR
29  6311 CONTINUE
30  WCOR=1.-WCOR
31  591 CONTINUE
32  ECOR=1.-EXP(-AL2*TEX/HALF(KK))
33  ETEST=AL2*TEX/HALF(KK)
34  IF(ETEST,GT,0.0001) GO TO 6120
35  KERR=1.
36  ECOR=0.
37  DO 6119 IND=1,5
38  KERR=KERR*FLOAT(IND)
39  ECOR=ECOR-(-ETEST)**IND/KERR
40  6119 CONTINUE
41  6120 IF(JA,NE,1)GO TO 293
42  XE=EFFSUM(JJ)/(A(JJ,KK)*TLIVE*3.7E-02*WCOR*CCOR)
43  ASAT=XE/ECOR
44  IF(JB,EQ,1)GO TO 210
45  WRITE(11,1116) COL(KK)
46  GO TO 209
47  293 XE=X(KK)/(WCOR*CCOR*TLIVE*3.7E-02)
48  ASAT=XE/ECOR
49  210 WRITE(11,1013)COL(KK)
50  209 DO 1181 I=1,NUMF
51  IFA(I,KK),LT,1.E-36)GO TO 1181
52  WRITE(11,1014)I,FITCH(I),ENERG(I)
53  1181 CONTINUE
54  CALL ORDER(6,JG,ACOL2(KK),ACOL3,XE,XINT,CONF(KK),XCONF,
55  ERROR,XER,ASAT,ACOL5,COL(KK),ITUNN)

```

56 CONTINUE
 57 RETURN
 58 176 ICHEC=1
 59 RETURN

1013 FORMAT('THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE',2X,
 6A8,/1H ,5X,6HNUMBER,5X,7HCHANNEL,5X,6HENERGY)

1014 FCRMAT(1H ,6X,14,6X,F7.2,4X,F7.2)

1116 FCRMAT('THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE',2X,6A8,
 1' ** CHECK **',/1H ,5X,6HNUMBER,5X,7HCHANNEL,5X,6HENERGY)
 END

--VARIABLE MAP--(L0=A)

NAME	ADDRESS	BLOCK	TYPE	SIZE	NAME	ADDRESS	BLOCK	TYPE	SIZE
A			OB /INTF/		JA	2	DUMMY-ARG		
ACOL2	51568		/COR/	2400	JB	1	DUMMY-ARG		
ACOL3	52148		/COR/	30	JFL	45408	/INTF/		
ACOL5	47668		/COR/	30	JG	5	DUMMY-ARG		30
AL2	3		DUMMY-ARG		JJ	4408			
ASAT	4558				K	4358			
B			OB /COR/		KERR	4468			
CCOR	4428			2400	KFL	45768	/INTF/		
CUL			OB //		KK	4378			
CONF	46728		/COR/	30	NUMF	4	DUMMY-ARG		30
ECOR	4518			30	ROW	45408	/COR/		
EFER	4548		/FITIN/	100	TCHECK	4438			30
EFFSUM	3108		/FITIN/	100	TCO	OB	/TIMES/		
ENERG	1448		/FITIN/	100	TEX	28	/TIMES/		
ERROR	4418		/FITIN/	100	TLIVE	38	/TIMES/		
ETEST	4528				TWA	18	/TIMES/		
ETOL	48		/TIMES/		WGOR	4448			
FITCH	OB		/FITIN/		WTEST	4458			
HALF	47308		/COR/	100	X	45768	/COR/		30
I	4568			30	XCONF	50628	/COR/		30
ICHEC	6		DUMMY-ARG		XE	4548			30
IL	46348		/COR/	30	XER	51208	/COR/		30
IND	4478				XINT	50248	/COR/		30
ITUNN	308		//	30					

--PROCEDURES--(L0=A)

NAME	TYPE	ARGS	CLASS
EXP	GENERIC	1	INTRINSIC
FLOAT	REAL	1	INTRINSIC
ORDER		14	SUBROUTINE
SQRT	GENERIC	1	INTRINSIC

UC=-LUNG/-OT,ARG=-COMMON/-FIXED,CS= USER/-FIXED,UB=-TB/-SB/-SL/ ER/-ID/-PMD/-ST,PL=5000
FTN5,I=IDEN,L=LID,B=NUCLIDE.

```

1 SUBROUTINE GLSQ(X,IL,N,M,ALPHA,E1,E2,A)
2 DIMENSION A(80,30)
3 DIMENSION X(30),IL(30)
4 MM=M+1
5 LL=1
6 DO 60 J=1,MM
7   IL(J)=0
8   I=1
9   DC 3 K=1,MM
10  II=I+1
11  DC 4 J=II,N
12  IF(ABS(A(J,K))-E1) 4,4,*6
13  T1=SORT((A(J,K))*2+(A(I,K))*#2)
14  S=A(J,K)/T1
15  C=A(I,K)/T1
16  DO 5 L=K,MM
17  T2=C*A(I,L)+S*A(J,L)
18  A(J,L)=-S*A(I,L)+C*A(J,L)
19  A(I,L)=T2
20  LL=LL+1
21 CONTINUE
22 IF (ABS (A(I,K))-E2)3,3,8
23 IL(K)=I
24 I=I+1
25 CONTINUE
26 X(MM)=-1.0
27 II=M
28 DO 35 I=1,M
29 X(I)=0.
30 DO 30 J=1,M
31 IF (IL(II))30,30,31
32 S=0.
33 LL=II+1
34 I=IL(II)
35 DO 32 K=LL,MM
36 S=S+A(I,K)*X(K)
37 X(II)=-S/A(I,II)
38 II=II-1
39 IF (IL(MM))50,51,50
40 ALPHA=0.
41 GO TO 52
42 I=IL(MM)
43 ALPHA=A(I,MM)
44 RETURN
45 END

```

VARIABLE	MAP	LO	HA	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
A	8	DUMMY-ARG		I	3318		INTEGER	
ALPHA	5	DUMMY-ARG		II	3348		INTEGER	
C	3408			IL	2	DUMMY-ARG	INTEGER	30
E1	6	DUMMY-ARG		J	3278		INTEGER	
E2	7	DUMMY-ARG		K	3328		INTEGER	

```

1 SUBROUTINE IDENT
2 CHARACTER*8 COL,ISOR,BLNK,ITUNN
3 COMMON/FITIN/FITCH(100),ENERG(100),EFFSUM(100),EFER(100)
4 COMMON/LIBR/THAR,APRD,ANEU,CRO,THR,EREF(30),GREF(30)
5 COMMON/LIB2/ISOR
6 COMMON/COR/B(80,30),ROW(30),X(30),YL(30),XCONF(30),
7 8HALF(30),ACOL5(30),XINT(30),XCONF(30),XER(30),
8 8ACOL2(30),ACOL3(30)
9 COMMON/TIMES/TCO,TWA,TEX,TLIVE,ETOL
10 COMMON/INTF/A(80,30),JFL(30),KFL(30)
11 COMMON COL(30),ITUNN(30)
12 READ(14,101)NUMF
13 FFORMAT(13)
14 IF(NUMF.LE.0) THEN
15 WRITE(6,*)'NO PEAKS ... CASE TERMINATED.'
16 STOP
17 ENDIF
18 DO 1000 I=1,NUMF
19 READ(14,200) FITCH(I),ENERG(I),EFFSUM(I),EFER(I)
20 FFORMAT((4E14,7))
21 1000 CONTINUE
22 WRITE(11,1015)
23 1015 FFORMAT(,
24 15X,'PEAK NO. CHANNEL ENERGY INTENS. PC-',
25 2'ERROR'/)
26 WRITE(11,1016)(I,FITCH(I),ENERG(I),EFFSUM(I),EFER(I),I
27 X=1,NUMF)
28 1016 FFORMAT(1H,6X,I7,ZF12.4,1E12.5,F12.4)
29 IF(ETOL.EQ.0.)ETOL=2.0
30 DO 10 J=1,30
31 DG 6 J=1,80
32 A(J,I)=0.
33 B(J,I)=0.
34 8 CONTINUE
35 CNF(I)=1.
36 ACOL2(I)=0.
37 ACOL3(I)=0.
38 10 CONTINUE
39 AL2=ALOG(2.)
40 DT=TCO+TWA
41 C
42 C START SEARCHING THE LIBRARY
43 C
44 JMAT=0
45 IP=0
46 9 CONTINUE
47 CALL LIBRAR(IP,LINE,BLNK,NR1,NOISO,LINES)
48 IP=1
49 IF(ISOR.EQ.BLNK) GO TO 70
50 C
51 C SEARCH FOR MATCHES BETWEEN LIBRARY AND SPECTRUM.
52 C
53 IRON=0
54 JA=1
55 CALL MATRIX(LINE,NUMF,ETOL,JMAT,DT,BLNK)

```

```

56 GO TO 9
57 JG=0
58 WRITE(11,7070) NRI,NOISO,LINES
59 FORMAT(1X,'/ LIBRARY NUMBER',I3,',',I4,' NUCLIDES',I4,' GAMMA
60 LINES')
61 WRITE(11,2001)
62 IF(JMAT.LE.0) GO TO 220
63
64 C
65 C
66 C
67 DETERMINE THE UNIDENTIFIED PEAKS
68
69 DO 110 J=1,NUMF
70 DO 100 K=1,JMAT
71 IF(A(J,K).GT.1.E-36)GO TO 110
72 CONTINUE
73 CALL ORDER(I,IR0W,FLOAT(J),ROW,DUM,DUM,DUM,DUM,DUM,DUM,DUM,
74 DUM,DUM,DUM1,DUM1)
75 CONTINUE
76 IF(JMAT.LE.0)GO TO 220
77 ICHEC=0
78 CALL INTRE(NUMF,JMAT,JB,JA)
79 IF(JB-1)187,175,151
80 C
81 C
82 C
83 SOLVE FOR ISOTOPES. LEAST SQUARES SOLUTION
84
85 IF(JA.E0.1) GO TO 198
86 DO 156 I=1,JA
87 JJ=JFL(I)
88 DO 155 K=1,JB
89 KK=KFL(K)
90 B(I,K)=100.*A(I,J,K)/(EFER(JJ)*EFFSUM(JJ))
91 B(I,K)=AMAX1(B(I,K),1.0E-38)
92 B(I,JB+1)=100./EFER(JJ)
93 CONTINUE
94 CONTINUE
95 E1=1.E-38
96 E2=1.E-38
97 CALL GLSQ(X,IL,JA,JB,ALPHA,E1,E2,B)
98 CALL DJAG(JB,B)
99 C
100 C
101 C
102 CHECK FOR NEGATIVE INTENSITIES
103
104 XPREV=1.E+06
105 I=1
106 IF(X(I).LT.0.)GO TO 177
107 IF(I.GE.JB)GO TO 300
108 I=I+1
109 GO TO 173
110 IF(X(I).LT.XPREV)GO TO 178
111 GC TO 174
112 XPREV=X(I)
113 ICHEC=I
114 GC TO 174
115
116 C
117 C
118 C
119 CHECK FOR LARGE ERRORS
120
121 DO 181 I=1,JB
122 EC=1./SORT(B(I,I))

```

```

113 IF(BC.LE.1.E-30.OR.X(I).LE.1.E-30)GO TO 6000
114 ERROR=100.*SORT(B(I,I))/X(I)
115 IF(ERROR.GT.50.)GO TO 182
116 CONTINUE
117 CALL CORR(JB,JA,AL2,NUMF,JG,ICHEC)
118 GO TO 184
119 CONTINUE
120 ICHEC=I
121 IF(ICHEC.EQ.0)GO TO 180
122 C
123 C CHECK FOR NEW UNIDENTIFIED PEAKS
124 C
125 M1=KFL(ICHEC)
126 DO 302 JJ=1,NUMF
127 IF(A(JJ,M1).LT.1.E-36)GO TO 302
128 DO 304 I=1,JMAT
129 IF(I.EQ.M1)GO TO 304
130 IF(A(JJ,I).GT.1.E-36)GO TO 302
131 CONTINUE
132 CALL ORDER(I,IROW,FLOAT(JJ),ROW,DUM,DUM,DUM,DUM,
133 1,DUM,DUM,DUM,DUM,DUM1,DUM1)
134 CONTINUE
135 C
136 C REMOVE THE DISCARDED ISOTOPE FROM THE WORKING MATRIX
137 C
138 DO 311 J=M1,JMAT
139 DO 310 I=1,NUMF
140 A(I,J)=A(I,J+1)
141 CONTINUE
142 COL(J)=COL(J+1)
143 CONF(J)=CONF(J+1)
144 ACOL2(J)=ACOL2(J+1)
145 HALF(J)=HALF(J+1)
146 CONTINUE
147 JMAT=JMAT-1
148 GO TO 75
149 C
150 C SOLVE FOR A SINGLE ISOTOPE
151 C
152 IF(JA.GT.1)GO TO 152
153 CALL CORR(JB,JA,AL2,NUMF,JG,ICHEC)
154 IF(ICHEC.NE.0)GO TO 300
155 DO 186 I=1,JA
156 JJ=JEL(I)
157 DO 185 K=1,JB
158 KK=KFL(K)
159 A(JJ,KK)=0.
160 CONTINUE
161 CONTINUE
162 IF(JG.LT.JMAT)GO TO 75
163 CONTINUE
164 WRITE(11,1003)
165 WRITE(11,1004)(I,ITUNN(I),XCONF(I),XINT(I),XER(I),ACO
166 XL5(I),I=1,JG)
167 SUM=0.
168 DO 1191 I=1,JG
169 SUM=SUM+XINT(I)

```



```

1  SUBROUTINE INTRF(NUMF, JMAT, JB, JA)
2  COMMON/INTF/A(80,30), JFL(30), KFL(30)
3  K=1
4  JA=0
5  JB=0
6  DO 115 J=1, NUMF
7  IF(A(J,K).LT.1.E-36) GO TO 115
8  JA=JA+1
9  IF(JA.EQ.1) JB=JB+1
10 JFL(JA)=J
11 KEL(JB)=K
12 CONTINUE
13 IF(JB.GE.1) GO TO 117
14 IF(K.GE. JMAT) RETURN
15 K=K+1
16 GO TO 113
17 K1=K
18 K1=K1+1
19 JCH=JA
20 IF(K1.GT. JMAT) RETURN
21 DO 120 JC=1, JA
22 JJ=JFL(JC)
23 IF(A(JJ,K1).LT.1.E-36) GO TO 120
24 DO 122 I=1, JB
25 IF(KEL(I).EQ.K1) GO TO 118
26 CONTINUE
27 GO TO 125
28 CONTINUE
29 GO TO 118
30 JB=JB+1
31 KFL(JB)=K1
32 DO 135 J=1, NUMF
33 IF(A(J,K1).LT.1.E-36) GO TO 135
34 DO 130 I=1, JA
35 IF(JFL(I).EQ.J) GO TO 135
36 CONTINUE
37 JA=JA+1
38 JFL(JA)=J
39 CONTINUE
40 IF(JA.GT. JCH) GO TO 117
41 GO TO 118
42 END

```

---VARIABLE MAP---(LO=A)		---PROPERTIES---		---TYPE---		---SIZE---	
NAME	ADDRESS	BLOCK	ADDRESS	BLOCK	PROPERTY	TYPE	SIZE
A	0B		4540B		/INTF/		
J	221B		220B			INTEGER	30
J	212B		2		DUMMY-ARG	INTEGER	
JA	4		211B			INTEGER	
JB	3		4576B		/INTF/	INTEGER	30
JC	216B		214B			INTEGER	
JCH	215B		1		DUMMY-ARG	INTEGER	
JFL			4540B		/INTF/	INTEGER	
JJ			220B			INTEGER	
JMAT			2		DUMMY-ARG	INTEGER	
K			211B			INTEGER	
KFL			4576B		/INTF/	INTEGER	
K1			214B			INTEGER	
NUMF			1		DUMMY-ARG	INTEGER	
REAL			2400			REAL	
INTEGER						INTEGER	
INTEGER						INTEGER	
INTEGER						INTEGER	
INTEGER						INTEGER	
INTEGER						INTEGER	

```

1  SUBROUTINE LIBRAR(IP,NGA,BLNK,NRI,NOISO,LINES)
2  COMMON/LIBR/THH,APR,ANE,CRO,THR,ENE(30),PCE(30)
3  COMMON/LIB2/ISO
4  CHARACTER*1 IHA
5  CHARACTER*8 ISO,BLNK,JUNK
6  IF(IP.GT.0) GO TO 890
7  NOISO=0
8  LINES=0
9  IF(NRI.EQ.0)NRI=1
10 READ(2,6000) UNK,BLNK
11 6000 FORMAT(A8,/,A8,124X)
12 892 READ(2,7000) LIB,BNR
13 7000 FORMAT(A8,2X,E10.0,112X)
14 890 READ(2,7008) ISO,THA,IHA,NGA,APR,ANE,CRO,THR
15 7008 FGRMAT(A8,2X,E10.0,A1,7X,12,4E10.0,62X)
16 IF(ISO.EQ.BLNK) RETURN
17 NOISO=NOISO+1
18 THH=THA
19 IF(IHA.EQ.'S') THH=THA/60.
20 IF(IHA.EQ.'H') THH=THA*60.
21 IF(IHA.EQ.'D') THH=THA*1440.
22 IF(IHA.EQ.'Y') THH=THA*1440.*365.25
23 IF(CRO.EQ.0.) CRO=1.
24 READ(2,7009) (ENE(I),PCE(I),I=1,NGA)
25 7009 FORMAT(8E10.0)
26 LINES=LINES+NGA
27 RETURN
28 END

```

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
ANE	28	/LIBR/		REAL	
APR	18	/LIBR/		REAL	
BLNK	3	DUMMY-ARG	*S*	CHAR#8	
BNR	2648			REAL	
CRO	38	/LIBR/		REAL	
ENE	58	/LIBR/		REAL	
I	2668			INTEGER	30
IHA	2618			CHAR*1	
IP	1	DUMMY-ARG		INTEGER	
ISO	08	/LIB2/		CHAR#8	
LIB	2638			LIB	
LINES	6			LINES	
NGA	2	DUMMY-ARG	*S*	INTEGER	
NOISO	5	DUMMY-ARG		INTEGER	
NRI	4	DUMMY-ARG		INTEGER	
PCE	438	/LIBR/		REAL	
THA	2658			REAL	
THH	08	/LIBR/		REAL	
THR	48	/LIBR/		REAL	
UNK	2628			CHAR*8	

NAME	ADDRESS	DEF	PROPERTIES	DEF
890	336	14	7000	1508
892	*NO REFS*	12	7008	1538
6000	1458	11	7009	1608
			FORMAT	FORMAT
			FORMAT	FORMAT
			FORMAT	FORMAT

---STATEMENT LABELS---(LO=A)

---LABEL-ADDRESS---PROPERTIES---DEF

```

1 SUBROUTINE MATRIX(LINE, NUMF, ETOL, JMAT, DT, BLNK)
2 CHARACTER*8 ISOR, BLNK, COL, ITUNN
3 COMMON/FITIN/FITCH(100), ENERG(100), EFFSUM(100), EFER(100)
4 COMMON/LIBR/THAR, APRD, ANEU, CRO, THR, EREF(30), GREF(30)
5 COMMON/COR/8(80, 30), ROW(30), X(30), IL(30), CONF(30),
6 HALF(30), ACOL5(30), XINT(30), XCONF(30), XER(30),
7 SACOL2(30), ACOL3(30)
8 COMMON/INTE/A(80, 30), JFL(30), KFL(30)
9 COMMON/LIB2/ISOR
10 COMMON COL(30), ITUNN(30)
11 EFMIN=1.E+38
12 DO 11 I=1, NUMF
13 EFMIN=AMINI(EFMIN, EFFSUM(I))
14 CONTINUE
15 TEST1=0.
16 DO 12 I=1, LINE
17 DO 12 J=1, NUMF
18 DIFF=ABS(ENERG(J))-EREF(I)
19 IF(DIFF.GT.ETOL) GO TO 12
20
21 C
22 C
23 C
24 C
25 C
26 C
27 C
28 C
29 C
30 C
31 C
32 C
33 C
34 C
35 C
36 C
37 C
38 C
39 C
40 C
41 C
42 C
43 C
44 C
45 C
46 C
47 C
48 C
49 C
50 C
51 C
52 C
53 C
54 C
55 C

```

FORM THE WORKING MATRIX

```

JPREV=1000
PREVC=1000.
JMAT=JMAT+1
CHECK=1000.
COL(JMAT)=ISOR
ACOL2(JMAT)=APRD*1000.+ANEU
HALF(JMAT)=THAR
EFREF=100.*EFFSUM(J)/GREF(I)
DIFF1=ENERG(I)-ETOL
DIFF2=ENERG(NUMF)+ETOL
DO 65 J1=1, LINE
IF(EREF(J1).LT.DIFF1-OR.EREF(J1).GT.DIFF2) GO TO 65
DO 50 JJ2=1, NUMF
DIFF=ABS(ENERG(JJ2))-EREF(J1)
IF(DIFF.GE.CHECK) GO TO 50
JCH2=JJ2
CHECK=DIFF
CONTINUE
50 IF(CHECK.GT.ETOL) GO TO 60
51 IF(JPREV.NE.JCH2) GO TO 56
IF(CHECK.LT.PREVC) GO TO 56
GO TO 65
60 CHECK=GREF(J1)*EFREF/100.
IF(CHECK.GT.EFMIN) GO TO 51
GO TO 65
56 A(JCH2, JMAT)=GREF(J1)/100.
TESTD=(0.16/ETOL)*CHECK*CHECK
TEST1=TEST1+TESTD
PREVC=CHECK
CHECK=1000.
65 CONTINUE
IF(TEST1.GT.70.) GO TO 6101

```

```

56 CONF(JMAT)=CONF(JMAT)*EXP(-TEST1)
57 GO TO 6102
58
59 6101 CONF(JMAT)=0.
60 6102 CONTINUE
61 TEST1=0.
62 TEST2=5.116856E-03*(DT/THAR)**2.0
63 IF(TEST2.GT.70.)GO TO 6201
64 CHECK=EXP(-TEST2)
65 GO TO 6202
66 CHECK=0.0
67 6201 CHECK=0.0
68 6202 CONTINUE
69 CONF(JMAT)=CONF(JMAT)*CHECK
70 IF(CONF(JMAT).GE.0.1) RETURN
71 HALF(JMAT)=0.
72 ACOL2(JMAT)=0.
73 COL(JMAT)=BLNK
74 CONF(JMAT)=1.
75 DC 44 KK=1,NUMF
76 A(KK,JMAT)=0.
77 CONTINUE
78 JPAT=JMAT-1
79 12 CONTINUE
80 RETURN
81 END

```

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
A	08	/INTF/			
ACOL2	51568	/COR/		REAL	2400
ACOL3	52148	/COR/		REAL	30
ACOL5	47668	/COR/		REAL	30
ANEU	28	/LIBR/		REAL	30
APRO	18	/LIBR/		REAL	
B	08	/COR/		REAL	2400
BLNK	6	DUMMY-ARG		CHAR*6	
CHECK	4248			REAL	
CHEC2	4358			REAL	
COL	08	//		REAL	30
CONF	46728	/COR/		REAL	30
CRO	38	/LIBR/		REAL	
DIFF	4218			REAL	
DIFF1	4268			REAL	
DIFF2	4278			REAL	
DT	5	DUMMY-ARG		REAL	
EFER	4548	/FITIN/		REAL	100
EFFSUM	3108	/FITIN/		REAL	100
EFMIN	4128			REAL	
EFREF	4258			REAL	
EMERG	1448	/FITIN/		REAL	100
EKEF	58	/LIBR/		REAL	30
ETDL	3	DUMMY-ARG		REAL	
FITCH	08	/FITIN/		REAL	100
GKEF	438	/LIBR/		REAL	30
HALF	47308	/COR/		REAL	30
I	4138			INTEGER	
IL	46348	/COR/		INTEGER	30
ISOR	08	/LIB2/		CHAR*8	
ITUNN	308	//		CHAR*8	30
J	4178			INTEGER	
JCH2	4348			INTEGER	
JFL	45408	/INTF/		INTEGER	30
JJ2	4328			INTEGER	
JMAT	4	DUMMY-ARG		INTEGER	
JPREV	4228			INTEGER	
JL	4308			INTEGER	
KFL	45768	/INTF/		INTEGER	30
KK	4408			INTEGER	
LINE	1	DUMMY-ARG		INTEGER	
NUMF	2	DUMMY-ARG		INTEGER	
PREVC	4238			REAL	
ROW	45408	/COR/		REAL	30
TESTD	4368			REAL	
TEST1	4158			REAL	
TEST2	4378			REAL	
THAR	08	/LIBR/		REAL	
THR	48	/LIBR/		REAL	
X	45768	/COR/		REAL	30
XCONF	50628	/COR/		REAL	30
XINT	51208	/COR/		REAL	30
XINT	50248	/COR/		REAL	30

NAME	ADDRESS	BLOCK	PROPERTIES	TYPE	SIZE
4	08	/INTF/		REAL	2400
ACOL2	51568	/COR/		REAL	30
ACOL3	52148	/COR/		REAL	30
ACOL5	47668	/COR/		REAL	30
ANEU	28	/LIBR/		REAL	30
APRO	18	/LIBR/		REAL	
B	08	/COR/		REAL	2400
BLNK	6	DUMMY-ARG		CHAR*6	
CHECK	4248			REAL	
CHEC2	4358			REAL	
COL	08	//		REAL	30
CONF	46728	/COR/		REAL	30
CRO	38	/LIBR/		REAL	
DIFF	4218			REAL	
DIFF1	4268			REAL	
DIFF2	4278			REAL	
DT	5	DUMMY-ARG		REAL	
EFER	4548	/FITIN/		REAL	100
EFFSUM	3108	/FITIN/		REAL	100
EFMIN	4128			REAL	
EFREF	4258			REAL	
EMERG	1448	/FITIN/		REAL	100
EKEF	58	/LIBR/		REAL	30
ETDL	3	DUMMY-ARG		REAL	
FITCH	08	/FITIN/		REAL	100
GKEF	438	/LIBR/		REAL	30
HALF	47308	/COR/		REAL	30

```

1  SUBROUTINE ORDER(K,N,XNEW,X,YNEW,Y,ZNEW,Z,WNEW,W,TNEW,T,
2  XSNEW,S)
3  CHARACTER*8 SNEW,S
4  DIMENSION X(30),Y(30),Z(30),W(30),T(30),S(30)
5  IF(N.LT.0.OR.N.GT.151)STOP
6  IF(N.GT.0)GO TO 20
7  M=N
8  GO TO 80
9  20 IF(XNEW.LT.X(N))GO TO 40
10 M=N
11 GO TO 80
12 GO TO 80
13 40 I1=0
14 50 I1=I1+1
15 IF(XNEW.GE.X(I1))GO TO 50
16 I2=N+2
17 60 I2=I2-1
18 GO TO(70,69,68,67,66,64),K
19 64 S(I2)=S(I2-1)
20 66 T(I2)=T(I2-1)
21 67 W(I2)=W(I2-1)
22 68 Z(I2)=Z(I2-1)
23 69 Y(I2)=Y(I2-1)
24 70 X(I2)=X(I2-1)
25 IF(I2.GT.I1+1)GO TO 60
26 M=I1-1
27 80 M=M+1
28 GO TO(90,89,88,87,86,84),K
29 84 S(M)=SNEW
30 86 T(M)=TNEW
31 87 W(M)=WNEW
32 88 Z(M)=ZNEW
33 89 Y(M)=YNEW
34 90 X(M)=XNEW
35 N=N+1
36 RETURN
    END
    
```

--VARIABLE MAP--(LO=A)		--VARIABLE MAP--(LO=A)	
--NAME--	--ADDRESS--	--BLOCK--	--SIZE
I1	2708		
I2	2718		
K	1	DUMMY-ARG	30
M	2678		
N	2	DUMMY-ARG	30
S	14	DUMMY-ARG	30
SNEW	13	DUMMY-ARG	30
T	12	DUMMY-ARG	30
TNEW	11	DUMMY-ARG	30
W	10	DUMMY-ARG	30
WNEW	9	DUMMY-ARG	30
X	4	DUMMY-ARG	30
XNEW	3	DUMMY-ARG	30
Y	6	DUMMY-ARG	30
YNEW	5	DUMMY-ARG	30
Z	8	DUMMY-ARG	30
ZNEW	7	DUMMY-ARG	30

APPENDIX-F. OUTPUT EXAMPLES

PEAK SEARCH BETWEEN 80 AND 4096 CHANNELS
 ATGE= .80 ALLT= .80 FAC= .80 ADEL= .80 ATEST= .80 PIEST= 1.00

SPECTRUM INPUT FROM FILE IAEAG2

THERE MAY BE A PEAK NEAR CHANNEL # 117
 THERE MAY BE A PEAK NEAR CHANNEL # 119
 THERE MAY BE A PEAK NEAR CHANNEL # 121
 THERE MAY BE A PEAK NEAR CHANNEL # 896
 THERE MAY BE A PEAK NEAR CHANNEL # 1026
 THERE MAY BE A PEAK NEAR CHANNEL # 1324
 THERE MAY BE A PEAK NEAR CHANNEL # 2096
 THERE MAY BE A PEAK NEAR CHANNEL # 2759
 THERE MAY BE A PEAK NEAR CHANNEL # 3268
 THERE MAY BE A PEAK NEAR CHANNEL # 3553
 THERE MAY BE A PEAK NEAR CHANNEL # 3750

INSPECT THE FIRST PEAK CAREFULLY...

NUMBER OF DETECTED PEAKS IN THIS REGION : 28

*** PEAKS FOUND ***

	MIN.CHN	MAX.CHN	PEAK AREA	COMP.COMT	STD.DEV	SIGMA	PEAK CHANNELS
1	84	126	2781715.	106205.	.1	2.126	97.895
2	150	168	139043.	498115.	.8	2.137	161.571
3	197	255	3826690.	1939408.	.1	2.151	246.203
4	345	382	5879803.	1210588.	.0	2.172	370.628
5	402	422	668428.	487835.	.2	2.179	414.249
	481	494	49887.	271748.	1.5	1.879	487.289
	671	683	26183.	175671.	2.3	1.877	676.503
	718	728	10626.	124306.	4.8	1.654	723.146
6	827	846	353095.	200239.	.2	2.249	837.380
	887	899	5607.	116141.	8.7	2.088	894.645
7	904	927	824838.	230736.	.1	2.262	917.378
	1021	1029	2360.	64143.	15.3	1.683	1024.760
8	1053	1089	2416940.	309599.	.1	2.289	1078.138
9	1152	1177	322953.	178488.	.3	2.303	1162.312
	1318	1328	4362.	59633.	8.1	1.943	1322.487
10	1533	1560	163485.	176391.	.4	2.367	1546.830
	1760	1770	4619.	69863.	8.2	1.668	1765.327
	1838	1851	5694.	99940.	4.7	2.160	1844.448
	2091	2099	2383.	32633.	10.9	1.720	2094.740
	2495	2539	1674852.	192073.	.1	2.529	2526.858
11	2753	2765	3804.	36464.	7.3	2.458	2757.633
	2928	2940	2473.	19593.	8.3	2.199	2933.249
	3263	3269	225.	3165.	35.9	.985	3266.173
12	3347	3389	1244116.	45019.	.1	2.670	3376.816
	3545	3557	1001.	2789.	8.1	2.553	3551.688
	3741	3756	1516.	3107.	5.8	2.902	3748.074
	385C	3867	3171.	2400.	2.8	2.482	3858.600
	402E	4041	1031.	1246.	5.8	2.353	4034.216

TOTAL NUMBER OF DETECTED PHOTOPEAK GROUPS 12

INUM INIT IFIN MUL II IVAR IRPT IGUES IDISK ISAVE ISET
6 827 846 1 3 5 0 0 0 1 0 0 0
INITIAL PARAMETERS:

COMPTON CONTINUUM
A0= 11451.5 A1= 86.47 A2= -6.32

STEP FUNCTION
HI= 12.00

PEAK HEIGHTS (GAUSS)
AG1= 72006.0

TAILING HEIGHTS
ATI= 7200.6

PEAK CHANNELS
X01= 11.422

B= .350 C= 1.000 SIGMAT= 1.500 SIGMAG= 1.868
INITIAL CHISQR= .303231E+02
GRADIENTS

.170850E+00 .878090E+00 .540057E+01 .166430E+00 .101907E-01
-.588223E+03 .225843E-01 -.806221E+03 .163815E+03 -.232799E+02
.109956E+04

FUNCTION MINIMUM IKNT= 12
GRADIENTS

.819678E-03 -.819766E-04 .259283E-01 -.474577E-03 -.375340E-04
-.466249E+00 .316635E-03 -.367606E+00 .246082E+00 -.120980E-01
.197060E+00

FINAL CHISQR= .171182E+02 CHISQR/(DEG.FREE)= .190203E+01

FINAL PARAMETERS:

COMPTON CONTINUUM
A0= 11447.8 +/- 62.7 A1= 85.05 +/- 23.9 A2= -6.23 +/- 1.5

STEP FUNCTION
HI= 11.90 +/- 2.1

PEAK HEIGHTS (GAUSS)
AG1= 72006.0 +/- 1.4

TAILING HEIGHTS
ATI= 7189.9 +/- 11.8

B= .386 +/- .044 C= .995 +/- .023 SIGMAT= 1.411 +/- .345 SIGMAG= 1.868 +/- .006 FWHM= 4.399

PEAK CHNL
1 837.422 +/- .012 TAILING AREA 9543.3 GAUSS AREA 337166.6 TOTAL AREA 346710.6 % ERROR .603

ERR.CORR=-1.0935052E+00

DATA 6Z PROGRAM #2 SPECTRUM
ENERGY CALIBRATION DATA

CHANNEL	ENERGY(KEV)
1	370.490
2	122.060
3	107.300
4	356.030
5	252.200
6	834.830
7	4032.500
8	1392.260

EFFICIENCY CALIBRATION DATA

ENERGY(KEV)	EFFICIENCY	EFF-EFFR
1	31.750	3.7580000E+00
2	81.000	4.8600000E-03
3	122.100	7.0200000E-03
4	356.000	2.8730000E-03
5	661.600	1.8630000E-03
6	834.800	1.3200000E-03
7	1173.200	9.2900000E-04
8	1332.500	6.1400000E-04

DATA INPUT FROM FILE FIT1

CALIBRATION RESULTS

PEAK#	CHANNEL	SPKOR-CHN	ENERGY(KEV)	EPKOR(KEV)	AREA	ERRCR(%)	INTENSITY	ERRR(%)
1	97.035	.035	31.800	.017	.7450E+C6	1.723	.1405E+10	5.959
2	106.343	.014	34.560	.014	.1253E+C7	.173	.1938E+10	3.927
3	101.952	.014	57.989	.013	.1125E+C6	.184	.6324E+08	3.014
4	246.250	.031	80.910	.015	.2451E+C7	1.756	.5657E+09	7.094
5	370.658	.007	122.111	.010	.5703E+C7	1.320	.8128E+09	3.458
6	414.292	.023	136.561	.012	.6620E+C6	1.421	.1041E+09	5.475
7	837.415	.013	276.645	.008	.3432E+C6	.825	.1006E+C9	5.049
8	917.376	.009	303.112	.008	.8120E+C6	.491	.2581E+C9	5.075
9	1078.145	.008	356.318	.008	.2307E+C7	.202	.8457E+C9	5.017
10	1162.313	.013	384.170	.008	.3085E+C6	.503	.1204E+C9	4.922
11	1546.815	.021	511.373	.011	.1567E+C6	.713	.7746E+C6	4.429
12	2526.842	.004	835.267	.010	.1638E+C7	.182	.1241E+10	2.704
13	3776.800	.008	1116.118	.008	.1625E+C7	.208	.1282E+10	2.118
14	37.95.00LPL, AA, P03							
15	37.95.00LPL, AA, P03							

***** BUCAASA/NUCLIDE REV 1.0 84/08/10. 15.05.52.*****

DB : IAEA G2 PROGRAM SOURCE #2

COUNT. TIME= 306.62(MIN) WAIT. TIME= 37926.00(MIN) EXSPR. TIME= 1.00 (MIN)LIVE C. TIME= 20000.00(SEC)

TABLE OF RESULTS

PEAK NO.	CHANNEL	ENERGY	INTENS.	PC-ERROR
1	97.9850	31.8004	1.4047E+10	5.9592
2	106.3430	34.5690	1.9381E+10	3.9369
3	161.9530	52.9892	6.3240E+08	4.6108
4	246.2500	80.9097	5.0575E+09	7.0991
5	370.6580	122.1112	8.1281E+09	4.4579
6	414.2920	136.5607	1.0410E+09	5.4755
7	837.4150	276.6455	1.0061E+09	5.0489
8	917.3760	305.1116	2.5808E+09	5.0262
9	1078.1450	356.3178	8.4566E+09	5.0141
10	1162.3130	384.1695	1.2038E+09	4.9223
11	1546.8150	511.3733	7.7597E+08	4.4291
12	2526.8420	835.3673	1.2415E+10	3.7040
13	3376.8600	1116.1180	1.1252E+10	2.1155

LIBRARY NUMBER 1, 137 NUCLIDES, 563 GAMMA LINES
ALL PEAKS CHECKED.

THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE NA-22

NUMBER	CHANNEL	ENERGY
11	1546.82	511.37

THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE MN-54

NUMBER	CHANNEL	ENERGY
12	2526.84	835.37

THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE CO-57

NUMBER	CHANNEL	ENERGY
5	370.66	122.11
6	414.29	136.56

THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE ZN-65

NUMBER	CHANNEL	ENERGY
13	3376.86	1116.12

THE FOLLOWING PEAKS ARE ATTRIBUTED TO ISOTOPE BA-133

NUMBER	CHANNEL	ENERGY
3	161.95	52.99
4	246.25	80.91
7	837.42	276.65
8	917.38	303.11
9	1078.15	356.32
10	1162.31	384.17

THE FOLLOWING ISOTOPES WERE IDENTIFIED

NUMBER	NUCLIDE	CONF. VALUE	SAMPLE ACT.	PC-ERROR SAT.	ACT. PCI
1	NA-22	0.9889	5.9050E+04	4.43	1.1730E+11
2	MN-54	0.9771	1.7789E+06	3.70	1.1550E+12
3	CO-57	0.9991	1.3562E+06	3.46	7.6524E+11
4	ZN-65	0.9717	3.6602E+06	2.12	1.8554E+12
5	BA-133	0.8219	1.8841E+06	2.18	1.5583E+13

TOTAL ACTIVITY ACCOUNTED FOR 8.7385E+06 PCI

THE FOLLOWING PEAKS WERE NOT IDENTIFIED

NUMBER	CHANNEL	ENERGY	INTENSITY	PC-ERROR
1	57.985	31.800	1.405E+09	5.96
2	166.343	34.569	1.938E+09	3.94
15	15.30.UCLP, AA, PC4		0.101KMS.	

REFERENCES

- 1- Hevesy, G., Levi, H., Mathematics, Physics and Medicine, Vol.14, No.5, p.3, 1936.
- 2- Adams, F., Hoste, J., "Non-destructive Activation Analysis" Atomic Energy Review, Vol.4, No.2, pp.113-180, 1966.
- 3- Çiftçioğlu, Ö., Ge(Li) Nükleer Radyasyon Detektörlerinden Elde Edilen Fotopikler İçin Analitik Bir Yaklaşım ve Yüksek Doğrulukta Otomatik Gamma Spektrum Analizi, İ.T.Ü., 1981.
- 4- Wainerdi, R.E., Beau, N.P.Du, Science, Vol.139, p.1027, 1963.
- 5- Hoste, J., et al., Instrumental and Radiochemical Activation Analysis,
- 6- Lederer, C.M., Hollander, J.M., Perlman, L., Table of Isotopes, New York: John Wiley, 1968.
- 7- Crouthamel, C.E., Applied Gamma-Ray Spectrometry, Oxford: Pergamon Press, 1960.
- 8- Koch, R.C., Activation Analysis Handbook, New York and London: Academic Press, 1960.
- 9- Laul, J.C., "Neutron Activation Analysis of Geological Materials", Atomic Energy Review, Vol.17, No.3, pp.603-695, 1979.
- 10- Nargolwalla, S.S., Przybylowicz, E.P., Activation Analysis with Neutron Generators, New York: John Wiley and Sons, 1973.
- 11- Anon., AQCS Programme, IAEA Lab/243, December 1983.
- 12- Glasstone, Sesonske, Nuclear Reactor Engineering, 1964.

- 13- Price, W.J., Nuclear Radiation Detection, McGraw Hill, 1964.
- 14- Gardner, R.P., Ely, R.L.Jr., Radio isotope Measurement Applications in Engineering, Reinhold, 1967.
- 15- Borak, F., Nuclear Engineering Laboratory Notes, B.Ü., 1982.
- 16- Adams, J.A.S., Gasparini, P., Gamma Ray Spectrometry of Rocks, Elsevier, 1970.
- 17- Ciftcioglu, Ö., "Further Note on The Analytical Approximation to the Peaks Obtained from Ge(Li) Detectors Used in Gamma Spectrum Analysis", Nuclear Instruments and Methods, Vol. 198, No.2,3, pp.391-398, July 1982.
- 18- Op de Beeck, J., "Gammaray Spectrometry Data Collection and Reduction by Simple Computing Systems", Atomic Energy Review, Vol.13, No.4, pp.743-806, 1975.
- 19- Quittner, P., Wainerdi, R.E., "Computer Evaluation of NaI(TR) and Ge(Li) Gamma Ray Spectra", Atomic Energy Review, Vol.8, No.2, pp.361-416, 1970.
- 20- Savitzky, A., Golay, M.J.E., "Smoothing and Differentiation of Data by Simplified Least Squares Procedures", Analytical Chemistry, Vol.36, No.8, pp.1627-1639, July 1964.
- 21- Yule, H.P., "Mathematical Smoothing of Gamma Ray Spectra", Nuclear Instruments and Methods, Vol.54, pp.61-65, 1967.
- 22- Barnes, V., "GASPAN-An Advanced Computer Code for the Analysis of High Resolution Gamma-Ray Spectra", IEEE Transactions on Nuclear Science, Vol.N5-15, No.3, pp.437-455, 1968.

- 23- Inouye, T., Harper, T., Rasmussen, N.C., "Application of Fourier Transforms to the Analysis of Spectral Data", Nuclear Instruments and Methods, Vol.67, pp.125-132, 1969.
- 24- Parr, R.M., Houtermans, H., Schaerf, K., "The IAEA Inter-comparison of Methods for Processing Ge(Li) Gamma-ray Spectra: A Preliminary Report", Transactions of the American Nuclear Society Conference on Computers in Activation Analysis and Gamma-Ray Spectroscopy, Mayaguez, May 1-4, 1978.
- 25- Mariscotti, M.A., "A Method for Automatic Identification of Peaks in the Presence of Background and Its Application to Spectrum Analysis", Nuclear Instruments and Methods Vol.50, pp.309-320, 1967.
- 26- Routti, J.T., Prussin, S.G., "Photopeak Method for the Computer Analysis of Gamma Ray Spectra from Semiconductor Detectors", Nuclear Instruments and Methods, Vol.72, pp.125-142, 1969.
- 27- Aarnio, P.A., Koskelo, M.J., Zambori, P., "A New Method for the Determination of Goodness-of-fit in Gamma Spectroscopy", Nuclear Instruments and Methods, Vol.184, pp.487-492.
- 28- Erdtman, G., Soyka, W., "The Radionuclide Gamma Ray Data File GAMDAT-78", KFA, Jul-Spez-34, April 1979.
- 29- Christensen, G.C., Koskelo, M.J., Routti, J.T., "Gamma Spectrum Storage and Analysis Program SAMPO 76 with Nuclide Identification", HS-RP/015/, European Organization for Nuclear Research, October 1978.
- 30- Koskelo, M.J., Aarnio, P.A., Routti, J.T., "SAMPO80: An Accurate Gamma Spectrum Analysis Method for Microcomputers", Nuclear Instruments and Methods, Vol.190, pp.89-99, 1981.