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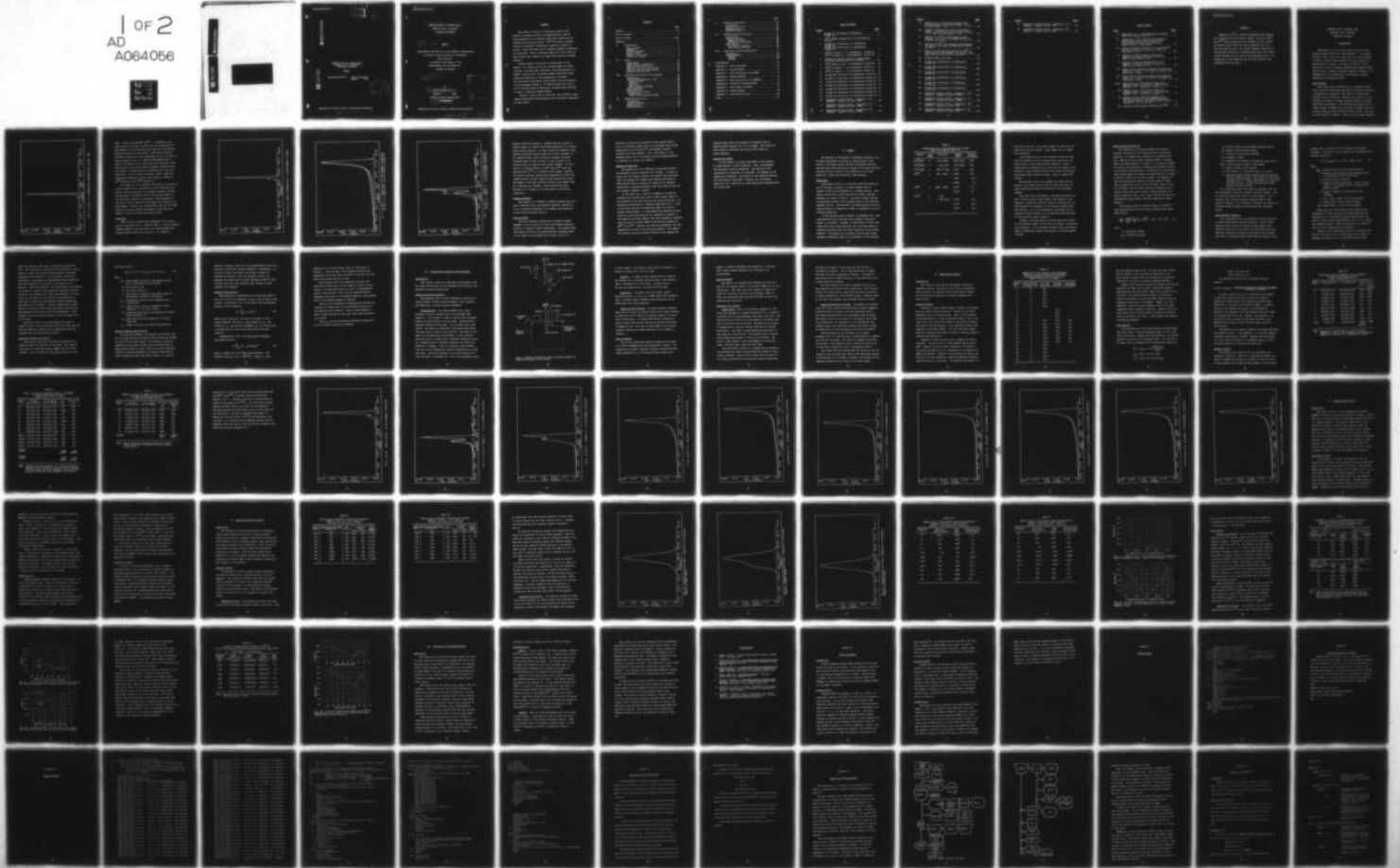
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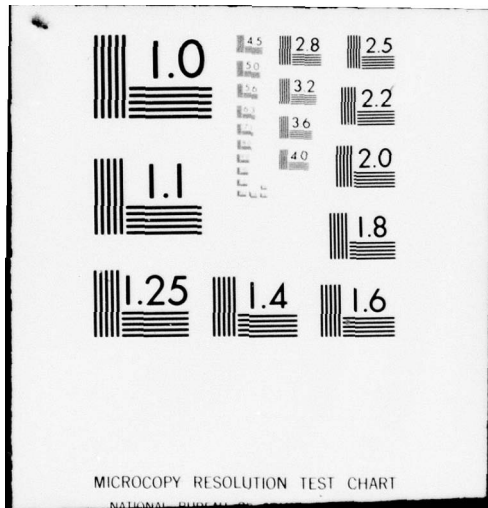
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COMPUTER CODE TO ANALYZE ALPHA
SPECTRA USING A SPECTRAL
STRIPPING APPROACH

THESIS

AFIT/GNE/PH/78D-16

John R. Harstine
Captain USAF

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COMPUTER CODE TO ANALYZE ALPHA
SPECTRA USING A SPECTRAL
STRIPPING APPROACH.

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master's THESIS,

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

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by

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Graduate Nuclear Engineering

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December 1978

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Preface

This thesis is part of a continuing study of the problem of computer analysis of alpha particle spectra. The performance of the program under ideal conditions was studied using Gaussian curves. Po^{210} was used to prepare sources of different thicknesses to obtain a library of curves. These were then used to analyze samples of americium and plutonium. Using a reference peak with a full width at half maximum that matched the sample gave the most accurate analysis.

Several people contributed to the success of this thesis. Dr. George John and Dr. Richard Hagee, my thesis advisors, provided ideas, resources, and encouragement all summer. Harold Kirby and Roland Armani contributed their ideas and experience in the preparation of sources. Dr. Dave Hardin and Captain Bruce Stinson were both helpful in my programming efforts. To them in particular, and to all of the AFIT physics laboratory and metal shop personnel as well, I extend my sincere thanks.

Finally, I would like to thank Mrs. Donna Hadley, whose typing contributed significantly to the successful completion of this thesis.

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Abstract

Sources of Po^{210} of varying thicknesses were prepared by an evaporative precipitation method. Sources of Am^{241} and Pu^{240} were analyzed with the spectra of these sources as reference peak functions using a modification of an existing computer code. The results showed a reduction of the residual from using a reference peak with a full width at half maximum close to that of the analyzed source. The performance of the computer code was also studied using randomized Gaussian peaks.

COMPUTER CODE TO ANALYZE ALPHA
SPECTRA USING A SPECTRAL
STRIPPING APPROACH

I. Introduction

This report is part of a continuing study of alpha spectra obtained from solid state detectors. The general purpose of this study is to learn how to use these spectra to obtain a more accurate analysis of small quantities of alpha-emitting nuclides. The specific purpose of this thesis was to take a computer program which analyzes alpha spectra using a spectral stripping approach and modify it to compensate for the differences in the shape of spectra obtained from different sources.

Basic Problem

Solid state alpha spectroscopy is a technique widely used to analyze microscopic quantities of unknown substances to determine the amounts in the sample of various heavy nuclides such as plutonium. However, the accuracy of this analysis is limited by several problems inherent in alpha decay and its detection. The spectrum from particles of a single energy is spread over the range of energies from the initial energy of decay practically down to zero. This can be seen clearly in Figure 1, which is a full-range spectrum

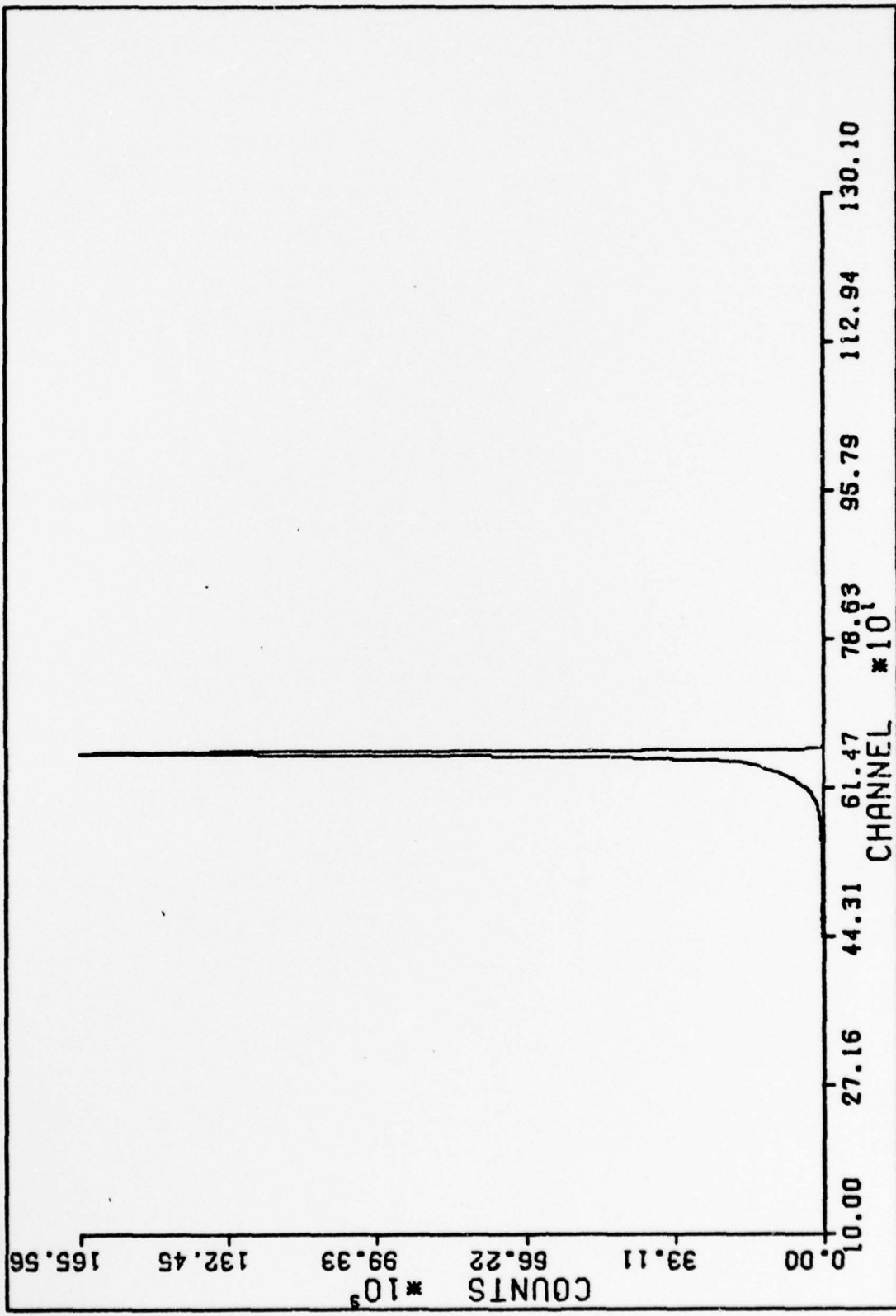


FIG 1. RA DEF # 15 (UNOXIDIZED) UNBIASED RUN 40,000 SEC.

from a source of Radium DEF (Po^{210}). In addition, most alpha emitters can decay to more than one energy state in the daughter nucleus yielding alpha particles of different discrete energies in the process. The spectra from the different energies are then overlapped, as seen in Figure 2, which represents part of a spectrum from Americium 241. Finally, the shape of the curves from the individual alpha energy peaks and of the resulting combined spectra varies from sample to sample because of differences in the self-absorption. This is shown in Figures 3 and 4, which are overlapping normalized spectra from different samples of Po^{210} (Figure 3) and Pu^{240} (Figure 4).

If a sample is to be analyzed accurately, the counts of a given energy must be separated into the individual components from the particles of different original energies. This requires a reference curve of the correct shape for the particular sample to be analyzed. The components of the entire energy range for each energy alpha particle are then summed. Finally, the contributions from all the alpha particles for each nuclide are summed to give the total number of decays for that particular nuclide.

Background

This study was specifically designed to be a continuation of work done by R. J. Hartley (Ref 5). He had prepared Program ALPHAFIT with the help of Dr. Philip Poirer from Program AUTOFIT which was written by J. R. Comfort of

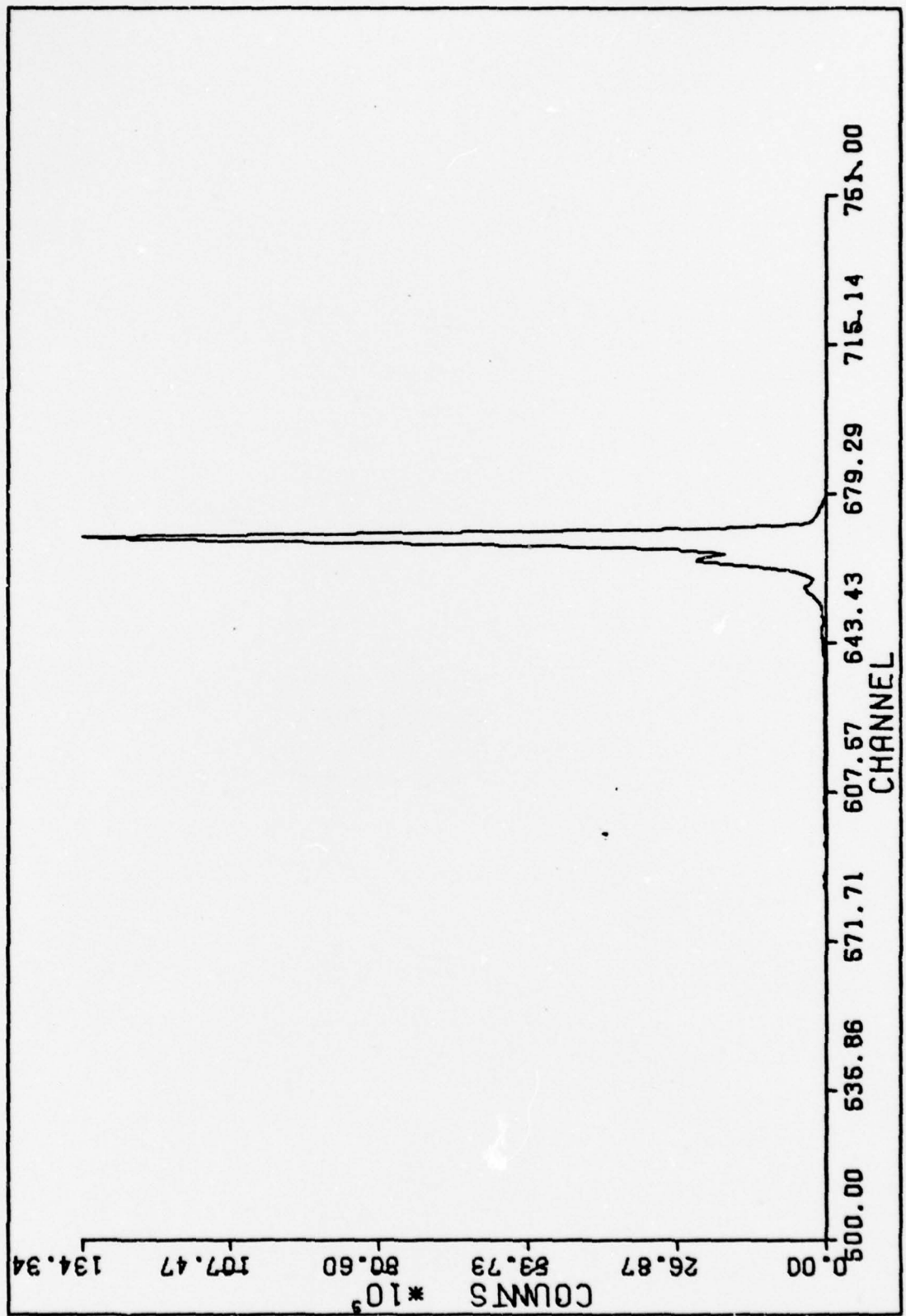


FIG 2. AM 241 (ORTEC) UNBIASED RUN 0.6 KEV/CHANNEL 10 KSEC.

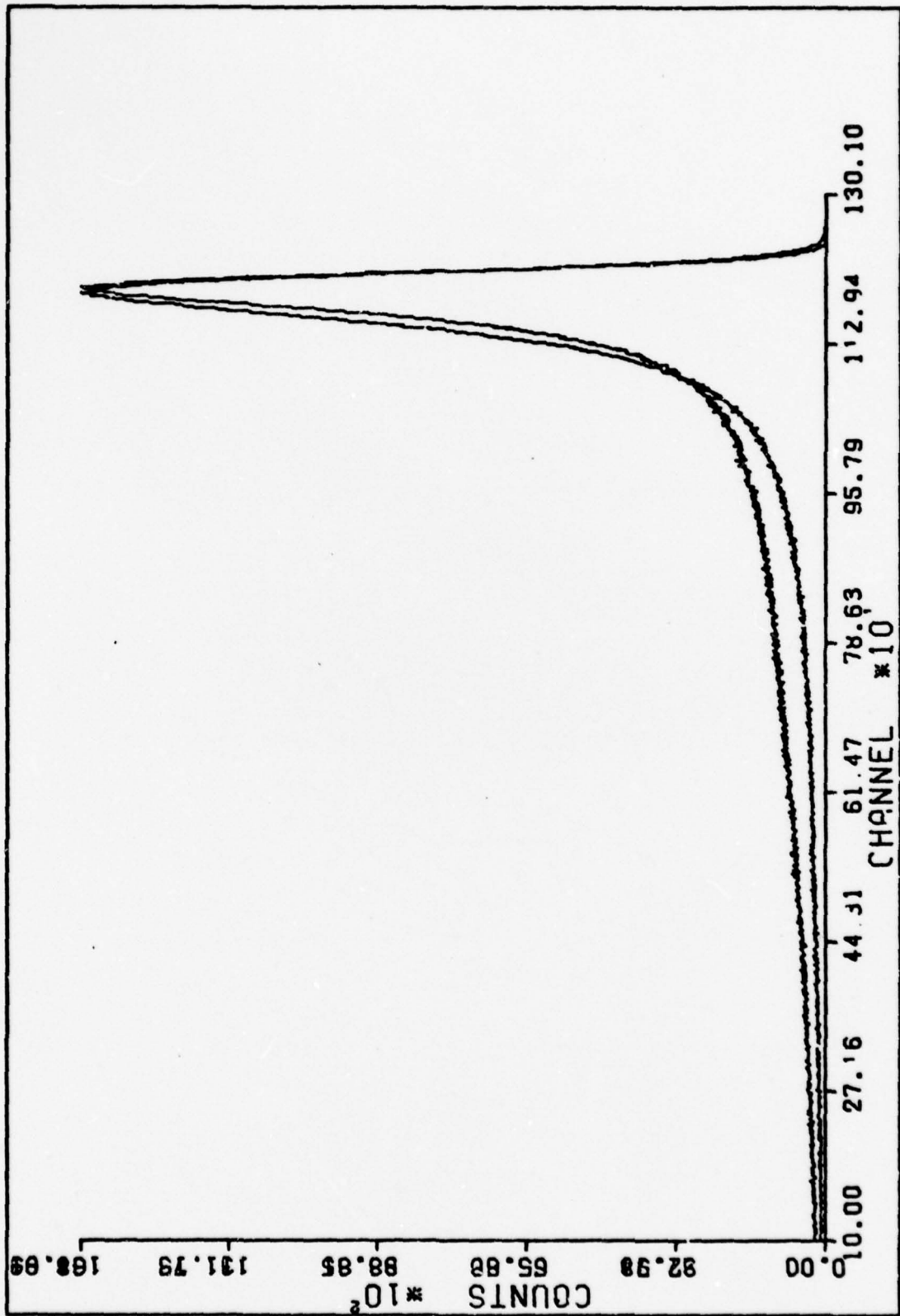


FIG 3 . RA DEF # 11 (UNOXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.
 RA DEF # 13 (UNOXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

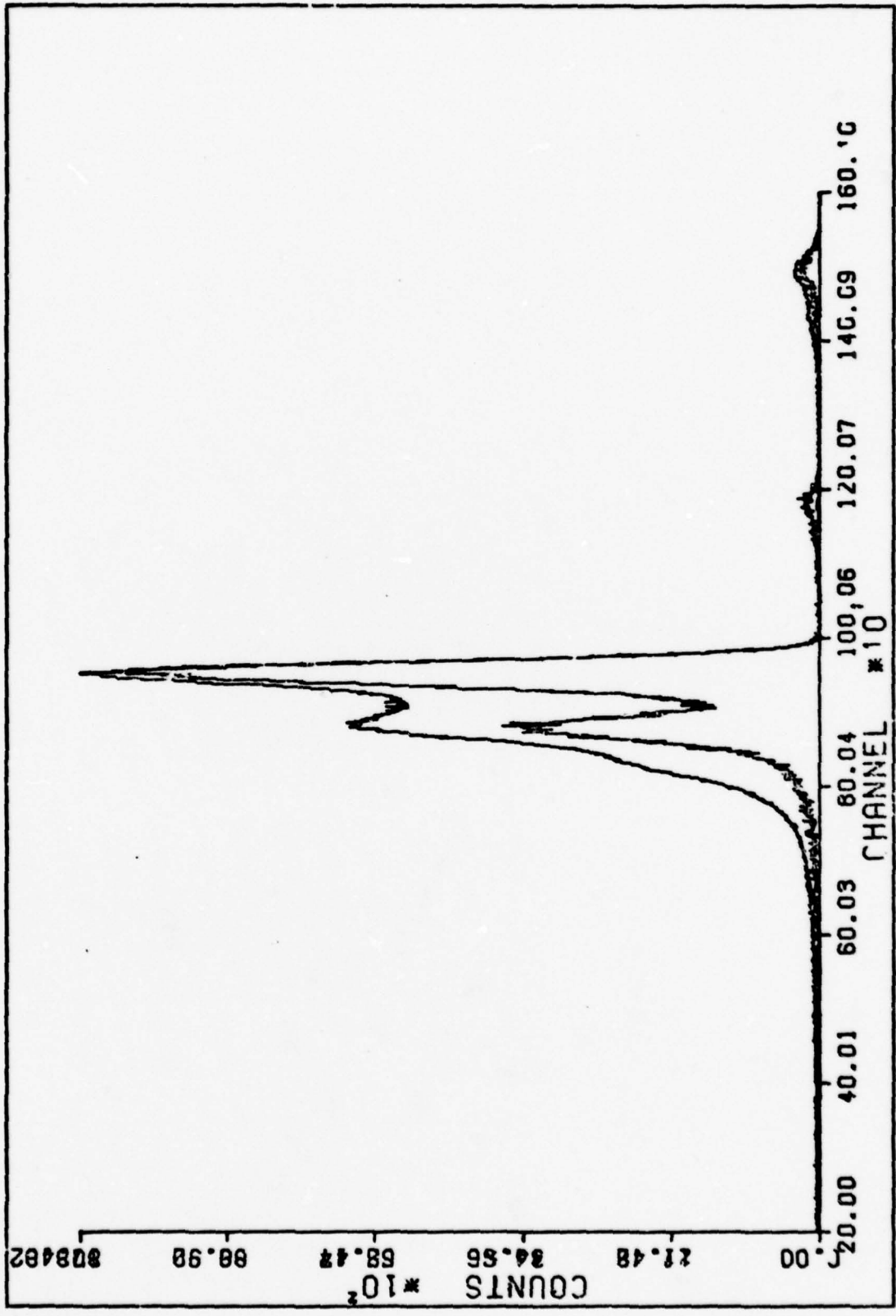


FIG 4 . PU 240 # 1 ARMANI 77 0.6 KEV/CHANNEL 20.000 SEC.
 PU 240 # 2 ARMANI 77 0.6 KEV/CHANNEL 10.000 SEC.

Argonne National Laboratory. AUTOFIT had been written to analyze gamma ray spectra and Hartley modified it to analyze alpha particle spectra. He then studied its behavior using computer generated Gaussian peaks and noted an anomaly in the computed error, which increased, dropped, and then increased again as the two peaks in the spectrum to be analyzed were set progressively closer together. He also used it to analyze samples of Am²⁴¹ and Pu²⁴⁰ using the spectrum from Po²¹⁰ as a reference curve shape. However, the results obtained showed large fluctuations in both the computed errors and the computed peak heights when either the sample of the same analyzed nuclide or the sample used as a reference was changed. These fluctuations were believed to be related to the variations in the source thicknesses.

Problem Statement

The problem is to develop a computer program that will take a spectrum from a multichannel analyzer, separate it into its separate components, and compute the quantities of the various nuclides present.

Plan of Attack

The basic approach selected was to modify Program ALPHAFIT to use a library of curves with shapes representative of a range of source thicknesses. The program would then choose the curve with characteristics matching those of the source to be analyzed and use that curve as a

reference to analyze the spectrum of the unknown sample. A set of reference samples were to be prepared using either Radium DEF or just Polonium²¹⁰ and reference spectra obtained from these samples. Also, the anomaly in the computed errors was to be studied and the program modified if necessary to correct the problem.

Summary of Work Done

The program was first modified to read data directly from magnetic tape or permanent disc storage. In order to reduce the core memory required and shorten the turnaround time, the program was changed from analyzing 20 peaks of 2048 channels each to analyzing 5 peaks of 512 channels. Subroutines to generate Gaussian peaks were then written and the program's behavior studied.

At the same time, a series of samples of Ra DEF was prepared with varying quantities of lead nitrate added to give samples of the same activity but varying thickness. An evaporative/precipitation technique developed by H. W. Kirby of the Mound Facility in Miamisburg, Ohio, was used to prepare these samples. An electroplating technique was also tried but sufficient time was not available to perfect it. The spectra from these samples were then recorded on magnetic tape and used to analyze spectra from existing samples of Am²⁴¹ and Pu²⁴⁰. However, the range of thicknesses was only appropriate for one of the plutonium samples. This sample was analyzed using the reduced version of the program and

analyzed again after the program was converted back to analyzing 2048 channels for up to 10 peaks. The results of these analyses confirmed the value of the library of curves approach.

Overview of Thesis

In this thesis, the theory pertinent to the analysis of alpha spectra is first discussed. Then, the equipment and procedures used are described. The results of the experiments are presented and analyzed. The changes to the program are explained. The results of the computer analyses are presented and discussed. Finally, the conclusions drawn from this study are set forth along with recommendations for future work.

II. Theory

The analysis of the amount of different nuclides by use of alpha spectrometry requires an understanding of the nature of the alpha spectra emitted by different nuclides, the processes which perturb the energy of the alpha particles emitted, and the response of the detector to the alpha particles. These are discussed in this chapter.

Alpha Decay

Alpha decay occurs as a transition from the nucleus of one of the heavy isotopes to a lower energy state in another isotope by the expulsion of a helium nucleus. Each parent nuclide emits alpha particles of certain specific energies, as listed in Table I. The exact energy released is determined chiefly by the quantum state of the resulting daughter nucleus. Once emitted, the alpha particle may lose varying amounts of energy by a number of processes up to and including detection.

If the emitting source material is extremely thin, some alpha particles may leave the source without losing any energy in collisions. However, if the source is even a few atoms thick, most alpha particles will lose some energy in ionizing collisions with the atomic electrons of the source material. The energy lost increases with the path length through the material which is the thickness of the material

Table I

Characteristics of Some Radioactive Isotopes
(Data from Lederer (Ref 10))

Isotope	Type Decay	Half-Life	Energy (MeV)	Percent of Decays
Pb ²¹⁰ (RaD)	β^-	20.4 years	0.061 (max)	100
Bi ²¹⁰ (RaE)	β^-	5.013 days	1.160 (max)	100
Po ²¹⁰ (RaF)	α	138.40 days	5.305	100
Am ²⁴¹	α	458 years	5.486	86
			5.443	12.7
			5.389	1.3
Pu ²⁴⁰	α	6580 years	5.168	76
			5.123	24
Pu ²³⁹	α	2.44 $\times 10^4$ years	5.157	73.3
			5.145	15.1
			5.107	11.5

divided by the sine of the angle between the path and the plane of the source surface. This energy loss is termed self-absorption.

A few alpha particles will initially be emitted away from the detector but will collide with a nucleus in the source itself or the source backing material. After a large change in direction and a large loss of energy in the collision, some of these particles will reach the detector and deposit their remaining energy. This is termed back-scatter.

Any material such as air between the source and the detector will absorb energy from the alpha particles, so alpha spectrometry should be conducted in an evacuated chamber.

When they reach the detector, the alpha particles may have to pass through a dead layer at the surface of the detector in which the electrons freed by collisions do not get collected to contribute to the pulse of current from the detector. As in self-absorption, the energy lost is dependent on the thickness of the dead layer and the angle of the particle's path through it.

Finally, the alpha particle reaches the active region of the detector, where it will lose its energy in collisions with electrons. These electrons produce a pulse of current which is amplified, shaped, and counted in a multi-channel analyzer.

Alpha Particle Interaction

The interaction of alpha particles with matter is strongly influenced by two characteristics of the alpha particle; its enormous mass relative to an electron mass ($M_\alpha \approx 7000 m_e$) and its double positive charge. The mass causes the alpha particle to travel in a virtually straight line except for Rutherford scattering with another nucleus. It also gives alpha particles a relatively low velocity for their high energy; for example, an alpha particle of energy 5 MeV has a speed only 3% that of light. An electron of the same energy would travel at 99% the speed of light. Thus an alpha particle has thirty (or more) times as long as an electron for its double charge to interact with an electron from each atom it passes. Alpha particles are easily stopped by only a thin layer of matter and may lose considerable energy before they even leave their source material.

The stopping power or specific energy loss dE/dX is given approximately by the following equation from Evans (Ref 40:637):

$$\frac{dE}{dX} = \frac{4\pi e^4 z^2}{m_0 v^2} \frac{N_A \rho}{GAW} Z \left[\ln \frac{2m_0 v^2}{I} - \ln(1 - \beta^2) - \beta^2 \right] \quad (1)$$

with

e = electronic charge

m_0 = electron rest mass

E = kinetic energy of the primary (alpha) particle
 ze = charge of the primary particle
 V = velocity of the primary particle
 N_A = Avogadro's number
 ρ = density of the material in grams per unit volume
GAW = the gram atomic weight of the element
 Z = atomic number of the absorber
 $\beta = V/C$, where C = velocity of light in a vacuum
 I = geometric-mean ionization and excitation potential for the absorbing atoms. This cannot be calculated accurately and is usually considered to be constant for each element. It must be determined experimentally for each element.

It is frequently more convenient to determine the loss per differential mass/area thickness traveled through. This is done by dividing both sides by ρ , the density. For a substance with several different elements such as lead nitrate, $Pb(NO_3)_2$, it is necessary to compute the energy loss for each element separately and then add the individual losses.

Alpha Particle Detection

This study deals with the detection of alpha particles by solid state surface barrier detectors. When an alpha particle enters the active region of the detector, the electrons with which it interacts and the holes left behind them move under the influence of the applied bias voltage. This gives a transient current which can be converted into a

voltage pulse and counted by the associated electronic equipment. The height of this pulse can be expressed by the following equation:

$$ph = [(E_{\text{dep}}/w) \times e \times \gamma]/C = N_e \gamma / C = q/C \quad (2)$$

where

E_{dep} = energy deposited by the alpha particle

w = average energy required for the production of an electron-hole pair (eV/e-h pair)

e = electron charge (coulombs)

γ = charge collection efficiency. This is essentially .1 in detectors made of high quality single crystals.

$N = E_{\text{dep}}/w$ = number of electron-hole pairs produced

$q = N_e \gamma$ = total charge collected (coulombs)

C = capacitance of the detector (farads)

ph = pulse height in volts at the detector

These pulses are then amplified and shaped by the preamplifier, linear amplifier and biased amplifier and transmitted to a multichannel analyzer which counts the number of pulses with height between h and $h + \Delta h$ during the acquisition time. These are collected in a number of bins to form a pulse-height distribution.

Because of the statistical nature of the energy loss process, the pulses will be distributed over a range of channels or energies even if the alpha particles have

precisely the same energy when incident on the detector face. This statistical spreading is not caused by a distribution of either the original alpha energy or the energy deposited in the detector. It is caused by statistical variations in the number of electron-hole pairs created by each alpha particle as it deposits its energy in the detector. Additional spread in the pulse height distribution is caused by a spread in the energy of the alpha particles caused by self-absorption in the source material, the dead layer at the surface of the detector, and variations in the angle at which the alpha particle passes through the dead layer and the source. Further, though minor, contributions to the total arise from large angle scatters from the backplate of the source and the surroundings. These combine to give the tailing effect on the low energy side of the peak.

Electronic noise in the electronics also gives a slight increase in the spread but this will be the same for both the reference source and the unknown when they are analyzed with the same detector system.

Relation of Counts to Activity

Each unknown spectrum is analyzed to determine the number of peaks and the area of each peak. This area is the number of counts per channel summed over all of the channels. This is related to the source activity by the

following formula:

$$N_t/t_c = A \times G \times f_{ss} \times f_w \times E \times f_t \times f_\alpha \quad (3)$$

where

N_t = total number of counts = the combined areas
for all the peaks of each isotope

t_c = the counting time

A = the source activity

G = solid angle subtended by the active layer of
the detector relative to the source

f_{ss} = surrounding scatter factor (negligible for
 α particles)

f_w = window factor, that is, absorption losses
(generally = 1 for zero losses)

E = intrinsic efficiency of the detector in counts/
alpha (generally 1)

f_t = dead time correction (generally 1 for zero
dead time)

f_α = number of alphas per nuclear transformation

Need for Computer Peak Analysis

In alpha spectrometry, the energies and relative numbers of alpha particles emitted by each nuclide are assumed to be known from other studies, the results of which are compiled and tabulated in works such as Lederer (Ref 7). These works provide an outer bound on the set of possible nuclides, which can frequently be further restricted by other information about the unknown source. If only one

nuclide is present, then all of the nonbackground counts are from that nuclide and computer analysis is unnecessary. It is only in those cases where the relative numbers of nuclides are unknown, while the possible nuclides and energies and proportions of alphas emitted by each of those nuclides are known, that computer peak analysis is both necessary and feasible.

Computer Peak Analysis

Each spectrum is represented by an array $[A_i]$ which is the sum of a set of N components $Z_i(x_n)$, one for each of the N peaks. Each element in A is the sum of the corresponding elements of each component

$$A_i = \sum_{n=1}^N a_n Z_i(x_n) \quad (4)$$

where $Z_i(x_n)$ represents the counts in channel i from a source component that has its peak located at x_n . The locations, x_n , and relative strengths, a_n , are varied until a satisfactory fit of the test array $[A]$ to the data array $[Y]$.

Mathematically, this is accomplished by forming a chi-squared function

$$F = \sum_{i=1}^N (Y_i - A_i)^2 / (\omega Y_i)^2 \quad (5)$$

which is summed over the region being analyzed. The weighting function ωY_i is $\sqrt{10 + Y_i}$, where Y_i is the

ordinate of the i th data point, that is, the counts in channel i . The inclusion of 10 slightly increases the weighting of the peak region relative to the tail and background and avoids division by zero.

Since Poisson statistics adequately describe the statistical fluctuations of the number of counts in each channel, the weighting function $(WY_i)^2$ is approximately equal to the variance. Thus, the chi-squared function represents the ratio of the observed spread in the analyzed data to the expected spread or variance.

The x_n 's are determined by computing the function for locations to either side of x_n and shifting the x_n 's in the direction that reduces F . When a local minimum is found or when directed by the input data, that particular x_n is fixed.

The a_n 's are then determined from direct solution of Eq (4) by matrix inversion techniques.

III. Experimental Equipment and Procedures

Introduction

This section covers the techniques and equipment used for alpha spectroscopy and the preparation and assay of the reference sources of Radium DEF.

Alpha Spectroscopy Equipment

The equipment used in these experiments consists of a vacuum chamber, surface barrier detector, power supplies and amplifiers, and multi-channel analyzers.

Vacuum Chamber. The vacuum chamber was a steel cylinder, 10 cm in diameter and 15 cm in height (See Figure 5). The cylinder is open at the top and is mounted around an O-ring clamp to the top plate. There are four openings through the top plate. Two of these lead to gas valves. One valve is connected to the vacuum pump, while the other can be opened to the room air. The third is the mount and connection for the detector. A BNC connector above the plate is electrically connected through the plate to a threaded mount or microdot connector into which the detector is screwed. A BNC "L" connector leads directly from this to the preamplifier which is supported by a clamp and stand. The fourth opening is an O-ring fitting for a thin rod which is attached to a 3 cm x 3 cm horizontal plate

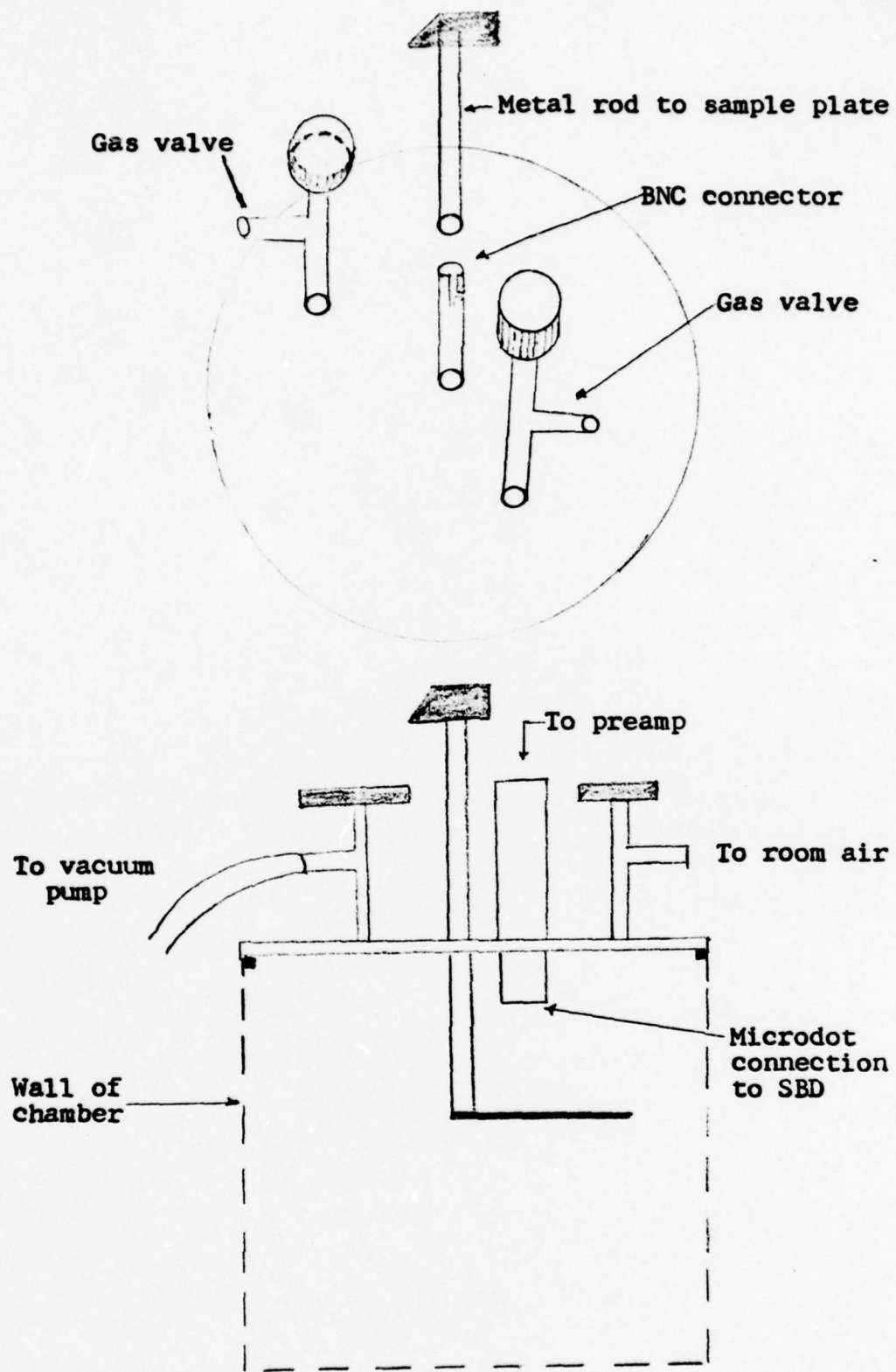


Fig. 5. Raised and Parallel Views of Vacuum Chamber for Alpha Spectroscopy (Not to Scale)

to hold samples. The distance from source to detector is varied by sliding this rod up or down.

Detector. An ORTEC 100 mm² surface barrier detector (SN 8-907A) with a microdot mount was used. This detector takes a maximum bias of 50.0 volts. A gross bias of 50 volts was applied for a net bias of 30-35 volts.

Amplifiers. The output from the surface barrier detector was fed, in turn, to an ORTEC Model 109-A preamplifier, a Tennelec Model TC203BLR linear amplifier, and an ORTEC Model 408 biased amplifier.

Multi-channel Analyzers. Two multi-channel analyzers were used to convert the output pulses into a count spectrum. An ND100 was used to obtain 512 channel spectra for preliminary observations. An ND2200 4096 channel analyzer was used to obtain 2048 channel spectra and record the results on magnetic tape. The tape was then taken to the central computer facility and stored there for use in computer analysis.

Assay Equipment

All of the radioactive samples prepared were assayed in an NMC 2 π geometry gas flow proportional counter. The associated electronic equipment included a Hewlett-Packard 5554A preamplifier, an NIM Standard high voltage power

supply, a Tennelec TC203BLR linear amplifier, a Tennelec TC444 single channel analyzer, and a Canberra 1772 counter/timer.

Assay Procedure

The sample to be assayed was inserted into the flow counter, the counter sealed, and the air flushed out by the flowing gas. Each sample was then counted at least five times for one minute at each of two voltages, 1000V to count just alpha particles and 1600 or 1800V to count both alpha and beta particles.

Preparation of Sources

Kirby Method. Most of the sources prepared for this study were prepared by a method developed by H. W. Kirby of the Mound Facility in Miamisburg, Ohio (Ref 4:134-135). The backing plate is rinsed for a few minutes in alcoholic KOH, then rinsed with water and dried. The area for the sample is masked with a circular rod while the plate is sprayed with Krylon. The plate is then warmed and dried under a heat lamp for a few minutes. The uncoated area is covered with 1N HNO₃ and allowed to stand for two minutes. The plate is then removed, rinsed thoroughly with distilled water, and dried again under the heat lamp.

The radioactive solution to be deposited is dropped on the uncoated area from a microsyringe and allowed to evaporate to dryness. This is then covered with two drops of 0.1 N HNO₃ and heated for two minutes without evaporating.

One drop of 3N NH_4OH is then added and the solution is evaporated to dryness. Two or three more drops of NH_4OH are added and again evaporated to dryness. The NH_4OH is then driven off by further heating on a hot plate until the visible fumes are observed.

The major change from Kirby's procedure was to use a heat lamp for the initial drying operations. This was done because the available hot plates were not able to maintain a steady temperature in the 90-100°C region. However, eight of the first nine samples were prepared using hot plates.

Armani Electroplating Method. One sample was prepared using the "high voltage" electroplating procedure suggested by Roland Armani of Argonne National Laboratory (Ref 1). One hundred microliters of the New England Nuclear Radium DEF solution lot #72-187, about 0.1 microcurie, were added to 10 milliliters of 2-propanol in a 14 millimeter inner diameter glass tube, which was clamped with rubber washers at either end to a plate cleaned as for the Kirby method.

Platinum gauze was not available, so a roughly octagonal plate of platinum about six millimeters in diameter was used for the anode. The anode was immersed just below the surface of the plating solution, which was then plated for two hours at 600 volts and 1.1 microamps current.

Only about 30% of the Radium DEF was plated out and the resolution was no better than that of the evaporated samples. It was decided not to attempt to perfect this method and the remaining samples were all made by the Kirby method.

IV. Experimental Results

Introduction

This chapter covers the Ra DEF samples prepared as reference sources, the results of the assay to determine their activity, the spectra obtained from those sources, and the relative sharpness of the peaks obtained from those sources.

Sources Prepared

Twenty-one sources were prepared, assayed, and counted with the surface barrier detector. Sources 1 and 2 were prepared to test the Kirby method. Source 3 was prepared by electroplating. It gave the broadest peak of any of the sources and only 20% of the Ra DEF in the plating solution was plated onto the planchet, so the remaining sources were prepared by the Kirby method. Two sets of Ra DEF samples were then prepared with varying amounts of $\text{Pb}(\text{NO}_3)_2$ added to increase self-absorption.

Samples 4-9 were the first set of samples of varying thickness. The activities of these samples agreed within $\pm 10\%$. However, as can be seen in Table II, the spread in the resulting spectra did not correspond to the quantity of added lead nitrate. Samples 7-9 were dried too long on the hot plate and this apparently caused considerable oxidation from the nitrate to the oxide. The spectra from samples 7-9

Table II

Comparison of Full Width at Half Maximum in
 2048 Channel Biased Spectra From 100 mm²
 Surface Barrier Detector with Quantity
 Added Pb(NO₃)₂ in the Sample

Sample #	Added Pb(NO ₃) ₂ x .525μg + 3%	KeV FWHM Unoxidized	KeV FWHM Oxidized	$\frac{\alpha \text{ Act (Ox)}}{\alpha \text{ Act(Unox)}}$
1	0	39.1		
2	0	35.2		
3	0	51.6		
4	0	39.6		
5	1	52.0		
6	2	44.6		
7	3		24.3	
8	4		20.4	
9	5		28.1	
10	0	39.3	34.7	.90
11	0	30.2	29.2	.60
12	1	29.0	35.3	.89
13	2	37.1	34.3	.87
14	3	32.8	34.9	.92
15	4	35.4	35.9	.98
16	5	32.9	32.8	.87
17	5	35.6		
18	0	39.4		
19	0	31.9		
20	5	34.2		
21	5	37.1		

had the sharpest peaks of all, but they had double peaks due to ringing in the line from the amplifier to the multi-channel analyzer (This was corrected by inserting a terminator.) and were not used for computer analysis.

Samples 10-21 were the second set prepared with varying quantities of added lead nitrate. These were prepared simultaneously and dried under a heat lamp instead of on a hot plate. The lead nitrate was added in solutions of varying concentration so that the same volume of water was evaporated from each of the samples. Samples 1-17 were prepared on stainless steel planchets, while 18-21 were prepared on small squares of platinum. Sources 10-16 were later heated over a Fisher burner to oxidize the deposit from the nitrate to the oxide. These sources were used for the computer analyses.

Assay Results

All activities are calculated based on the NIC Radium DEF sample #A110, with one microcurie equal to 2.22×10^6 counts per minute. Sample A110 was measured at 514 disintegrations per second on 28 September 1961. The activity on 24 August 1978 is computed from the exponential decay law.

$$A(t) = A(t_0) \times e^{\frac{-(.693)(t-t_0)}{t_{1/2}}}$$

$$t_{1/2} = 20.4 \times 365 \frac{1}{4} \text{ days}$$

$$t-t_0 = 330 + 16 \times 365 \frac{1}{4} \text{ days}$$

$$A(t_0) = 514 \text{ dps} \pm 5\%$$

$$A(t) = 289 \text{ dps} \pm 5\%$$

The remaining activities are calculated from the formula,

$$\text{Activity (Sample)} = \frac{\text{Counts/min (Sample)} \times \text{Activity (Standard)}}{\text{Counts/min (Standard)}}$$

As seen in Tables III and IV, which give the averages of five one-minute counts plus or minus the standard deviation of those counts, the unoxidized samples agreed fairly well in activity from sample to sample. As seen in Table IV, the standard deviations of the averages of activities for samples on the same backing (stainless steel or platinum) were only 1-2%. However, the combined $\alpha + \beta$ activity divided by three for the three nuclides in the decay chain was always several percent higher than the α only activity.

The results of the assay of samples 10-16 after oxidizing are listed in Table V. The combined $\alpha + \beta$ activity remained consistent from sample to sample. However, the fluctuation in α only counts increased to a standard deviation of 15% as varying amounts of polonium were driven off.

Spectral Results

The widths of the spectra from all the samples are compiled in Table II. There was no correlation between the amount of added lead nitrate in a sample and the full width at half maximum of the peak from that sample. Most of these

Table III

Results of Assay of Samples 1-9 in 2π Geometry
 Gas Flow Proportional Counter at
 1000V (α) and 1600V ($\alpha + \beta$)

Sample	α Counts/60 sec	$\alpha + \beta$ cts/60 sec	Activity μC_1	
			α	$(\alpha + \beta)/3$
1	78,490 \pm 170	295,300 \pm 2100	.0721	.0846
2	77,800 \pm 230	336,920 \pm 640	.0715	.0966
3	21,730 \pm 170	112,990 \pm 290	.0200	.0324
4	122,640 \pm 390	470,150 \pm 780	.113	.135
5	122,570 \pm 460	466,580 \pm 510	.113	.134
6	120,520 \pm 300	474,200 \pm 1300	.111	.136
7	102,030 \pm 250	455,450 \pm 470	.0938	.131
8	123,960 \pm 220	483,180 \pm 480	.114	.138
9	99,500 \pm 300	402,830 \pm 680	.0914	.115
A110	8,512 \pm 92	27,291 \pm 165	.00782	.00782
			\pm .00039	

NOTE: Samples 1-9 were prepared on stainless steel
 planchets. Sample 3 was prepared by electroplating.
 Sample A110 was used as a calibration standard.

Table IV

Results of Assay of Samples 10-21 in 2π Geometry
Gas Flow Proportional Counter at
1000V (α) and 1800V ($\alpha + \beta$)

Sample #	α Counts per 60 seconds	$\alpha + \beta$ Counts per 60 seconds	α Act μC_1	$(\alpha + \beta)/3$ Act μC_1
10	109,780 \pm 180	363,120 \pm 560	.101	.104
11	107,470 \pm 230	359,490 \pm 800	.0988	.103
12	109,310 \pm 200	373,910 \pm 660	.100	.107
13	111,740 \pm 170	377,640 \pm 560	.103	.108
14	108,740 \pm 310	371,480 \pm 520	.0999	.106
15	110,770 \pm 320	369,880 \pm 670	.102	.106
16	108,450 \pm 280	352,250 \pm 850	.0997	.101
17	110,860 \pm 140	363,600 \pm 6300	.102	.104
18(p1)	116,210 \pm 150	393,780 \pm 380	.107	.113
19(p2)	113,410 \pm 450	390,340 \pm 490	.104	.112
20(p3)	115,090 \pm 320	403,070 \pm 470	.106	.116
21(p4)	113,730 \pm 240	398,810 \pm 650	.105	.114
Average 10-17			.1008 \pm .0014	.1049 \pm .0023
Average 18-21			.1055 \pm .0013	.1138 \pm .0017

NOTE: Samples 10-17 were prepared on 1.25-inch diameter stainless steel planchets, while 18-21 were prepared on 14 mm square platinum planchets, which were then placed on stainless steel planchets for counting.

Table V

Results of Assay of Samples 10-16 in 2π Geometry
 Gas Flow Proportional Counter at
 1000V (α) and 1800V ($\alpha + \beta$)

Sample #	α Counts per 60 seconds	$\alpha + \beta$ Counts per 60 seconds	Activity, α μC_1	Activity, $(\alpha+\beta)/3$ μC_1
10	99,080 \pm 460	381,680 \pm 120	.0911	.109
11	64,860 \pm 220	342,390 \pm 180	.0596	.0981
12	97,070 \pm 240	367,080 \pm 540	.0892	.105
13	97,300 \pm 310	381,660 \pm 610	.0894	.109
14	99,860 \pm 200	361,360 \pm 510	.0918	.104
15	108,980 \pm 310	371,930 \pm 790	.100	.107
16	94,260 \pm 590	368,150 \pm 480	.0866	.106
Average			.087 \pm .013	.1054 \pm .0037

NOTE: These samples were gently heated over a Fisher burner to convert the deposit from the nitrate to the oxide.

peaks were 10-15 KeV wider than the 21 KeV wide peaks from the Am²⁴¹ and Pu²⁴⁰ #2 samples, which are plotted in Figures 6 and 7. However, there was a good selection of widths in the region of Pu²⁴⁰ #1. Its full width at half maximum was about 32 KeV, but could not be determined precisely because the notch between the two main peaks did not come down to one-half the maximum (See Figure 7). Because of this good match, Pu²⁴⁰ #1 was selected as the "unknown" to be analyzed by the computer program using as reference peaks the spectra from the oxidized sources 10-16, which are plotted in Figures 8-15.

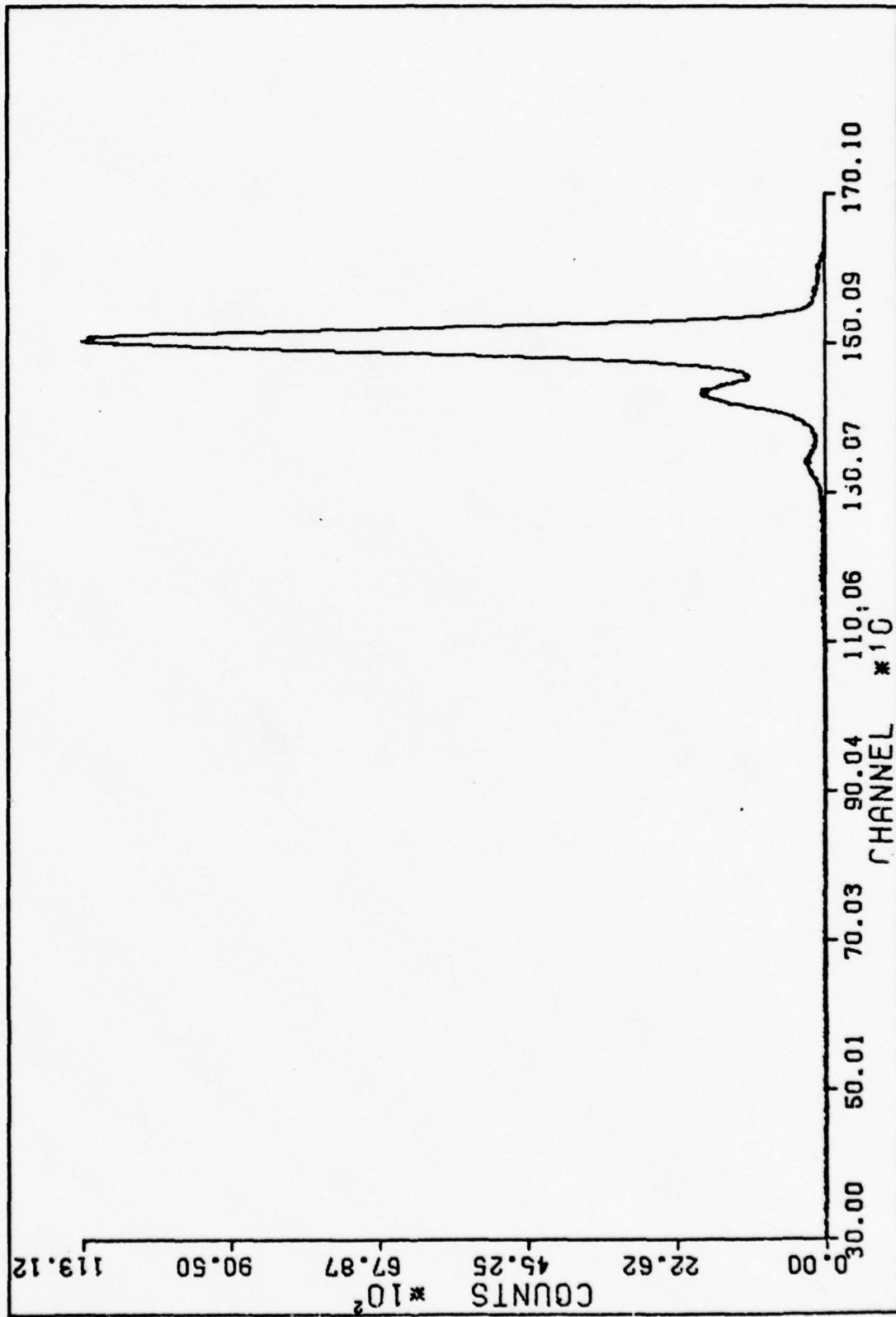


FIG 6 . AM 241 GRTEC 1/21/69 0.6 KEV/CHANNEL 10.000 SEC.

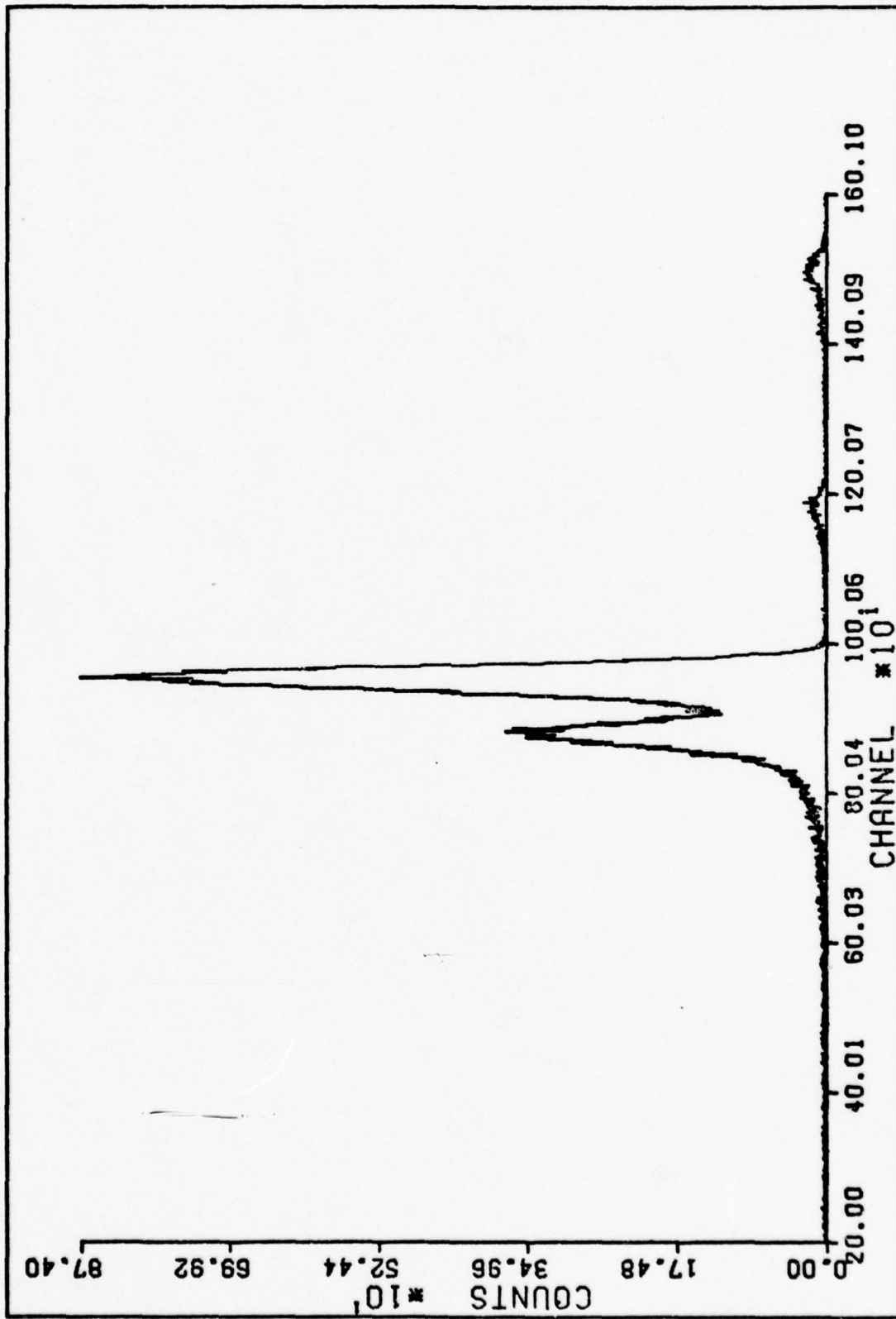


FIG 7. PU 240 # 2 ARMANI 77 0.6 KEV/CHANNEL 10.000 SEC.

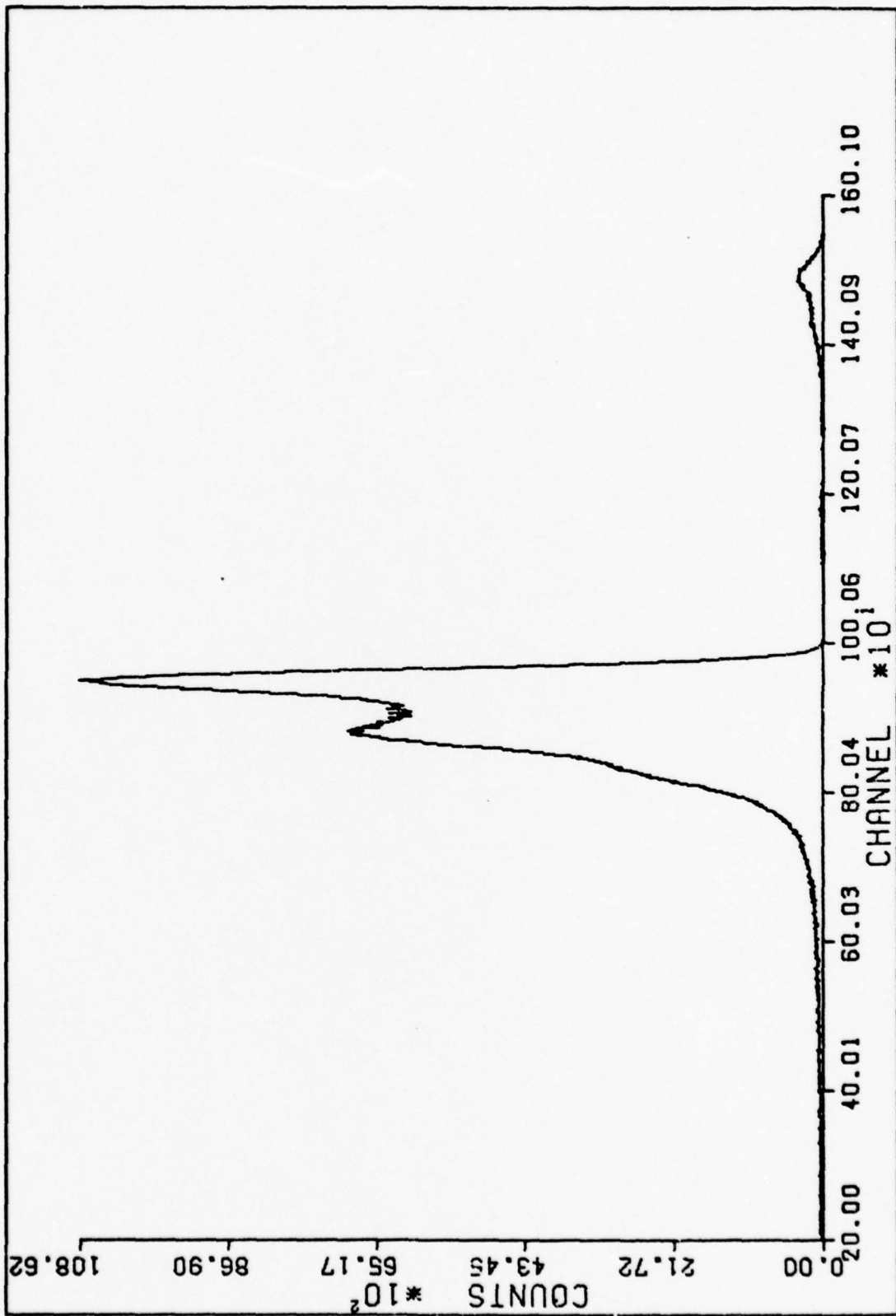


FIG 8 . PU 240 # 1 ARMANI 77 0.6 KEV/CHANNEL 20.000 SEC.

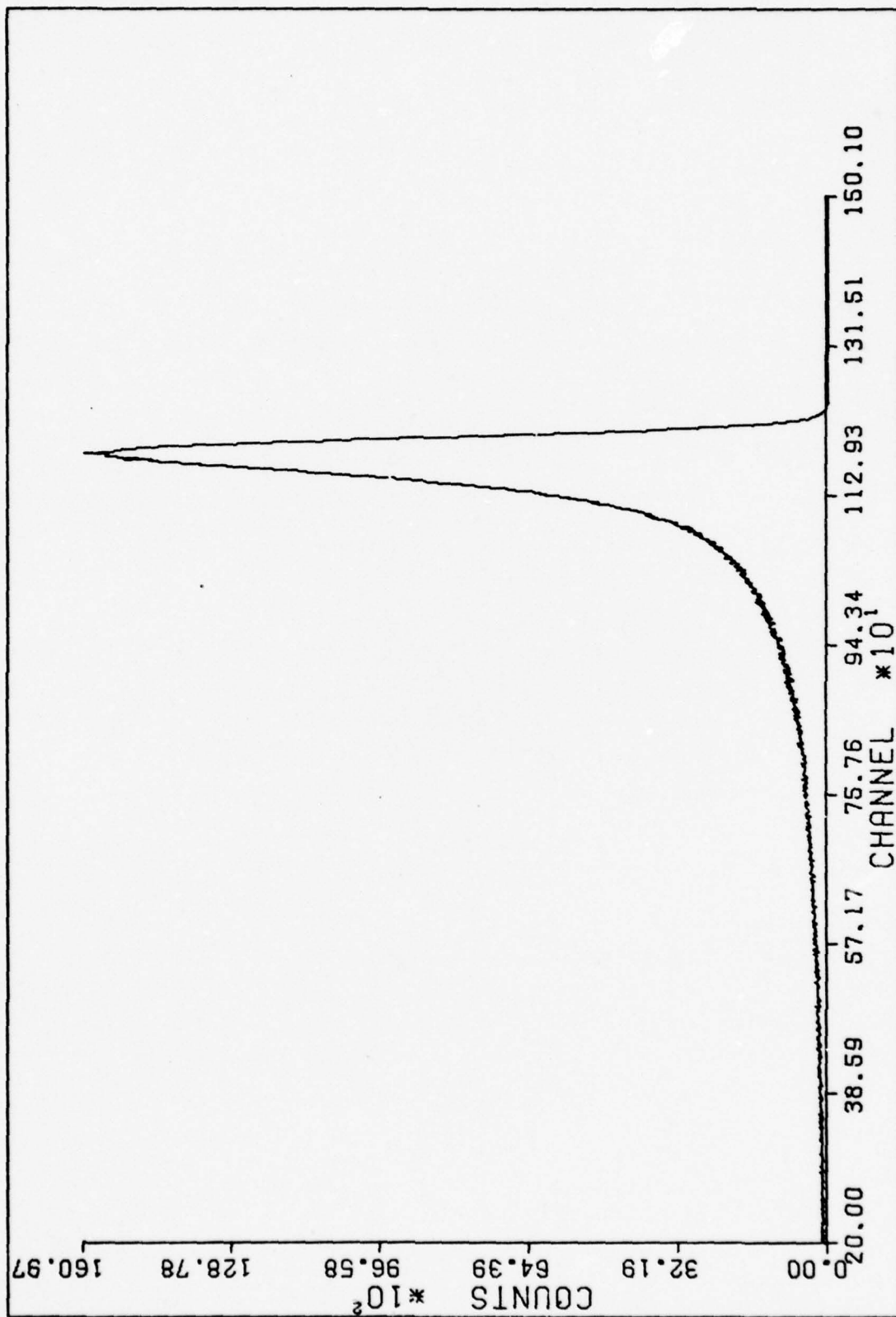


FIG 9. RA DEF # 10 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

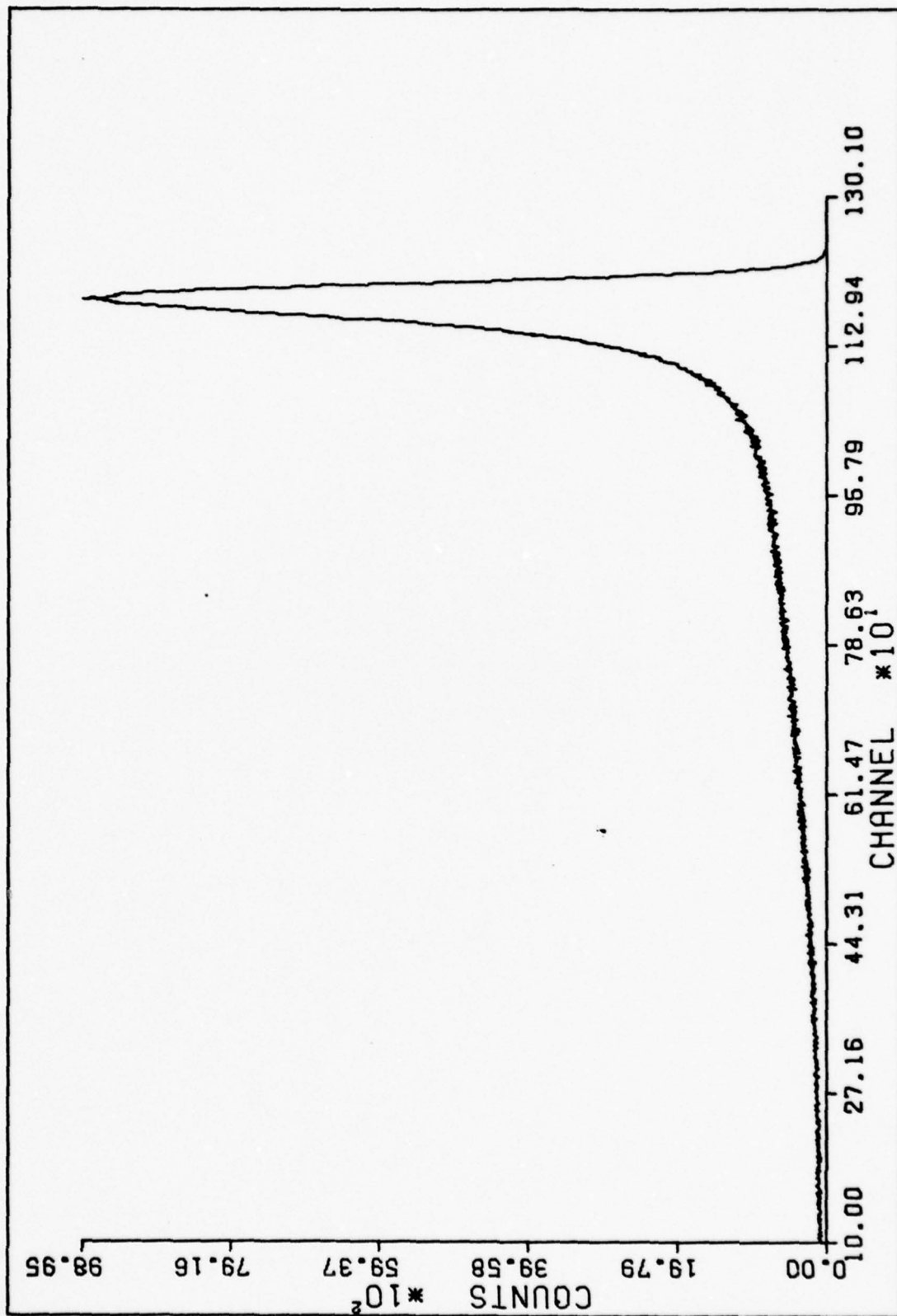


FIG 10. RA DEF # 11 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

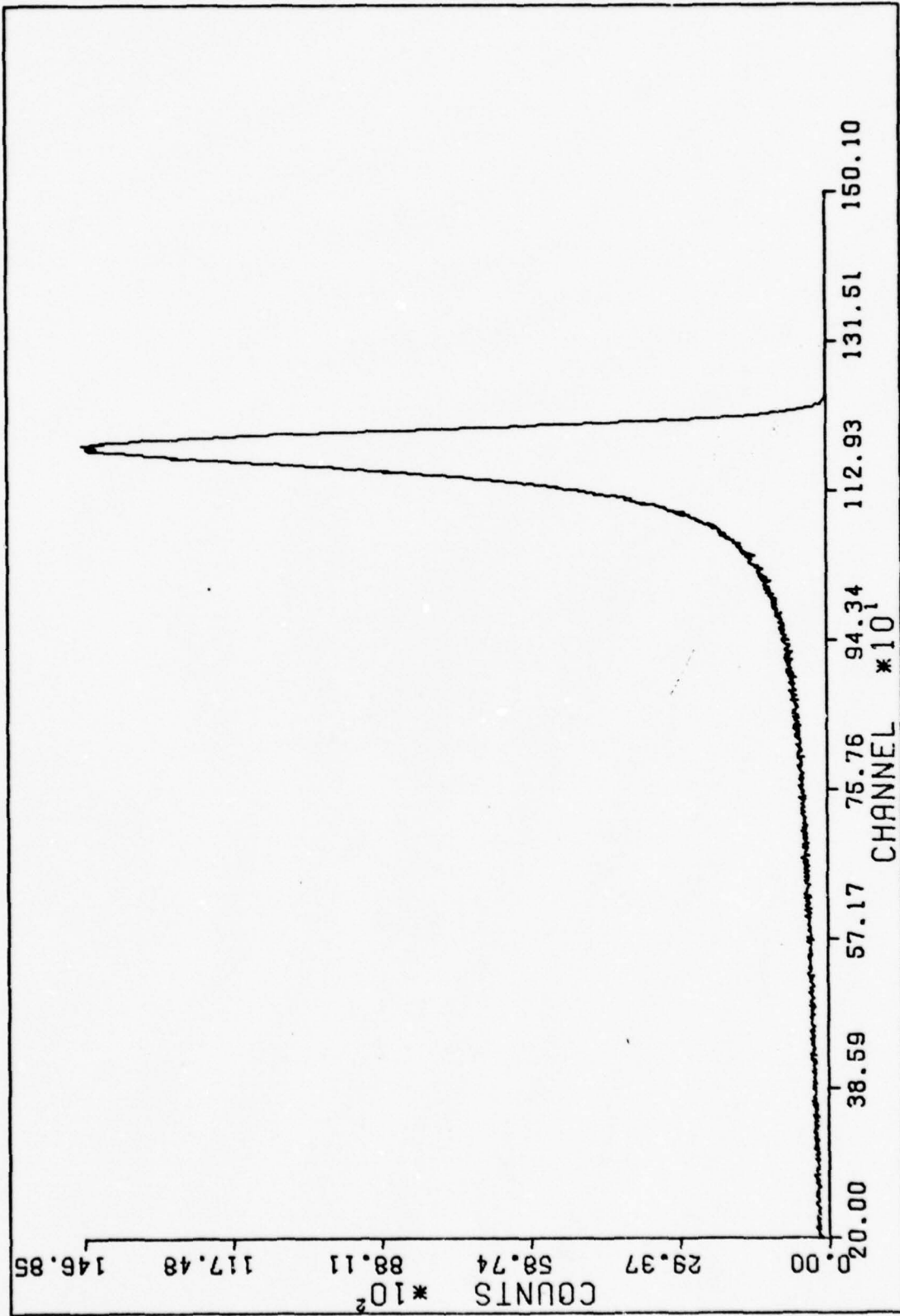


FIG11. RA DEF # 12 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

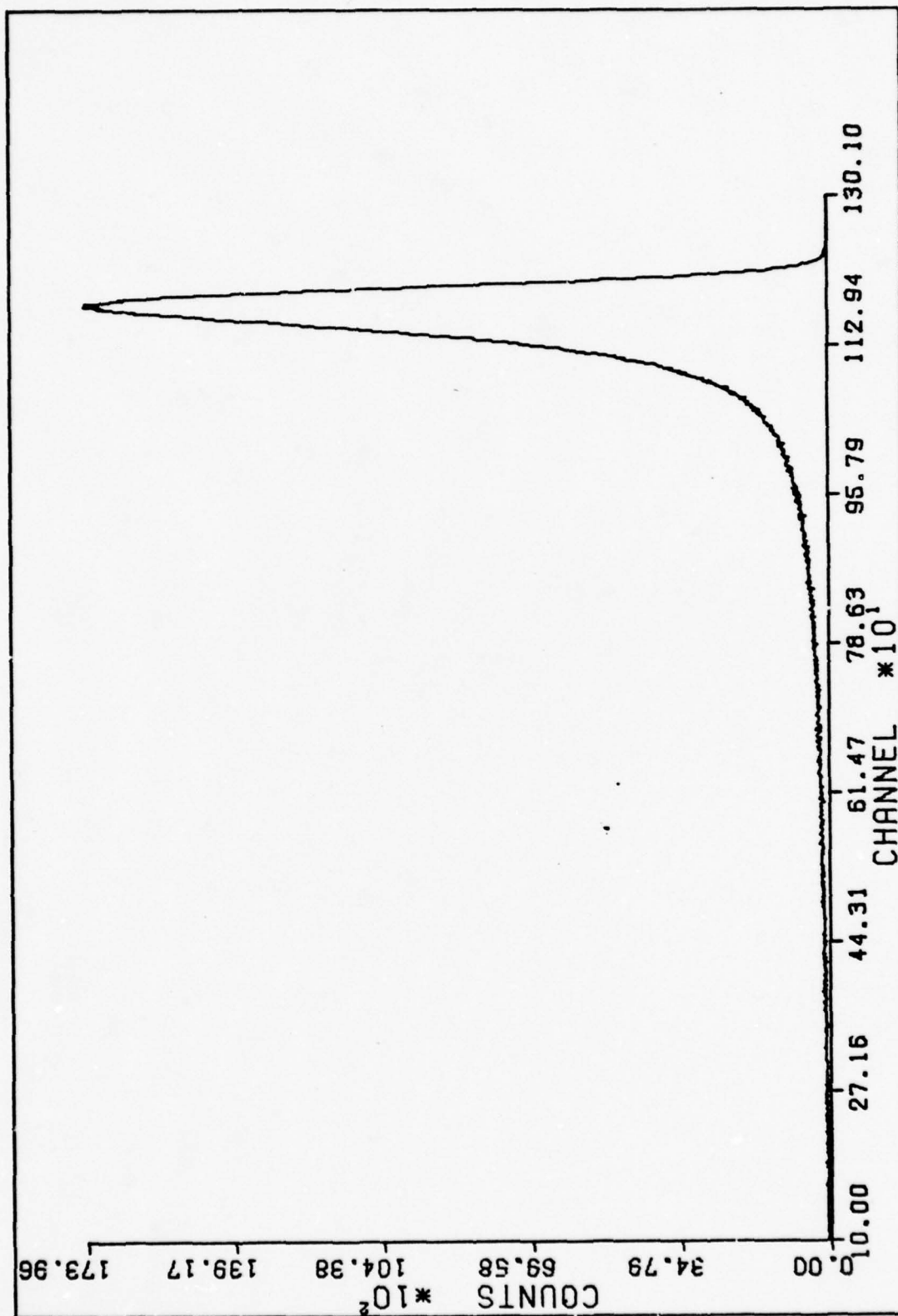


FIG 12. RA DEF # 13 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

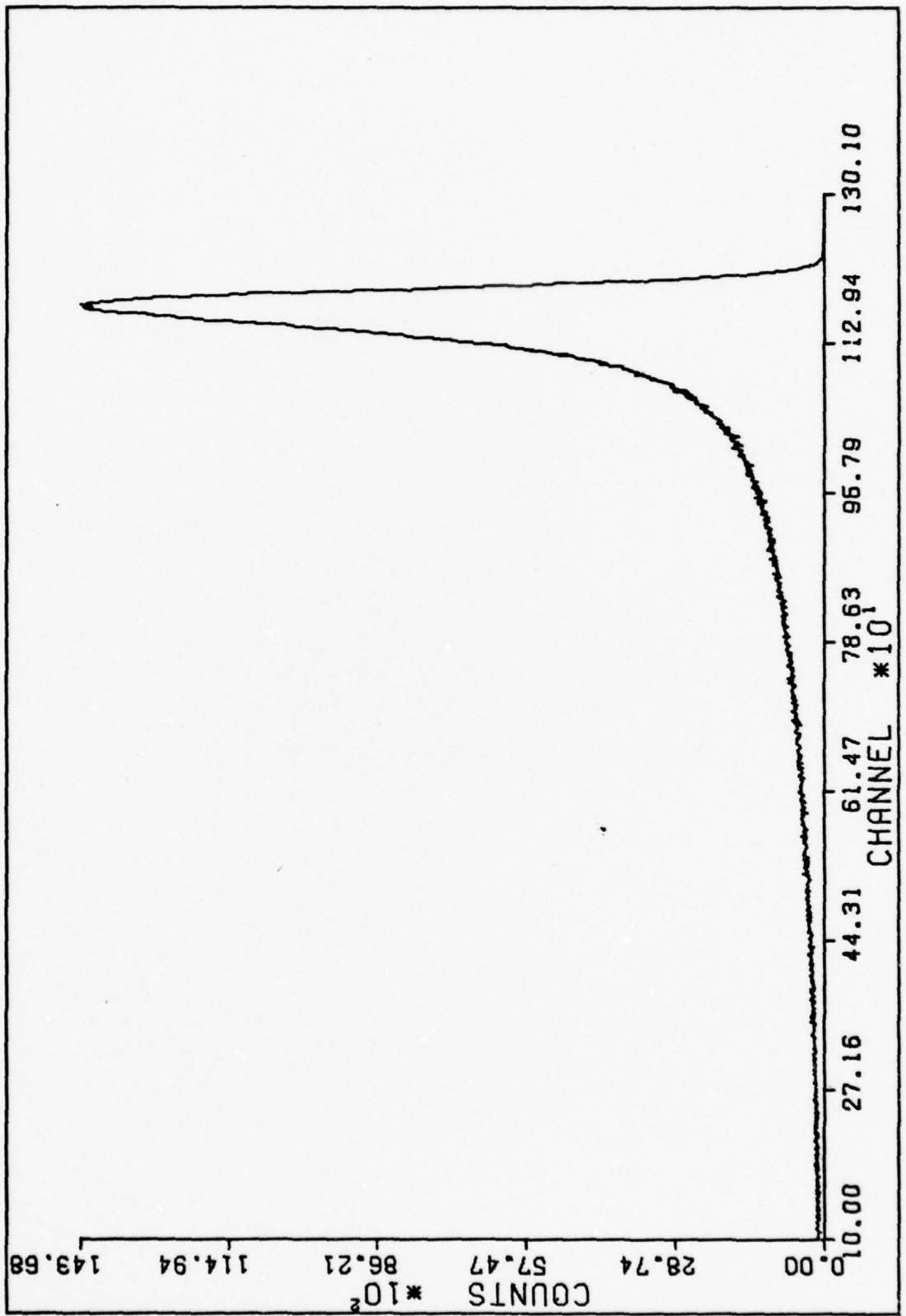


FIG 13. RA DEF # 14 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

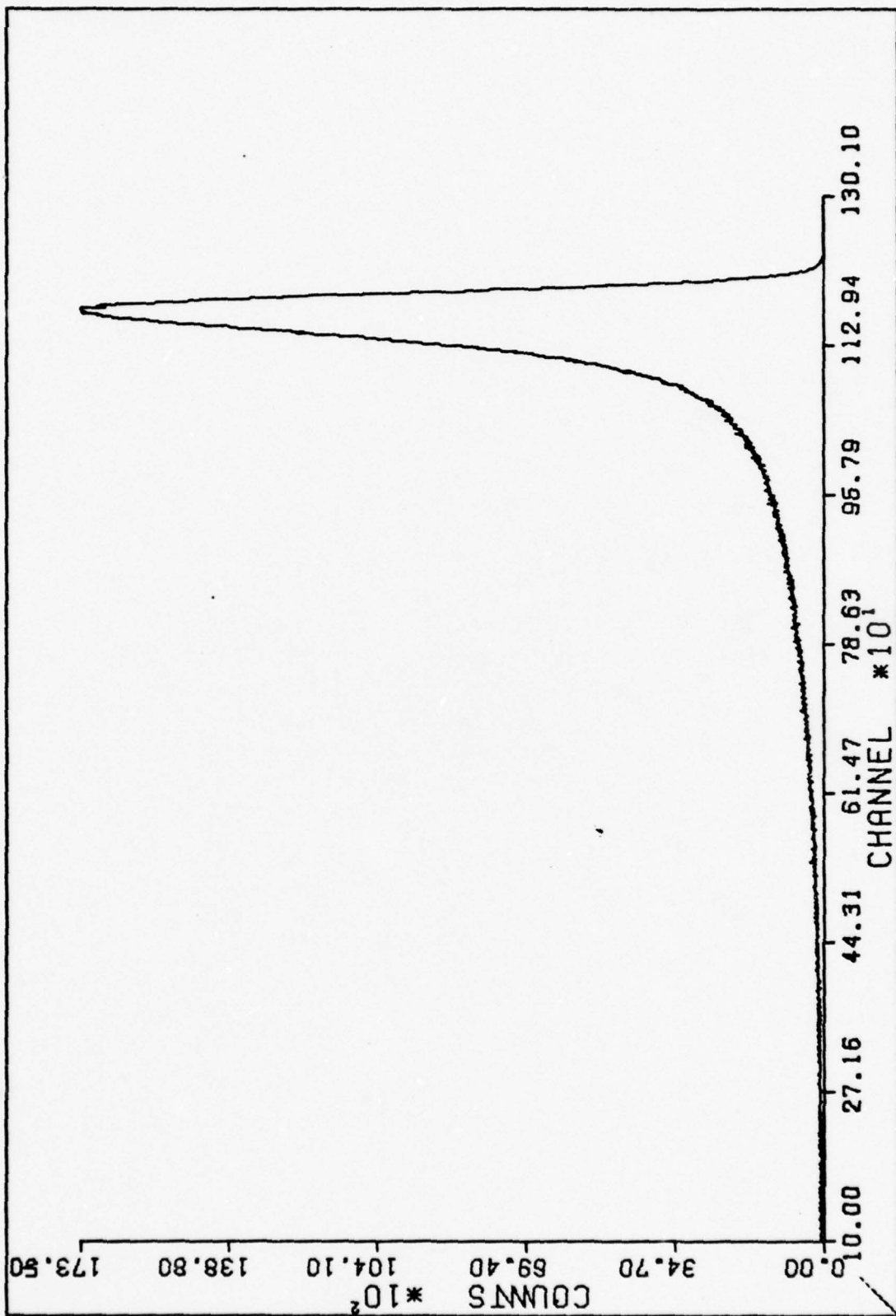


FIG 14. RA DEF # 15 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

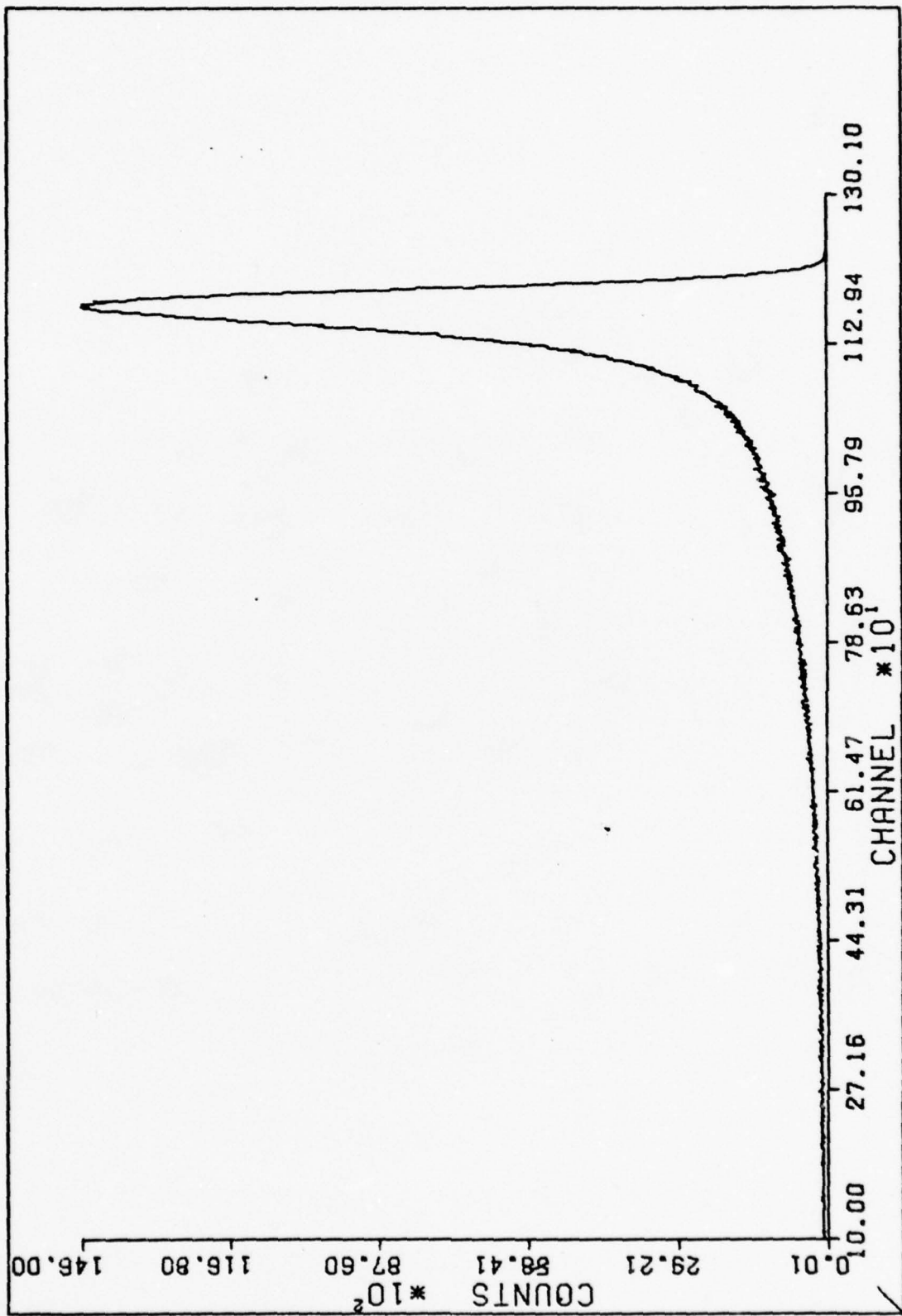


FIG 15. RA DEF # 16 (OXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

V. Program Modifications

Introduction

The starting point for these programs was Program ALPHAFIT, which was produced by Lieutenant Richard S. Hartley with the help of Phil Poirier from Program AUTOFIT written by J. R. Comfort (Ref 5). Two specific modifications were originally planned, to convert the program to read the spectral data directly from magnetic tape or disc storage, and to use a library of curves to choose the curve which will give the best analysis and use it to analyze the unknown spectrum. In addition, subroutines were written to create Gaussian spectra modified by a Poisson distribution for counts in each channel and these spectra were used in place of detector spectra to study the program's performance.

Conversion to Tape

It was desired to convert the program to read the spectral data directly from the magnetic tape on which they were written by the multi-channel analyzer. Two programs, SCRIPT and SPECTRA were written by H. Careway (Ref 3) to use the FORTRAN BUFFER IN and DECODE statements to read these data into an array. SCRIPT then prints out the numbers, while SPECTRA produces a CALCOMP plot. The READ section of these programs was extracted and modified into subroutine RDSPEC. RDSPEC was then called directly from the main

program to read the reference spectra and from subroutine SPCTRM to read the unknown spectrum.

Reading the data in this manner is not without difficulty. First, the spectra to be read must be placed in order on file TAPE1 by using the SKIPF and COPYCF control card statements. Then, the statement FILE, TAPE1, FO=SQ, BT=C, RT=S, BFS=1000. is used to tell the computer this is a stranger tape (RT=S) and the buffer size (BFS=1000). This must be followed by a LOAD-SET statement such as LDSET, FILES=TAPE1, PRESET=ZERO.

Second, perhaps because of a stray bit or an unclean tape, a datum would be rejected by the computer dumping the program immediately. RDSPEC was modified with the statement, ERRSET (KOUNTS,100), so that the program would not dump for just one such datum. The numbers read in this way were always satisfactory, but occasionally the bottom section of a spectrum would be rejected by the computer.

Reorganization

Program ALPHAFIT analyzed spectra of 2048 channels for up to 20 separate peaks. This is necessary for analyzing a spectrum with several isotopes over a wide range of energies but requires an enormous (over 250K) quantity of core storage. This requirement impedes studying the behavior of the program, making changes, and troubleshooting, so the program was reduced to analyzing 512 channels out of the 2048 containing up to five peaks. This reduced the

core requirements to 120-124K, which allowed several runs each evening. However, this reorganization imposed certain limits. With the biased amplifier spreading the spectrum out to 0.48 or 0.60 KeV per channel, a range of only 250-300 KeV could be studied. This was adequate for Am^{241} but insufficient for the Pu^{240} spectra taken, so only the two largest peaks in Pu^{240} were analyzed. More than five peaks would have to be analyzed in most unknown spectra.

The second change was to have the program read and store five reference spectra to analyze each unknown spectrum. This was done simply by copying each spectrum into the array REFSTO (520,5) before using the reference to analyze the unknown.

Artificial Spectra

In order to study the performance of the program's analyzing routines, it was desired to generate spectra of arbitrary characteristics to simulate alpha spectra. Subroutine CONJUR was written to use several routines written by Bevington (Ref 2) to generate Gaussian peaks of specified height, standard deviation and position, add them to create a spectrum, then randomly modify the counts in each channel according to an approximate Poisson distribution. CONJUR and the associated subroutines were then substituted for subroutine RDSPEC. The resulting program was called ALFAIC.

VI. Program Computation Results

Introduction

The program's analyzing performance was extensively tested under idealized conditions by using generated Gaussian type spectra. Samples of americium and plutonium were analyzed by the 512 channel version using the best of the samples prepared (after oxidizing). One of the plutonium samples was also analyzed using the 2048 channel version of the program. These analyses showed that a difference of only one channel between the widths of the reference and unknown peaks caused significant reduction in the accuracy of the analysis.

Conjured Spectra

The program was used to analyze spectra composed of two Gaussian peaks with a standard deviation (σ) of 20 channels. The separation between these peaks was varied from one quarter to two and a half times the standard deviation (5-50 channels) to investigate the anomaly reported by Hartley (Ref 5:22). The width of the reference peak was varied from 15 to 25 channels to observe this effect.

Separation Effect. The program was tested with peaks of 5:10 and 1:10 relative heights (Tables VI and VII). None

Table VI

Errors Versus Separation Distance for Gaussian
 Peaks 1/2 = 5:10, $\sigma = 20$, Peak 1 in
 Channel 250, True Area ≈ 572000

Center Peak 2	$\frac{\text{Area}(\text{true}) - \text{Area}(\text{comp})}{\text{Area}(\text{true})}$	RMS Error %	Estimated Error		Ratio $\frac{\text{Peak 2}}{\text{Peak 1}}$
	%		Peak 1, Peak 2		
255	.064	.035	805	865	.238
260	.065	.038	525	543	1.933
265	.065	.037	355	390	2.358
270	.062	.051	313	357	2.233
275	.0604	.046	254	301	2.120
280	.0581	.035	196	236	1.986
290	.0538	.033	164	209	2.007
300	.0480	.035	152.5	202.4	2.0008

Table VII

Errors Versus Separation Distance for Gaussian
 Peaks 1/2 = 1:10, $\sigma = 20$, Peak 1 in
 Channel 250, True Area ≈ 417000

Center Peak 2	$\frac{\text{Area(true)} - \text{Area(comp)}}{\text{Area(true)}}$ %	RMS Error %	Estimated Error Peak 1, Peak 2		Ratio Peak 2 Peak 1
255	.084	.043	285	222	.0047
260	.079	.079	348	218	.012
265	.087	.129	173	460	81
270	.078	.045	169	236	10.7
275	.075	.044	134	211	10.3
280	.072	.043	107	191	10.2
300	.083	.043	78	195	10.04
350	.049	.042	52	161	10.06

of these peaks were sufficiently separated to show a drop in counts between the two peaks (Figures 16-17). (Compare with the americium and plutonium spectra in Figures 6 and 8.)

The absolute difference between the computed and true areas rises gradually as the two peaks approach. When the peaks are separated by less than one standard deviation, the Root Mean Square difference between the computed approximation and the analyzed spectrum declines as the smaller peak vanishes into the larger, while the computed error in each peak is generally larger and the computed ratio of the two peaks fluctuates wildly.

These results show the program is unable to resolve two peaks accurately when they are so close as to appear to be one (See Figure 18). Nevertheless, both the difference between the absolute areas of the unknown and resolved spectra, the absolute residual, and the Root Mean Square of the difference at each point, the average residual, remain less than 0.1%. The two peaks have merged and are indistinguishable. The only indication that the spectrum is composed of more than one peak is the 1-10% difference between the left and right half widths at half maximum.

Reference Width Effect. The analysis of peaks of fixed width with references of various widths show (See Tables VIII and IX and Figures 19-20) that matching the spread of the reference to that of the unknown can reduce the residuals

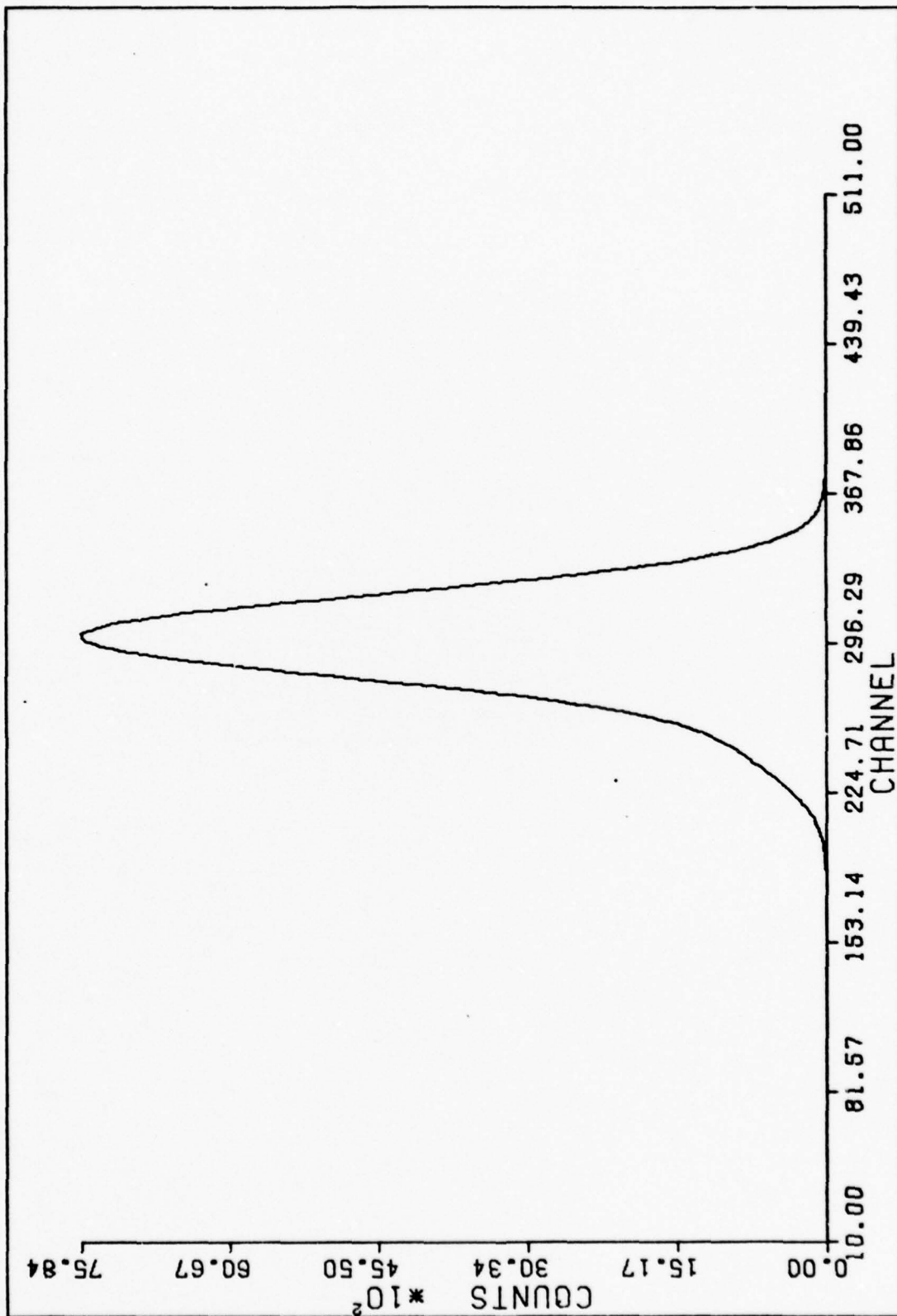


Fig. 16. Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 1000, 10000.

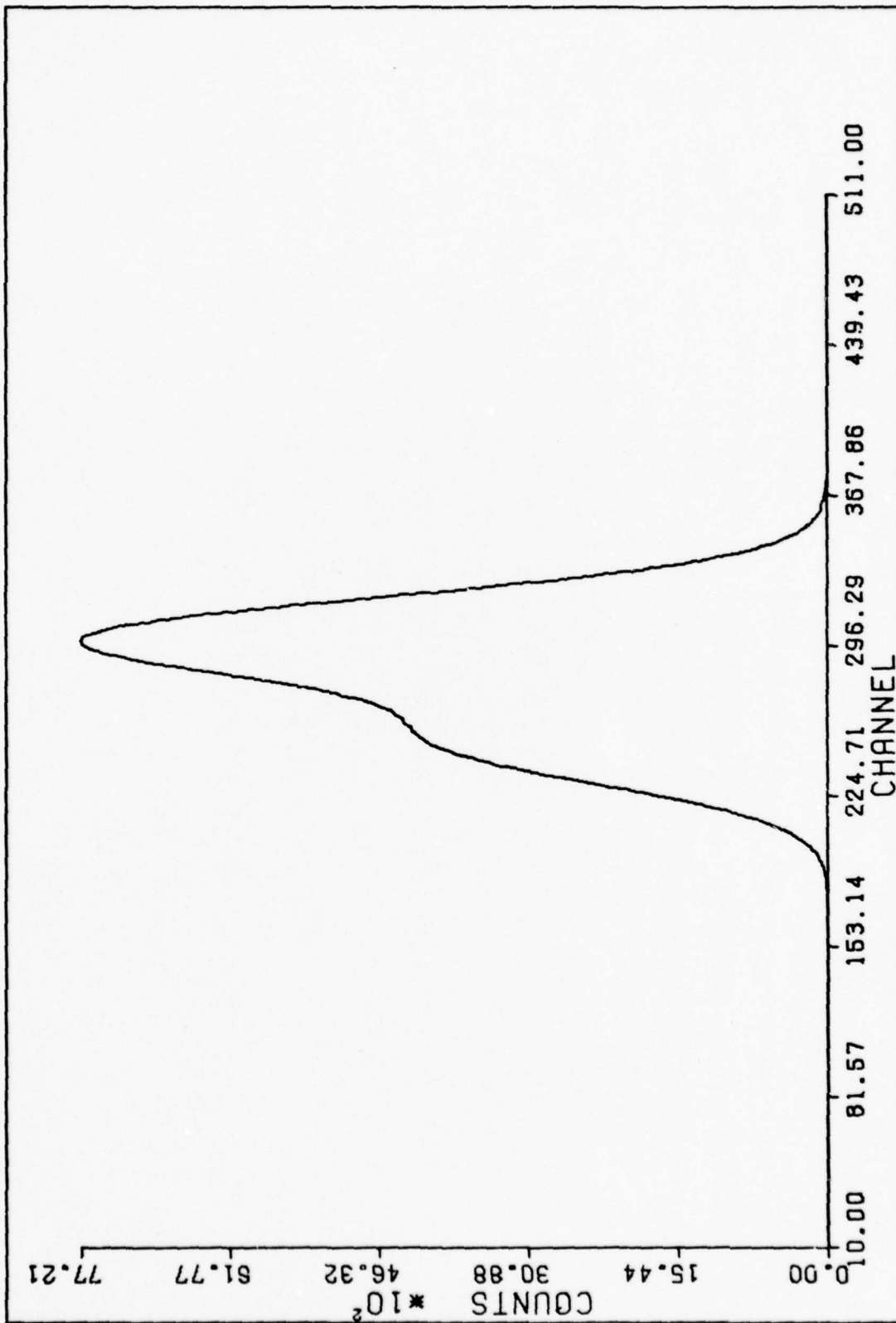


Fig. 17, Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 5000, 10000.

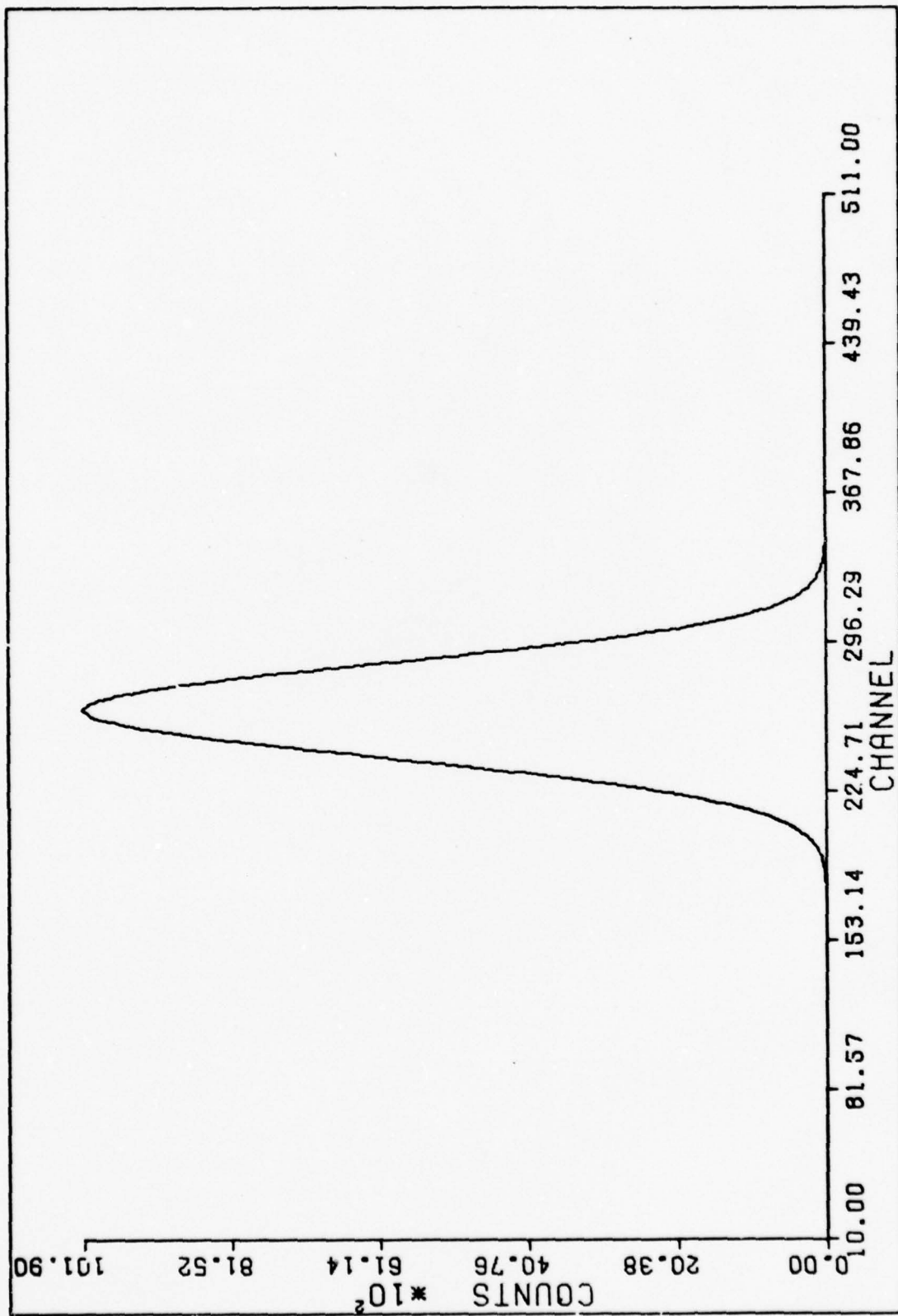


Fig. 18. Randomized Gaussian Peaks. Separation = 20 Channels.
 Heights are 5000, 10000.

Table VIII

Analysis of ($\sigma = 20$) Gaussian Peaks with Reference
 Peaks of Varying σ . Ratio of Peak
 Heights = 10:1 Separation = $50(2.5 \sigma)$

Reference σ	True Area -Resolved Area	RMS Error	Resolved Ratio of Two Peaks
15	2092	10299	7.1
16	1175	7857	7.6
18	134	3570	8.6
19	296	1374	7.9
19.5	4.2	703	8.8
20.0	237	171	10.05
20.5	353	761	11.1
21.0	436	1492	12.3
22	564	2954	13.5
24	731	5363	18.3
25	703	11297	-66

Table IX

Analysis of ($\sigma = 20$) Gaussian Peaks with Reference
Peaks of Varying σ . Ratio of Peak
Heights = 10:5 Separation = $50(2.5 \sigma)$

Reference σ	True Area -Resolved Area	RMS Error	Resolved Ratio of Two Peaks
15	4392	13127	1.72
16	2527	10130	1.77
18	623	4724	1.88
19	6.4	1926	1.939
19.5	168.6	964.8	1.9699
20.0	272.8	198.4	2.0008
20.5	394.6	927.8	2.046
21.0	500.2	1728.8	2.11
22	678	4154	2.23
24	952	7856	2.56
25	1072	9580	2.76

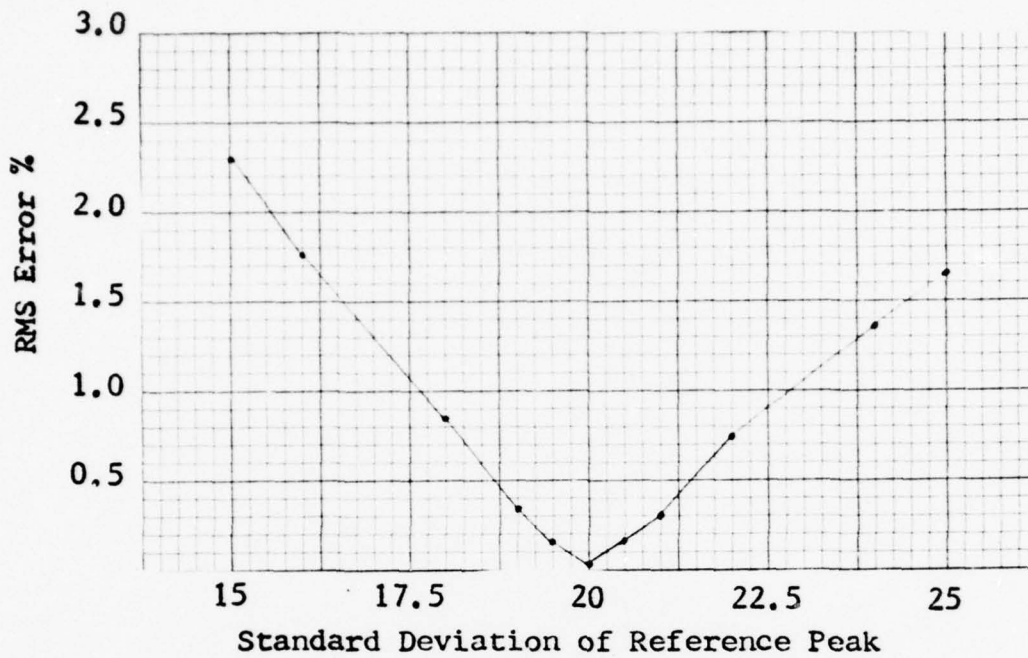


Fig. 19. Analysis of ($\sigma = 20$) Gaussian Peaks with Reference Peaks of Different Widths. Ratio of Peak Heights = 10:1.

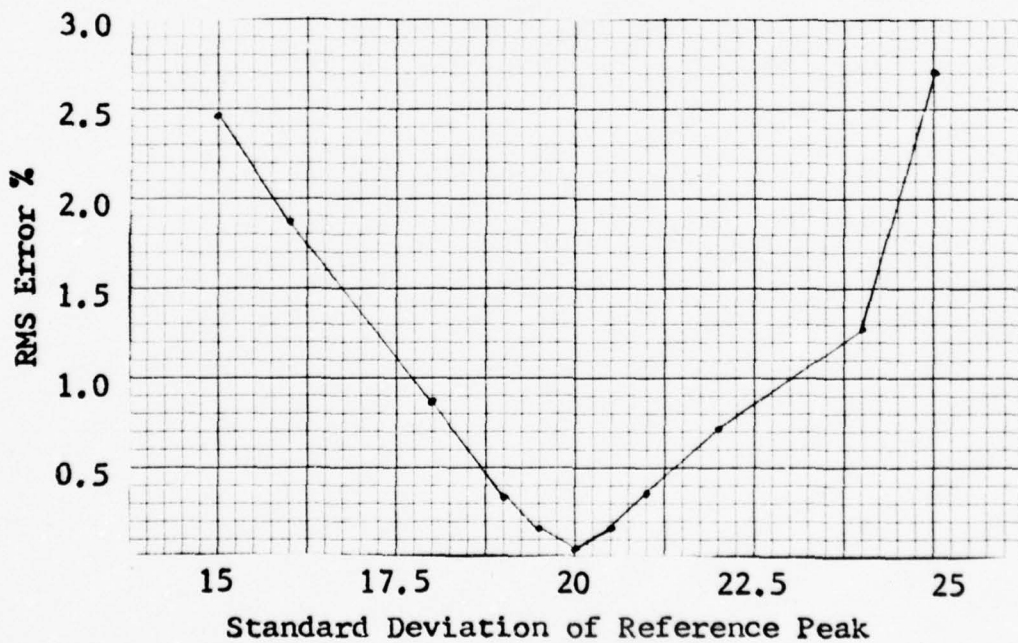


Fig. 20. Analysis with Reference Peaks of Different Widths. Standard Deviation of Peaks Analyzed = 20. Ratio of Peak Heights = 10:5.

by two or three orders of magnitude under ideal conditions. A difference of only 0.5 in the standard deviation produces a clear increase in the RMS error.

Real Spectra

512 Channel Analyses. The first group of analyses were conducted on a 512 channel segment out of the full 2048 channel spectrum. Five spectra were used to analyze two samples, Am²⁴¹ and Pu²⁴⁰ #1. The spectra from the oxidized Ra DEF samples 10, 11, 12, 13, and 16 were selected because they had the sharpest peaks. Although these peaks could not be placed in sequence showing a continuous regular change in the curve shape, they could be placed in order of their full width at half maximum. As shown in Table X and Figures 21 and 22, the RMS error corresponded directly to the fit between the FWHM's of the unknown and the reference used for analysis. It first dropped and then rose as the FWHM increased for the plutonium sample and rose steadily for the americium sample.

Other measurements of the accuracy of the fit were not as well correlated to the FWHM. The difference in areas when analyzing Pu²⁴⁰ #1 showed the same trend as the RMS error except for sample #10, but there was no agreement when analyzing americium. The computed ratio of the two main peaks in Pu²⁴⁰ was too low except for sample 16.

2048 Channel Analyses. The analyses on the full 2048 channel spectrum of Pu²⁴⁰ showed good correlation between

Table X

Analysis of Plutonium and Americium with Polonium
Spectra of Varying Self-Absorption. All
Spectra from 100 mm² ORTEC Surface Barrier
Detector at 30-35 V Net Bias

Unknown = Pu ²⁴⁰ #1		FWHM = about 32		
Reference Spectrum from Sample #	FWHM (KeV)	Δ Area Error (counts)	RMS Error (counts)	Computed Ratio
11	29.2	9318	11244	2.79
16	32.8	7833	10618	3.06
13	34.3	7206	6943	2.42
10	34.7	23038	5942	2.67
12	35.3	7773	9616	2.71

Unknown = Am ²⁴¹		FWHM = 21.1		
Reference Spectrum from Sample #	FWHM (KeV)	Δ Area Error (counts)	RMS Error (counts)	
11	29.2	29140	18325	
16	32.8	24330	20954	
13	34.3	15630	21835	
10	34.7	9642	21709	
12	35.3	19826	23368	

NOTE: Only 512 channels of these spectra containing the two or three chief peaks were analyzed. The ratio for plutonium is for the 5.168 and 5.123 meV peaks. The true ratio is 3.167.

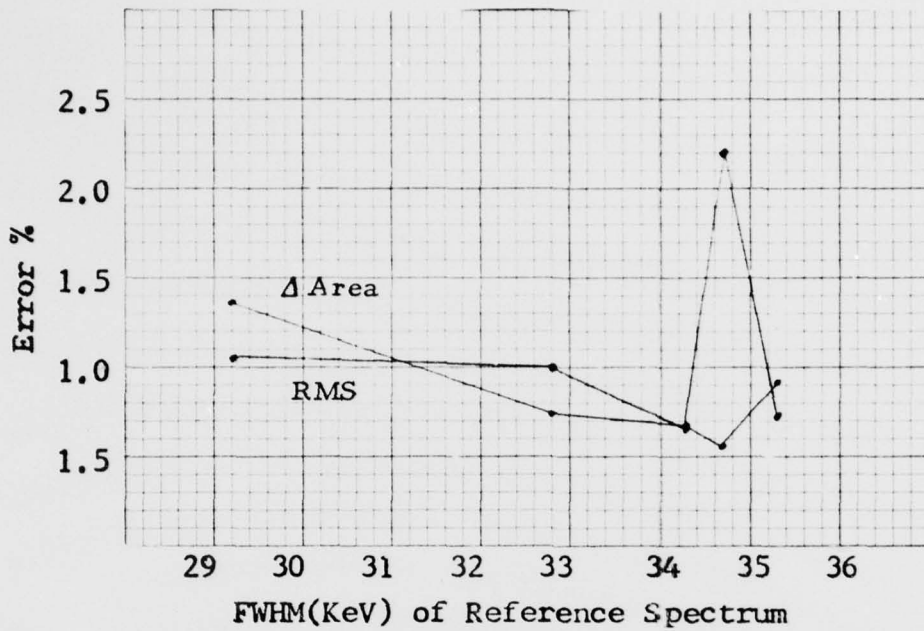


Fig. 21. Analysis of Pu²⁴⁰ #1 with Various Ra DEF Samples. All Spectra From ORTEC 100 mm² SBD at 30-35 V Net Bias.

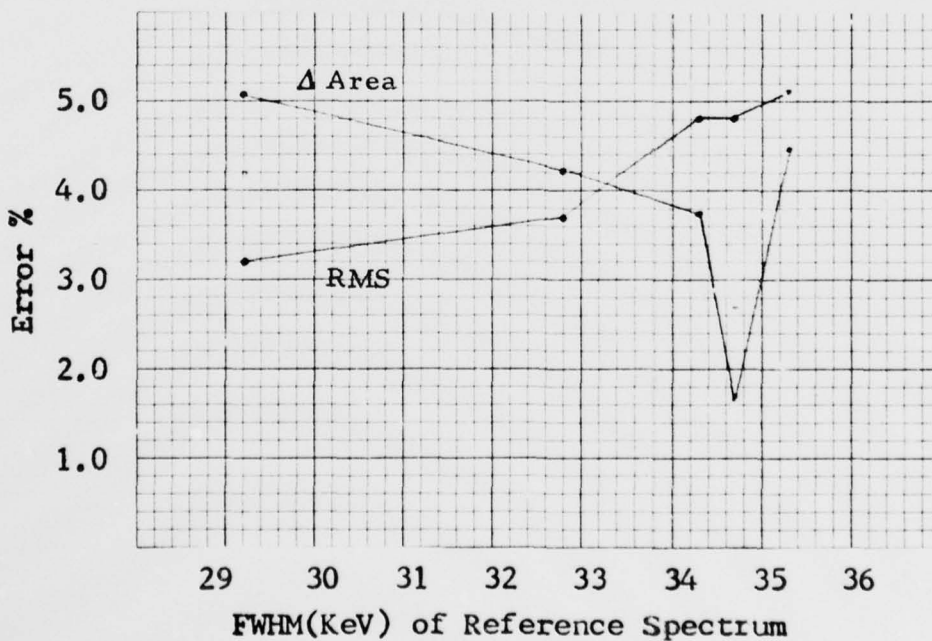


Fig. 22. Analysis of Am²⁴¹ with Various Ra DEF Samples. All Spectra From ORTEC 100 mm² SBD at 30-35 V Net Bias.

all three measures of the fit and the match of the FWHM's except for reference sample #15 (See Table XI and Figure 23). This had the largest FWHM but gave the second best fit. The resolved composite areas were 50% to 150% too large and the composite now gave too large a percentage of the counts to the largest peak. These results confirm that matching the reference curve shape to the spectrum being analyzed gives a more accurate analysis.

The results of these analyses show the potential of the library of curves approach to produce a more accurate analysis of alpha spectra. However, the program remains unstable and capable of producing bizarre results even under good conditions. The peak locating routines will sometimes shift the locations of two clearly separated peaks to only a few channels apart and at other times will shift one or more peaks completely out of the spectrum. The routines which compute the relative multipliers for each peak (See Eq (4)) will at times return a negative value for one of the peaks. These problems need to be solved in future work with this program before it can be considered completely reliable. Even then, the program's performance will be limited by the reference spectra available.

Table XI

Results of 2048 Channel Analyses of Pu²⁴⁰ #1

Pu ²⁴⁰ FWHM = 103.58 Channels				
Reference Sample	FWHM Channels/KeV	Δ Area Counts/%	RMS Counts/%	Peak Ratio
110x	50.68/29.2	1624448/142	75965/6.6	16.4
160x	57.07/32.8	1033675/90	53577/4.7	7.3
130x	59.59/34.3	551953/48	37264/3.25	4.42
100x	58.05/34.7	902232/79	46422/4.05	5.8
120x	60.59/35.3	1203889/105	63790/5.6	17.4
140x	60.63/35.3	1375767/120	63419/5.5	12.4
150x	62.47/36.4	831737/73	43413/3.8	4.98

NOTE: The peak ratio is for the 5.168 and 5.123 meV peaks.
The true ratio is 3.167.

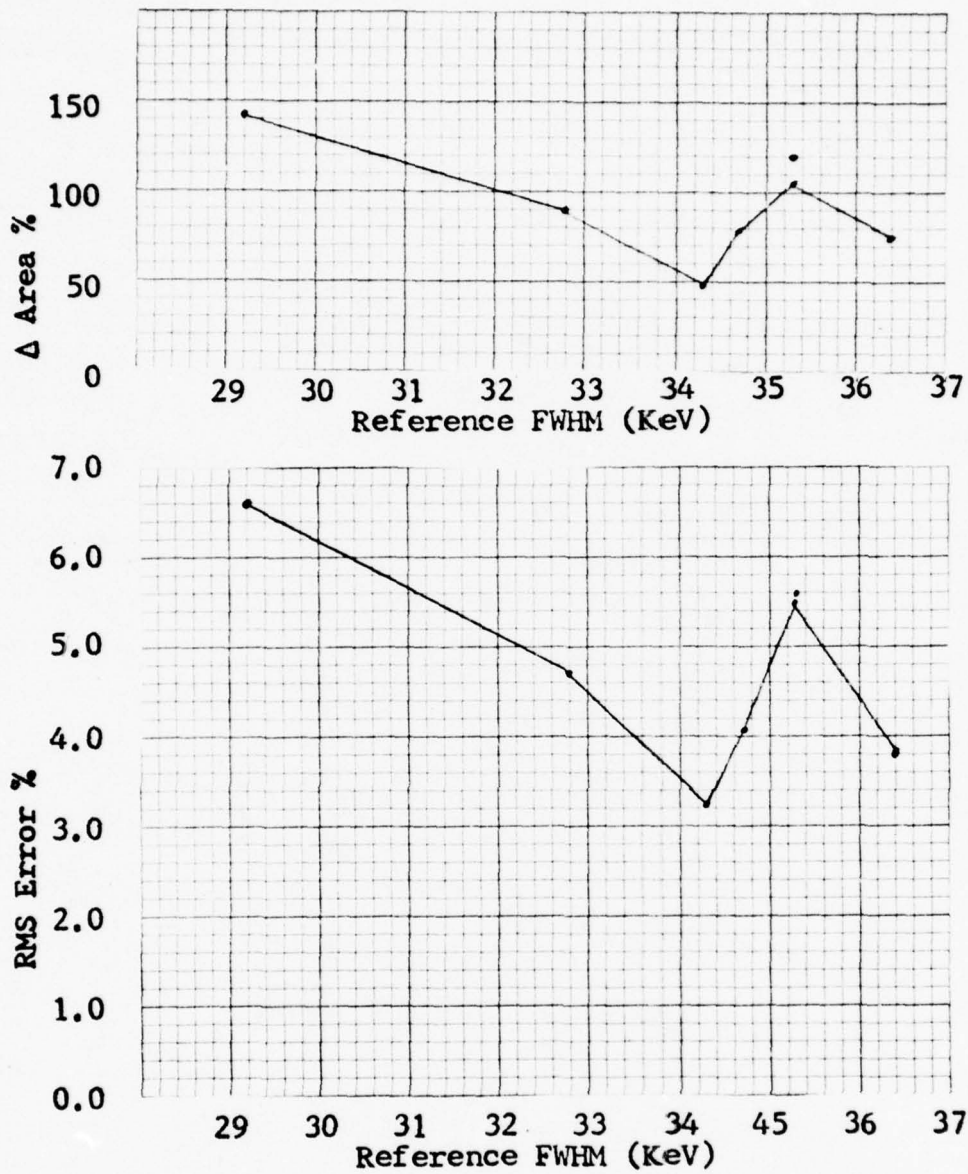


Fig. 23. Results of 2048 Channel Analyses of Pu²⁴⁰ #1 with Various Ra DEF Samples. All Spectra From ORTEC 100 mm² SBD at 30-35 V Net Bias.

VII. Conclusions and Recommendations

Conclusions

The analyses with generated spectra clearly show that, at least under ideal conditions, matching the FWHM of the reference peak to the FWHM of the spectrum to be analyzed gives a better analysis. Differences of only one channel in these FWHM's were shown to increase the RMS error by a factor of 3 to 5. This strongly supports the need for a library of reference curves to use in analyzing various alpha spectra.

The analyses with real spectra also support these conclusions. The reduced range (512 channel) analyses of americium and plutonium both show a reduction in the RMS error as the FWHM of the reference peak is made closer to the FWHM of the spectrum analyzed. The full range (2048 channel) analyses of plutonium confirm this reduction of the RMS error and, in addition, show a corresponding reduction in the absolute residual area and more accurate resolution of the relative areas in the two chief peaks.

These analyses show that the use of a library of reference spectra can give a several percent reduction in error provided that reference spectra with the correct characteristics are available. The chief need at this time is for a consistent set of smoothly varying spectra,

including a range of FWHM's as low as 20 KeV or better.

Recommendations

Samples. The main need is for better reference samples. Po^{210} is clearly the isotope to use. It may be possible to prepare adequate Ra DEF samples, but these will have to be the oxide or perhaps bare metal. The nitrate samples have too much self-absorption, even with no added lead. An electroplating technique will probably be required to produce samples with low enough self-absorption.

There are two further studies that could be made with the samples prepared for this thesis. New spectra should be obtained from samples 7-9. If the peaks from these have FWHM's as narrow as indicated in Table II, they should be used to analyze samples with correspondingly low self-absorption such as the americium²⁴¹ sample used in this study. Additional spectra from the later set (10-21) should also be taken in another year or two to check for changes in the curve shapes due to a more even distribution in the polonium²¹⁰ as a result of radioactive decay.

Program. There are also improvements that can be made in the program. A big problem is how to store and access a large library of 2048 channel reference spectra. These will probably have to be stored on magnetic tape, so some means of conveniently reading a particular record is needed.

The operation of the main program could be considerably streamlined by eliminating some of the unused options. The following sequence should be adequate. First, controlling data are read. Second, the spectrum to be analyzed and a background spectrum are read. The FWHM is computed for the largest peak in the unknown spectrum and a reference spectrum is selected and read. The program then passes these three arrays to the analysis routines and conducts the analysis. The automatic and interpolated background options and the computer-derived peak shape options could then be eliminated.

It would also be useful to modify the analyzing routines so that the spectrum for each peak extends all the way to zero, perhaps using a computed average of the lower channels to fill the gap from the bottom channel down to zero. Finally, the analysis routines should be carefully studied to verify their correct operation and make useful modifications such as rejecting negative peaks and limiting the shifting of the specified peaks to a fixed range about the specified location. These routines are the subroutines PREPAR and DAVIDN and all the subroutines called by these two.

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Appendix A

Utility Programs

Introduction

Several programs besides ALPHFT (alpha fit) were used during the work on this thesis. It was decided to read the multi-channel analyzer generated data from magnetic tape (or tape-derived permanent disc) storage. Captain Harold A. Careway (Ref 3) had written two programs, SCRIPT and SPECTRA, to perform this operation using the FORTRAN BUFFER IN and DECODE statements.

Program SCRIPT

Program SCRIPT was designed to read in a series of L consecutive spectra, then print out the first IC channels of each spectrum. In the form developed by Careway, both SCRIPT and SPECTRA were quite sensitive to some phenomenon which caused the code for a number to be interpreted as the code for {, @, ", or some other character. This would cause the computer to dump the program without reading, writing, or plotting any more spectra. At the suggestion of Captain Stinson, these programs were modified using the CALL ERRSET statement to allow the computer to accept a few such events before dumping the program. This allowed subsequent spectra to be read and written or plotted on the

same computer run. By printing out only the first few lines from a spectrum, program SCRIPT could easily be used to investigate which spectra contain bad data. However, when the full spectrum was printed out after such an occurrence, no bad data were observed.

Program SPECTRE

Program SPECTRA, the plotting routine, was extensively modified so that it could be used to plot the graphs for this thesis. It was then renamed SPECTRE. In the original form, it generated only a large graph of variable dimensions similar to the type 2 plot in SPECTRE but with no title. The program always plotted channels 70 to IC, an input variable. The spectra to be plotted had to be placed in order on the file TAPE1 by correct use of the SKIPF, COPYCF, and REWIND control cards. Provision was made to edit erroneous data prior to plotting.

Modifications

The program was first modified using CALL ERRSET as was SCRIPT. It was then modified using additional CALL PLOT statements and a CALL SYMBOL statement to generate a smaller plot enclosed in a box with boundaries marked for cutting with a title at the bottom of the page (after cutting). The titles were initialized in the array ITITLE by a series of DATA statements and the correct title was determined from the tagword of the data to be plotted. Finally, the program was heavily modified to allow the user to read the 4XN array

NTAG, which specified the spectrum/tagword to be plotted, a choice of the old and new formats, and the first and last channels to be plotted. It is still desirable to register the first spectrum to be plotted by using the SKIPF control card in order to reduce Input/Output time, but this is not necessary. The tagwords to be plotted may be read in any order but will be plotted in ascending order.

Appendix B

Program SCRIPT

```

PROGRAM SCRIPT(INPUT,OUTPUT,TAPE1)
DIMENSION Y(4100),X(256),MW(160)
C THIS PROGRAM PRINTS OUT SPECTRA
C THE FIRST SPECTRA TO BE PRINTED OUT MUST BE REGISTERED BY USE OF
C THE SKIP CONTROL CARD
C THE FIRST DATA CARD IS IN FORMAT ***** L= NUMBER OF SPECTRA
C THE SECOND DATA CARD IS IN FORMAT ***** IC= NUMBER OF CHANNELS
C*****
READ 1000,L
READ 1000,IC
DO 100 J=1,L
N=1
KK=1
10  BUFFER IN(1,0)(MW(1),MW(160))
    KK=UNIT(1)
    CALL ERSET(KOUNT,100)
    DECODE(100,50,MW)M,M,X
    IF(KOUNT.GT.0) GO TO 100
50  FORMAT(2X,I1,2X,A4,23F6.0,9(/25F5.0),/,8F5.0)
    DO 80 I=1,256
        Y(N)=X(I)
80  N=N+1
    IF(KK.NE.0)GO TO 10
    PRINT*, " UNIT(1) = ",KK," N = ",N
    PRINT 1010,M
    NN=(IC/10)+1
    DO 90 K=1,NN
        IN=(K-1)*10
        II=IN+1
        PRINT 1020,IN,Y(II),Y(II+1),Y(II+2),Y(II+3),Y(II+4),Y(II+5),Y(II+
C6),Y(II+7),Y(II+8),Y(II+9)
90  CONTINUE
100  CONTINUE
1000  FORMAT(I5)
1010  FORMAT(14I,15I,"TAGWORD NUMBER",155,I5)
1020  FORMAT(1X,I5,10F10.0)
STOP
END

```

Appendix C

User Instructions for SCRIPT

Program SCRIPT is simple to use. The spectra to be read are placed on file TAPE1. The FILE and LDSET statements tell the computer the buffer size for the file and load it to be read. Two data cards are required in I5 format. The first should contain L, the number of spectra to be read and printed. The second should give IC, the number of channels to be printed out for each spectrum starting with channel 0. A typical control card sequence would be the following.

FTN.

ATTACH, TAPE1, XFILE, MR=1.

FILE, TAPE1, FO=SQ, BT=C, RT=S, BFS=1000.

LDSET, FILES=TAPE1, PRESET=ZERO.

LGO.

Appendix D

Program SPECTRE

PROGRAM SPECTRE(INPUT,OUTPUT,PLOT,TAPE1)

C*****

C PROGRAM SPECTRE IS AN ELABORATED VERSION OF PROGRAM SPECTRA,
 C WHICH WAS PROVIDED BY DR. GEORGE JOHN.
 C IT ALLOWS THE PLOTTING OF TWO DIFFERENT PLOTS INTERCHANGEABLY:
 C ONE IS A SMALL BORDERED PLOT IN AFIT THESIS FORMAT.
 C THE OTHER IS A LARGER VERSION, WHICH MAY BE MORE SUITABLE
 C FOR DIRECT COMPARISONS.

C

DIMENSION X(4100),Y(4100),Z(256),M(160)
 DIMENSION ITITLE(6,100)
 DIMENSION NTAG(4,20),XA(2),YA(2)

C*****

DATA ITITLE(1,42)/60HFIG	. RA DEF # 17 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,43)/60HFIG	. RA DEF # 17 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,44)/60HFIG	. RA DEF # 18 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,45)/60HFIG	. RA DEF # 18 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,46)/60HFIG	. RA DEF # 19 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,47)/60HFIG	. RA DEF # 19 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,48)/60HFIG	. RA DEF # 20 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,49)/60HFIG	. RA DEF # 20 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,50)/60HFIG	. RA DEF # 21 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,51)/60HFIG	. RA DEF # 21 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,52)/60HFIG	. AM 241 ORTED 1/21/69	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,53)/60HFIG	. AM 241 ORTED 1/21/69	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,54)/60HFIG	. AM 241 ORTED 1/21/69	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,55)/60HFIG	. AM 241 ORTED 1/21/69	0.6 KEV/CHAN
CNEL 10000 SEC. /		
DATA ITITLE(1,56)/60HFIG	. RA DEF # 15 (JNOXIDIZED)	UNBIASED RUN
C 40,000 SEC. /		
DATA ITITLE(1,57)/60HFIG	. RA DEF # 15 (JNOXIDIZED)	UNBIASED RUN
C 40,000 SEC. /		
DATA ITITLE(1,58)/60HFIG	. RA DEF # 15 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,59)/60HFIG	. RA DEF # 15 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,60)/60HFIG	. RA DEF # 14 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40000 SEC. /		
DATA ITITLE(1,61)/60HFIG	. RA DEF # 14 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40,000 SEC. /		
DATA ITITLE(1,62)/60HFIG	. RA DEF # 13 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40,000 SEC. /		
DATA ITITLE(1,63)/60HFIG	. RA DEF # 13 (JNOXIDIZED)	0.6 KEV/CHAN
CNEL 40,000 SEC. /		

DATA ITITLE(1,64)/60HFIG CNEL 40,000 SEC./	. RA DEF # 12 (JNOXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,65)/60HFIG CNEL 40,000 SEC./	. RA DEF # 12 (JNOXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,66)/60HFIG CNEL 40,000 SEC./	. RA DEF # 11 (JNOXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,67)/60HFIG CNEL 40,000 SEC./	. RA DEF # 11 (JNOXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,68)/60HFIG CNEL 40,000 SEC./	. RA DEF # 15 (JNOXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,69)/60HFIG CNEL 40,000 SEC./	. RA DEF # 15 (JNOXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,70)/60HFIG CNEL 10,000 SEC./	. AM 241 ORTED 1/21/69 0.6 KEV/CHAN
DATA ITITLE(1,71)/60HFIG CNEL 10,000 SEC./	. AM 241 ORTED 1/21/69 0.6 KEV/CHAN
DATA ITITLE(1,72)/60HFIG CNEL 10,000 SEC./	. PU 240#2 ARMANI 77 0.6 KEV/CHAN
DATA ITITLE(1,73)/60HFIG CNEL 10,000 SEC./	. PU 240 # 2 ARMANI 77 0.6 KEV/CHAN
DATA ITITLE(1,74)/60HFIG CNEL 20,000 SEC./	. PU 240 # 1 ARMANI 77 0.6 KEV/CHAN
DATA ITITLE(1,75)/60HFIG CNEL 20,000 SEC./	. PU 240 # 1 ARMANI 77 0.6 KEV/CHAN
DATA ITITLE(1,76)/60HFIG CEL 40,000 SEC. /	RA DEF # 10 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,77)/60HFIG CEL 40,000 SEC. /	RA DEF # 10 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,78)/60HFIG CEL 40,000 SEC. /	RA DEF # 11 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,79)/60HFIG CEL 40,000 SEC. /	RA DEF # 11 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,80)/60HFIG CEL 40,000 SEC. /	RA DEF # 12 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,81)/60HFIG CEL 40,000 SEC. /	RA DEF # 12 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,82)/60HFIG CEL 40,000 SEC. /	RA DEF # 13 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,83)/60HFIG CEL 40,000 SEC. /	RA DEF # 13 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,84)/60HFIG CEL 40,000 SEC. /	RA DEF # 14 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,85)/60HFIG CEL 40,000 SEC. /	RA DEF # 14 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,86)/60HFIG CEL 40,000 SEC. /	RA DEF # 15 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,87)/60HFIG CEL 40,000 SEC. /	RA DEF # 15 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,88)/60HFIG CEL 40,000 SEC. /	RA DEF # 16 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,89)/60HFIG CEL 40,000 SEC. /	RA DEF # 16 (OXIDIZED) 0.6 KEV/CHAN
DATA ITITLE(1,90)/60HFIG CHANNEL 10 KSEC./	. AM 241 (ORTED) UNBIASED RUN 0.6 KEV/C
DATA ITITLE(1,91)/60HFIG CHANNEL 10 KSEC./	. AM 241 (ORTED) UNBIASED RUN 0.6 KEV/C
DATA ITITLE(1,92)/60HFIG	. BACKGROUND COUNT (BIASED) 40000 SEC

```

C.
DATA ITITLE(1,93)/604FTG . BACKGROUND COUNT (BIASED) 40000 SEC
C.

```

```

C*****
C THE FIRST SPECTRUM TO BE PLOTTED MUST BE REGISTERED BY THE USE OF THE
C SKIP CONTROL CARD
C           NTAG(1,N) IS THE TAGWORD TO BE PLOTTED
C           NTAG(4,N) IS THE LAST CHANNEL TO BE PLOTTED
C           NTAG(3,N) IS THE FIRST CHANNEL TO BE PLOTTED
C           NTAG(2,N) IS THE TYPE OF PLOT:      1 = SMALL FOR PUBLICATION
C                                           2 = LARGE
C

```

```

C*****
C READ, YA(1),XA(1),YA(2),XA(2)
C FIRST, THE TAGWORDS TO BE PLOTTED AND OTHER DATA (NTAG)
C ARE READ
C

```

```

      J=0
      5 J=J+1
      READ, (NTAG(I,J),I=1,4)
      IF(NTAG(1,J).GT.0) GO TO 5
      J=J-1
      PRINT, " TAGWORDS ", (NTAG(1,JJ),JJ=1,J), " TO BE PLOTTED "
      CALL ARYODR(NTAG,J)
      N=J
      DO 900 I=1,N
      XAXIS=XA(NTAG(2,I))
      YAXIS=YA(NTAG(2,I))
      APLE = XAXIS + 4.0
      K=NTAG(4,I)-NTAG(3,I)+1

```

```

C BEGIN WORKING ON SPECTRA
      11 NN=1
      KK=1

```

```

C*****

```

```

C READ IN THE Y VECTOR
      40 BUFFER IN(1,0)(MW(1),MW(160))
      KK=UNIT(1)
      CALL EPRSET(KCOUNT,100)
      50 DECODE(150,60,MW)M,4M,7
      60 FORMAT(2X,I4,2X,A4,23F6.0,3(/25F5.0),/,8F5.0)
      PRINT, " TAGWORD NUMBER ",M," READ "
      IF(M -NTAG(1,I)) 11,70,900
      70 CONTINUE
      IF(KCOUNT.GT.0) GO TO 100
      71 CONTINUE
      DO 100 J=1,256
      Y(NN)=7(J)
      100 NN=NN+1
      IF(KK.NE.0)GO TO 40

```

```

C
C SET UP THE X VECTOR
      X(1) = FLOAT(NTAG(3,I))
      DO 10 II=2,K
      10 X(II)=X(II-1)+1.0
      X(K+1) = X(1)
      X(K+2) = FLOAT(K)/XAXIS

```

```

C *****
C
C ERROR EDIT SEE PROGRAM SCRIPT
C IF IE EQUALS ZERO THEN THERE ARE ERRORS IN THE Y VECTOR FROM SCRIPT
C NE IS THE NUMBER OF ERRORS IN THE VECTOR Y
  READ 1000,IE,NE
  IF(IE.EQ.0)GO TO 300
C *****
C SET UP PLOTTER
  CALL PLOT(0.0,-3.0,-3)
  IF(NTAG(2,I).GT.1) GO TO 20
  CALL PLOT(1.0,3.0,3)
  CALL PLOT(1.0,8.0,2)
  CALL PLOT(4.0,9.5,3)
  CALL PLOT(9.0,9.5,2)
  CALL PLOT(12.0,8.0,3)
  CALL PLOT(12.0,3.0,2)
  CALL PLOT(9.0,1.0,3)
  CALL PLOT(4.0,1.0,2)
  CALL PLOT(2.25,2.0,3)
  CALL PLOT(2.25,8.0,2)
  CALL PLOT(11.0,3.0,2)
  CALL PLOT(11.0,2.0,2)
  CALL PLOT(2.25,2.0,2)
  CALL PLOT(2.75,2.5,-3)
  GO TO 21
190 PRINT*," BAD DATA READ, TAGWORD # ",M
  GO TO 71
  20 CALL PLOT(1.0,2.0,-3)
  21 CONTINUE
C
C SCALE Y VECTOR
200 DO 210 J=1,K
  210 Y(J) = Y(J+NTAG(3,I)+NOFF-1)
  T=B=Y(1)
  DO 220 J=1,K
  IF(Y(J).GT.T)T=Y(J)
  IF(Y(J).LT.B)B=Y(J)
220 CONTINUE
  Y(K+1)=B
  Y(K+2)=(T-B)/YAXIS
C
C PLOT RESULTS
C
  CALL AXIS(0.0,0.0,74CHANNEL,-7,YAXIS,0.0,X(K+1),X(K+2))
  CALL AXIS(0.0,0.0,64COUNTS,6,YAXIS,90.0,Y(K+1),Y(K+2))
  CALL LINE(X,Y,K,1,0,1)
  PRINT 1030,M
  CALL SYMBOL(1.0,SYM,0.105,ITITLE(1,M),0.0,50)
  CALL PLOT(ASLE,0.0,-3)
300 CONTINUE
  CALL PLOTE
  STOP
C
300 DO 310 J=1,NE
  READ 1010,IC,AC
  IC=IC+1

```

```

310 Y(IC)=AC
GO TO 200
1000 FORMAT(2I5)
1010 FORMAT(I5,F10.0)
1020 FORMAT(2F10.0)
1030 FORMAT(1X,"TAGWORD PLOTTED",T18,I5)
END

```

```

SUBROUTINE ARYOP(NARRAY,N)
DIMENSION NARRAY(+,N),ISAV(4)
NP=N-1
DO 50 I=1,NP
K=I+1
DO 50 J=K,N
IF(NARRAY(1,I).LE.NARRAY(1,J)) GO TO 50
DO 30 M=1,4
ISAV(M) = NARRAY(M,I)
NARRAY(M,I) = NARRAY(M,J)
30 NARRAY(M,J) = ISAV(M)
50 CONTINUE
RETURN
END

```

```

SUBROUTINE HALVE(SPEC,FWHM,RWHM)
REAL LWHM,RWHM
DIMENSION SPEC(2100)
PKMAX=100.
DO 100 I=10,2100
IF(SPEC(I).LE.PKMAX) GO TO 100
PKMAX=SPEC(I)
IPEAK=I
100 CONTINUE
HAFMAX=PKMAX/2.
J=IPEAK
150 J=J+1
200 IF(SPEC(J).GT.HAFMAX) GO TO 150
RWHM=J+(SPEC(J)-HAFMAX)/(SPEC(J-1)-SPEC(J))
J=IPEAK
250 J=J-1
IF(SPEC(J).GT.HAFMAX) GO TO 250
LWHM=J+(HAFMAX-SPEC(J))/(SPEC(J+1)-SPEC(J))
FWHM = RWHM-LWHM
PRINT*," PKMAX = ",PKMAX," LWHM = ",LWHM," FWHM = ",FWHM," RWHM = "
C,RWHM
RETURN
END

```

Appendix E

User Instructions for SPECTRE

Program SPECTRE is designed to allow the user to select the tagword to be plotted, choose a large or small format, and select the range of channels for the plot with one card for each spectrum to be plotted. A set of title statements are initialized by the use of DATA statements.

The file containing the spectra to be read must be placed on file TAPE1 as for Program SCRIPT, but the first spectrum need not be registered. It is more efficient to advance the file pointer to just before the smallest tagword to be plotted, but this is not absolutely necessary.

A series of $2N+1$ data cards are required to plot N spectra. The first card must have the axial dimensions in inches for the two plot formats in the following order: counts (small), channel (small), counts (large), channel (large). These are normally 5.0, 7.0, 8.0, 12.0. In the large format, the counts axis is limited by the width of the plotter to less than nine inches but the channel axis is unlimited. The small format dimensions should not be changed.

Next should come a series of cards with the information for each spectrum to be plotted. Each card should contain in order the tagword to be plotted, the type of plot (1 = small, 2 = large), and the first and

last channels to be plotted.

Finally, error data cards are added for each spectrum to be plotted. Each card should contain IE and NE in 2I5 format with

IE = Is there an error?

0 = Yes

Not 0 = No

NE = Number of errors

If IE = 0 there should be NE cards containing the channel number and new value for each error in format I5, F10.0. These will be read before the next error data card.

The order of the tagword cards is unimportant since they will be placed in sequence from smallest to largest by subroutine ARYODR. However the error edit cards must be in correct sequence to match the tagwords after the tagwords are ordered by ARYODR.

The SCOPE control cards required are similar to those for SCRIPT.

Appendix F

Overview of Program ALFAIC

This appendix is a discussion of the general flow of action in program ALFAIC. Refer to the block diagram in Figure 24.

The main program first reads certain controlling data including the run TITLE card, NAMELIST CONTRL, and the background values BACK, which are then sent to ARYODR to be placed in correct sequence. The program then calls RDSPEC to read in a reference spectrum from file TAPE1. Subroutine HALVE computes the FWHM for this spectrum. The program then calls SPCTRM, which in turn calls RDSPEC to read the spectrum to be analyzed. Then the tentative positions of peaks to be resolved are read into PEKPOS and sent to ARYODR for ordering. On subsequent iterations, the program will read in a specified number of reference spectra to use to analyze this same unknown.

Now the program calls BGRND, which can perform one of three options. BGRND can automatically compute the background using subroutines LSQPOL and MATINV. It can also compute an interpolated background function through a designated set of points. The third option, which was used throughout this study, is to compute a number of regions of

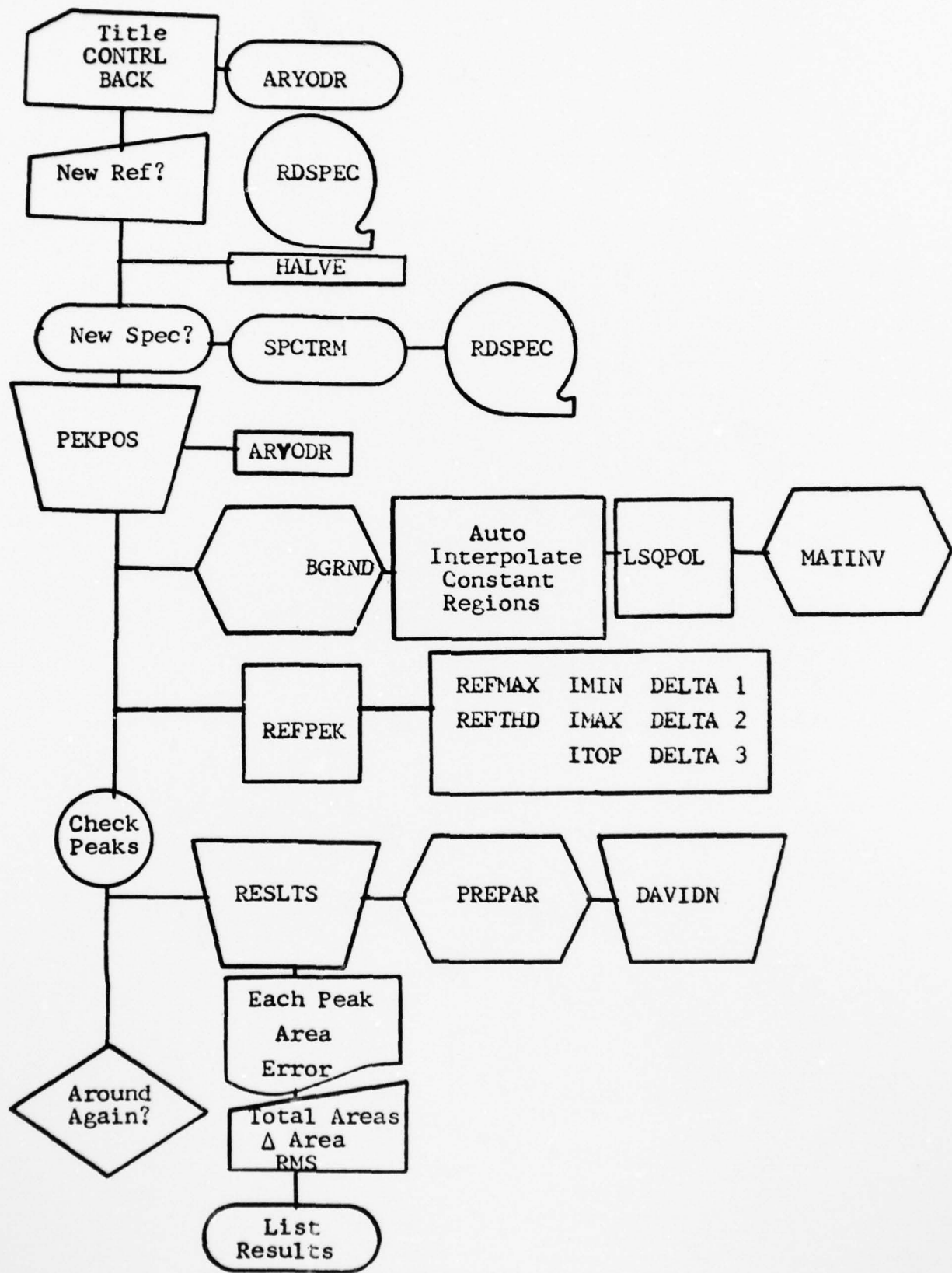


Fig. 24. ALFAIC Overall Flow Chart

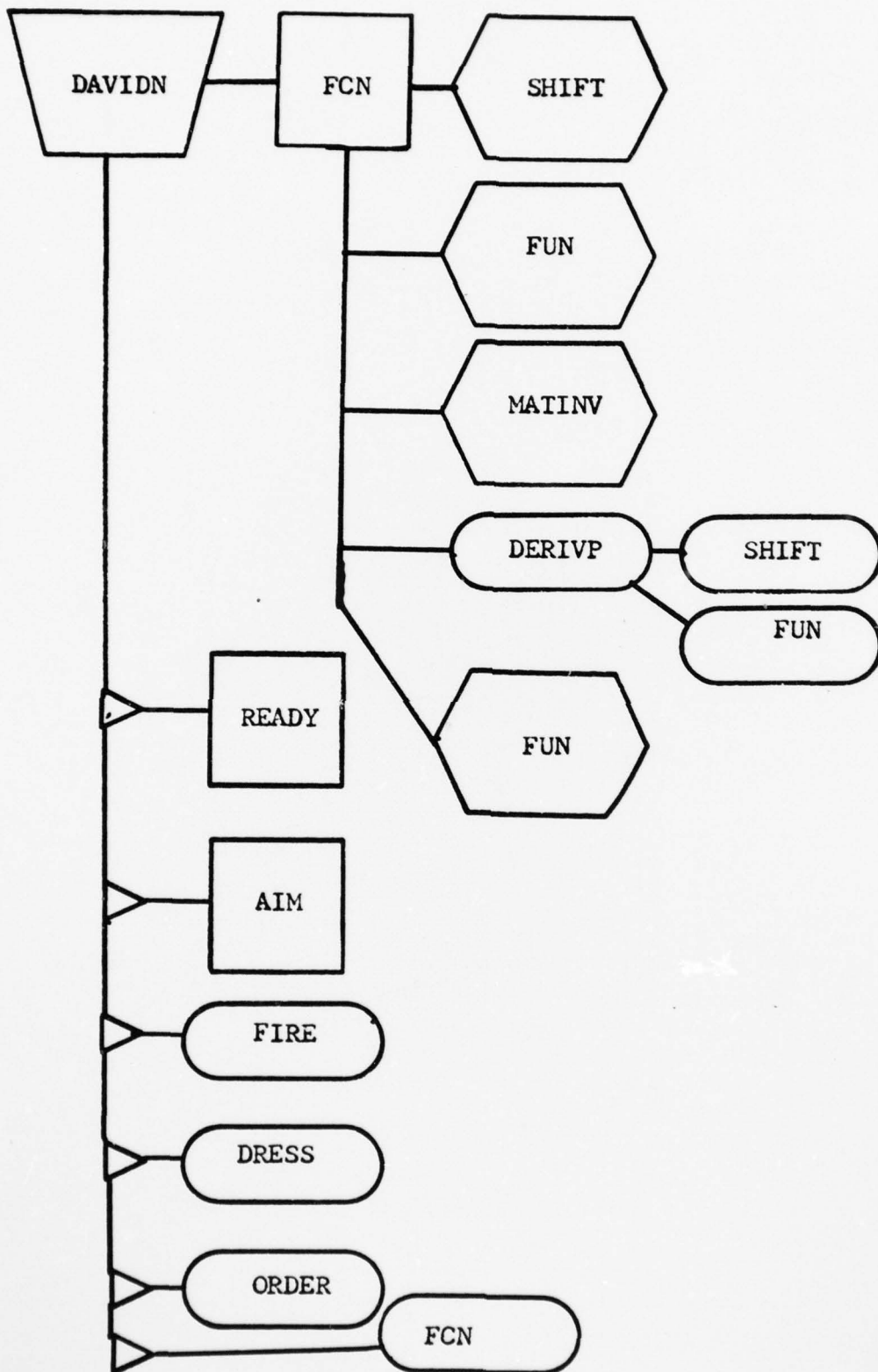


Fig. 24 (continued)

constant background from data in BACK.

Next, the program calls REFPEK which computes certain parameters for the reference peak. These may instead be specified and the program will compute a reference to match or the program can compute a reference from the spectrum to be analyzed. The parameters are based on the highest and lowest nonzero values in the reference spectrum, the maximum value in the reference peak and the one-third maximum point to the right of the peak.

The program then checks the peaks to determine if they can be fitted within the range of the spectrum using a reference peak of the length computed in REFPEK.

Finally, the program calls RESLTS, which passes the data on to PREPAR. When the computed spectrum is returned from PREPAR, RESLTS computes the areas and estimated errors for each peak and the total areas of both the unknown and the resolved or calculate spectra and the square root of the sum of the square of the difference between these two spectra at each point.

PREPAR sets up the problem for DAVIDN, which calls FCN and then, as required, calls READY, AIM, FIRE, DRESS, ORDER, and FCN again. FCN utilizes SHIFT, FUN, MATINV, and DERIVP to help it search for the minimum Chi-Squared Function. These routines collectively do the work of calculating a spectrum which is the result of a constant for each peak multiplied by the reference spectrum at each point relative to that peak location. These individual components are then added to give the combined spectrum.

Appendix G

Input Cards for ALFAIC

Introduction

ALFAIC allows the user a plethora of options, but placing the input cards in the correct order is critical if the program is to function as desired. The program can be run in two main ways, analyzing real data or internally generated data.

Conjur Option Conversion

As listed, the program analyzes real data from file TAPE1 and the routines CONJUR, FACTOR, PPOISS, PGAUSS, and OUTPUT are not used. By replacing the calls to RDSPEC with calls to CONJUR, the program may be converted to analyzing randomized Gaussian spectra. Input 6 should be substituted for Input 5 if this version is used.

Standard Version

The unknown spectrum and NRSPEC reference spectra should be placed in file TAPE1 in the following order:

Reference spectrum 1

Unknown spectrum

Reference spectra 2- NRSPEC

FILE and LDSET control cards are needed as for Programs SCRIPT

and SPECTRE.

Input Cards

Input 1. Title Card

FORMAT (8A10)

The title for this complete sequence is read from the first card. End of file or blank terminates the run.

Input 2. NAMELIST CONTRL

NBACK = 0

Background determined automatically by program.

= +n

Background option I. The X and Y coordinates for n background points will be read in i program calculates a curve passing through all points.

= -n

Background option II. n background intervals will be read in (background is a constant between the limits of each interval).

Note 1: $|n| \leq 50$

If $n > 50$, the program will truncate it to 50.

Note 2: $n \geq 3$ for background Option I (positive sign).

NPKRD \geq +1

Initial peak positions to be read, as values of channel number.

NREF = 0

Reference peak to be selected from the spectrum. (This option is generally not recommended.)

= -1

Reference peak spectrum to be read from tape.

NSSW1 = 1

Print the results from variable-metric-minimization routines.

= 0

Suppress the above.

AD-A064 056

AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OHIO SCH--ETC F/6 7/2
COMPUTER CODE TO ANALYZE ALPHA SPECTRA USING A SPECTRAL STRIPPI--ETC(U)
DEC 78 J R HARSTINE

UNCLASSIFIED

AFIT/GNE/PH/78D-16

NL

2 OF 2
AD
A064056





MICROCOPY RESOLUTION TEST CHART

NATIONAL BUREAU OF STANDARDS-1963-A

NSSW2 = 1	List the raw data, resolved peaks, and composite spectra.
= 0	Suppress the above.
MAXREF =	The maximum number of channels in the reference peaks.
KEPREF = 0	Read in NRSPEC new reference spectra.
= 1	Use the reference spectra from the last analysis.
KEPDAT = 0	Read in a new spectrum to be analyzed.
= 1	Analyze the last data spectrum again.
STDEV =	The standard deviation of the Gaussian spectra to be analyzed.
STDEL =	The amount the different refer- ence spectra are varied around STDEV.
NRSPEC =	The number of reference spectra to be used.

Input 3. Background Data Cards (not used for NBACK=0).

DB(I), BACK(I), I = 1, NBACK
FORMAT (16F5.0)

1-5 DB(I) = For NBACK > 0 (option I)

11-15, etc.

DB(I) is the channel number at
which a background value is to
be specified.

For NBACK < 0 (option II):

DB(I) is the channel number at the
lower end of the Ith interval for
which a background value is to be
specified. DB(1) is supplied by
the program and may be left blank.

6-10 BACK(I) = The value of the background for the Ith background position (NBACK > 0), or for the Ith background interval (NBACK < 0).

Note 1: The pairs DB(I), BACK(I) may be given in any order. The program will rearrange them in increasing order of DB(I).

Note 2: For NBACK > 0, the program requires backgrounds for the first and last channels of data. If not given explicitly, the program will use BACK(1) for the first channel, and BACK(NBACK) for the last channel. These program-supplied values may be counted for meeting the minimum requirement of 3 background points.

Input 4. Peak extraction channel

IPK = The desired channel number of the maximum count in the 512 channel segment to be analyzed.

Input 5. DO Loop Sequential data

Five sequences of these cards will be required for each analysis.

Input 5a. Reference Peak Parameter Card (Use only if NREP=0.)

STOIPR, DELTA1, DELTA2, DELTA3

FORMAT (4F10.5)

1-10 STOIPR = The channel number of the maximum count in the reference peak.

11-20 DELTA1 = Channels from the front (high-energy) edge of the reference peak to the "third-height" position on the front edge.

21-30 DELTA2 = Channels from the back (low-energy) edge of the reference peak to the third-height position.

31-40 DELTA3 = Channels from STOIPR to the third-height position.

Note: For MCA operation, the "third-height" position is defined as STOIPR and hence the program sets DELTA3=0.0.

Input 5b. Peak Position Cards (Use with NPKRD > +1.)

PEKPOS(I), IFIXPK(I)

UNFORMATTED (LIST DIRECTED)

PEKPOS(I) = The estimated third-height location of the Ith peak to be considered by the program, specified in channel number.

IFIXPK(I) = 0 or blank The program will adjust PEKPOS(I) for the best fit to the data. (Standard option.)

> i PEKPOS(I) will be held fixed by the program.

Note: The cards may be in any order. The program will rearrange them into ascending order of PEKPOS(I).

Input 5c. Peak Position Termination Card

PEKPOS(I) < -1.0. This will terminate peak locations and the program will process a new set of data, beginning with Card 1.

Input 6. Conjured Data Sequence Cards

These are used instead of INPUT5 when running the program using data to be created by Subroutine CONJUR and the associated functions. The two statements in ALFAIC and SPCTRM calling RDSPEC must be replaced with calls to CONJUR for these options.

Input 6a. Channels of desired peak(s)

IPEAK(N), N=1, NPEAK

UNFORMATTED (LIST DIRECTED)

IPEAK = The center channel of the Gaussian peak to be created by calling function PGAUSS.

Input 6b. Heights of desired peaks

IHITE(N), N=1, NPEAK

UNFORMATTED (LIST DIRECTED)

IHITE(N) = The approximate height in counts
of the peak in channel IPEAK(N).

Input 6c. Peak position cards

These are the same as Inputs 5b and 5c.

Appendix H

Program ALFAIC

```

PROGRAM ALFA10(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,PUNCH,
1 TAPE7=PUNCH,TAPE8,TAPE1)
C PROGRAM ALPHAFIT WAS OBTAINED FROM PROGRAM AUTOFIT WRITTEN BY
C J.R. COMFORT OF ARGONNE NATIONAL LABORATORY
C THIS PROGRAM ALLOWS THE FOLLOWING:
C A MAXIMUM OF 2100 CHANNELS FOR A REFERENCE PEAK
C A MAXIMUM OF 2100 CHANNELS FOR A SPECTRUM
C A MAXIMUM OF 50 CHANNELS FOR A BACKGROUND INPUT
COMMON /A00/ VM1(582),NSSW1,NSSW2
COMMON /A02/ DUMXNS(161),STORV1(2100),RA4X(2100),ITIMES,NNX
COMMON/A03/ TITLE(20),PEKPOS(20),IFIXPK(20),BETA,GSTATE,
1 GSOVAL,NT,NCALC,IGS,LQ
COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
1 STCIER,REF1AX,I01,I02,IDT,N3,NE,NREF
COMMON /A05/ BACK2(2100),DB(50),BACK(50),NJ,NBACK,NPKRD
COMMON /DATA/ DIST(2100),COUNTS(2100),RJVID,TODAY,FREQ,OFTEN,
1 NOFTEN,NCHAN1,IT,TJ,ISPECT,IFMT,IERR,MAXREF,MAXP2
COMMON /OPTN/ KEPREF,KEPDAT
DIMENSION REFSTO(2100,10),FWHM(10,2)
EQUIVALENCE (IBLNK,3LNK,DBLNK)
DATA(DBLNK=8H )
NAMELIST/CONTRL/NBACK,NPKRD,NREF,NSSW1,NSSW2,MAXREF,KEPREF,KEPDAT
C,STDEV,STDEL,NPSPEC
C ...START CALCOMP AND GET DATE...
IERR = 0
CALL DATE(TODAY)
GO TO 50
C ...TERMINATE PROGRAM...
45 WRITE(6,101)
101 FORMAT(3X,18H ENDPLOT EXECUTED)
STOP
C ...READ AND WRITE TITLE CARD. EXIT ON E.O.F...
50 READ(5,10) (TITLE(I),I=1,3)
IF(EOF(5))45,49
49 IF(TITLE(1).EQ.DBLNK) GO TO 45
WRITE(6,30) (TITLE(I),I=1,3),TODAY
C ...INPUT OF DATA...
READ(5,CONTRL)
IF(EOF(5))45,51
51 PRINT CONTRL
C KEPREF IS AN OPTION TO ALLOW THE USER TO KEEP THE SAME REFERENCE
C PEAK FOR ALL ANALYSIS
C KEPREF.GT.0 ALLOWS THE USE OF THE SAME REFERENCE PEAK FOR ENTIRE
C ANALYSIS
C KEPREF.EQ.0 REQUIRES A NEW REFERENCE PEAK WITH EACH SPECTRUM
C ANALYZED
C KEPDAT IS AN OPTION TO ALLOW THE SAME DATA SET TO BE USED FOR ALL
C ANALYSIS.
C KEPDAT .GT.0 ALLOWS THE SAME DATA SET TO BE USED FOR THE ANALYSIS.
C KEPDAT .EQ.0 REQUIRES A NEW DATA SET FOR EACH ANALYSIS.
MAXP2 = MAXREF + 2
IF (NREF.GT.10) NREF = 10
IF (NBACK) 70,100,81
70 NJ = -NBACK
NBACK = 2
GO TO 90
80 NJ = NBACK

```

```

NRACK = 1
90 IF (NJ.GT.50) NJ = 50
READ(5,14) (DB(I),BACK(I),I=1,NJ)
DO 91 I=1,NJ
91 PRINT*, "DB(",I,") = ",DB(I)," BACK(",I,") = ",BACK(I)
IF (NJ.GT.1) CALL ARYOPR(DB,BACK,NJ,2)
C
...INITIALIZATION...
100 CONTINUE
LQ=0
NADJ=0
STOIPR = 0.0
DO 105 I=1,20
105 IFIXPK(I) = 0
DO 110 I=1,MAXREF
110 STOREF(I) = 0.0
C
...MORE DATA INPUT...
IF (NREF) 120,130,150
120 IF (KEFREF.GT.0) GO TO 778
PRINT*, " CALLING RDSPEC FOR REFERENCE PEAK "
DO 1001 IJK=1,NRSPEC
CALL RDSPEC(STOREF,N,NTAG,MAXREF)
NSTOR = N
DO 77 I = 1,N
REFSTO(I,IJK)=STOREF(I)
77 CONTINUE
CALL HALVE(REFSTO(1,IJK),FWHM(IJK,1))
FWHM(IJK,2) = IJK
1001 CONTINUE
GO TO 1000
778 DO 99 I = 1,NSTOR
STOREF(I)=REFSTO(I,IJK)
99 CONTINUE
1000 CONTINUE
GO TO 150
130 READ(5,18) STOIPR, DELTA1, DELTA2, DELTA3
150 CONTINUE
C
...GET A STANDARD SPECTRUM DATA SET...
IF (KFPDAT.GT.0) GO TO 175
170 CALL SPCTRM
175 IF (JERR.GT.0) GO TO 45
WRITE(6,34) NCHANV
DELTA3 = 0.0
C
...READ PEAK POSITIONS, DISTANCE
200 DO 220 I=1,21
210 READ, PEKPOS(I), IFIXPK(I)
IF (PEKPOS(I).LE.-1.) GO TO 230
PRINT*, " PEAK# ",I, " = ",PEKPOS(I)
220 CONTINUE
NT = 20
GO TO 240
230 NT = I - 1
240 IF (NT.GT.1) CALL ARYOPR(PEKPOS,IFIXPK,NT,2)
IPK1=PEKPOS(1)
330 DO 350 I=1,NCHANV
350 RAWX(I) = COUNTS(I)
C
...CALC. BACKGROUND, SELECT REFERENCE PEAK AND PICK PEAKS...
CALL HALVE(RAWX,FWHM1)

```

```

DIFMIN = 50.
DO 300 I=1,NRSPEC
DIFF=ABS(FWHM1-FWHM(I,1))
IF(DIFF.GT.DIFMIN) GO TO 300
DIFMIN=DIFF
IJK=I
300 CONTINUE
IF(DIFMIN.LT.50.) GO TO 301
PRINT*, " UNSATISFACTORY REFERENCES, FWHM OF UNKNOWN IS ",FWHM1,
C" CHANNELS "
GO TO 10
301 CONTINUE
DO 302 I=1,NSTOR
STOREF(I)=REFSTO(I,IJK)
302 CONTINUE
NNX = 0
IF ((NBACK.EQ.0).AND.(NPKRD.EQ.0)) GO TO 440
IF (NBACK.EQ.0) GO TO 370
IF (DB(1).LT.DIST(1)) DB(1) = DIST(1)
IF (DB(NJ).GT.DIST(NCHANN)) DB(NJ) = DIST(NCHANN)
370 CALL BGRN:
NNX = NNX + 1
DO 420 I=1,NCHANN
IF (RAWX(I)) +20,+20,410
410 RAWX(I)=RAWX(I)-BACK2(I)
IF(RAWX(I).LT.0.0) RAWX(I) = 0.0
420 CONTINUE
440 CALL REFPEK
IF (NPK(I).NE.0) GO TO 500
460 DO 470 I=1,NT
470 PEKPOS(I) = PEKPOS(I) + DELTA3
IF (NNX) 370,370,520
500 WRITE(1,38)
GO TO 520
520 WRITE(3,-0)
C ... MAKE SURE THAT ALL PEAKS ARE IN THE RANGE OF THE SPECTRUM
530 M = 1
DO 550 I=1,NT
IF ((PEKPOS(I)-DELTA2-2.*OFTEN).LT.DIST(1)) GO TO 550
IF ((PEKPOS(I)+DELTA1+2.*OFTEN).GT.DIST(NCHANN)) GO TO 550
M = M + 1
550 CONTINUE
PRINT*, " NADJ = ",NADJ, " M = ",M
IF (M.(E.NT) GO TO 580
DO 560 I=1,50
560 STOREF(I)=0.0
NADJ = NADJ+1
IF(NADJ.LT.10) GO TO 440
PRINT*, " UNSATISFACTORY PEAKS"
GO TO 15
580 NT = 1
WRITE(6,42) (PEKPOS(I),I=1,NT)
DO 600 I=1,NCHANN
600 STORV(I) = BACK2(I)
CALL RESULTS
KEPDA* = 1
GO TO 50

```

```

10  FOR Y,T(=A10)
12  FORMAT ( I4,4I2,I4 )
14  FORMAT (11F5.0)
16  FORMAT (I1,15F5.0)
18  FORMAT (4F10.5)
24  FORMAT (F4.4,I1,F10.5)
30  FORMAT (1H1,1X,8A10,10Y,A10)
32  FORMAT (10H0          4X8HNBACK = I4,4X34NPKRD = I2,4X7HNREF = I2
      1,4X9H          4X8HNSSW1 = I2,4X34NSSW2 = I2,4X9HMAXREF = I4)
34  FORMAT (11H0 NCHANN = I1,5X7H )
38  FORMAT (15H0 INITIAL GUESSES OF PEAK POSITIONS)
40  FORMAT (10H0 CALCULATED ESTIMATES OF PEAK POSITIONS)
42  FORMAT (10F12.3)
44  FORMAT (1H0,I4,14H PEAKS DELETED)
      END

```

```

      FUNCTION FACTOR(N)
      DOUBLE PRECISION FI,SUM
11  FACTOR = 1.
      IF (N-1)40,40,13
13  IF (N-10)21,21,31
21  DO 23 I=2,N
      FI=I
23  FACTOR=FACTOR*FI
      GO TO 40
31  SUM=0.
      DO 34 I=11,N
      FI=I
34  SUM=SUM+DLOG (FI)
35  FACTOR=3628800.*DEXP (SUM)
40  RETURN
      END

```

```

      FUNCTION PGAUSS(X,AVERAG,SIGMA)
      DOUBLE PRECISION Z,ZSQ
1  Z=(X-AVERAG)/SIGMA
      ZSQ=(Z**2)/2.
      IF (ZSQ.GE.200.) GO TO 10
      PGAUSS=0.3989422804/SIGMA*DEXP(-ZSQ)
      GO TO 11
10  PGAUSS=0.
11  RETURN
      END

```

```

SUBROUTINE CONJUR(SPEC,NPEAK,STDEV,NCHANN)
DIMENSION SPEC(4000),DIST(4000),PDISS(200),IPEAK(5)
DIMENSION IHITE(5)
PRINT*," NPEAK = ",NPEAK," STDEV = ",STDEV," NCHANN = ",NCHANN
READ*,(IPEAK(N),N=1,NPEAK)
PRINT*," IPEAK = ",(IPEAK(N),N=1,NPEAK)
READ*,(IHITE(N),N=1,NPEAK)
PRINT*," IHITE = ",(IHITE(N),N=1,NPEAK)
DO 100 I=1,NCHANN
100 SPEC(I)=0.0
DO 1000 J=1,NPEAK
AVERAG=IPEAK(J)
SIGMA=STDEV
A=37.878 * IHITE(J)
DO 200 I=1,NCHANN
X=I
SPECTR=A*PGAUSS(X,AVERAG,SIGMA)
IF( X .LT. AVERAG ) GO TO 101
IF(SPECTR.GE. 0.1) GO TO 101
SPECTR = 0.0
GO TO 102
101 IF(SPECTR.LT. 1.0) SPECTR = 1.0
102 SPEC(I) = SPEC(I) + SPECTR
200 CONTINUE
1000 CONTINUE
NSEED=2001
CALL RANSET(NSEED)
AVERAG = 20.
IMAX=2*AVERAG
DO 400 I=1,IMAX
400 DIST(I)=PPOISS(I,AVERAG)
IOLD=1
NP=0
DO 500 L=1,IMAX
A=DIST(L)*IMAX
IF(A.LT. 1.0) GO TO 500
INFW=IOLD+A
DO 450 J1=IOLD,INFW
PDISS(J1) = L
NP=NP+1
450 CONTINUE
IOLD=INFW+1
500 CONTINUE
DO 600 I=1,NCHANN
IJ=RANF(N)*NP
IF(IJ.LT.1) GO TO 600
SPEC(I)=SPEC(I)+SQRT(SPEC(I))*(PDISS(IJ)/AVERAG-1.0)
600 CONTINUE
RETURN
END

```

```

SUBROUTINE HALVE(SPEC,FWHM,RWHM)
REAL LWHM,RWHM
DIMENSION SPEC(2100)
PKMAX=100.
DO 100 I=10,2100
IF(SPEC(I).LE.PKMAX) GO TO 100
PKMAX=SPEC(I)
IPEAK=I
100 CONTINUE
HAFMAX=PKMAX/2.
J=IPEAK
150 J=J+1
200 IF(SPEC(J).GT.HAFMAX) GO TO 150
RWHM=J+(SPEC(J)-HAFMAX)/(SPEC(J-1)-SPEC(J))
J=IPEAK
250 J=J-1
IF(SPEC(J).GT.HAFMAX) GO TO 250
LWHM=J+(HAFMAX-SPEC(J))/(SPEC(J+1)-SPEC(J))
FWHM = RWHM-LWHM
PRINT*," PKMAX = ",PKMAX," LWHM = ",LWHM," FWHM = ",FWHM," RWHM = "
C,RWHM
RETURN
END

```

```

SUBROUTINE RDSPEC(Y,N,M,MAX)
DIMENSION Y(4100),X(256),MW(160),Z(520)
N=1
KK=1
10 BUFFER IN(1,0)(MW(1),MW(160))
KK=UNIT(1)
CALL EPRSET(KOUNT,100)
DECODE(150,60,MW)4,4M,X
IF(KOUNT.GT.0) GO TO 10
50 FORMAT(2X,I4,2X,A4,23F6.0,9(/25F5.0),/,8F5.0)
IF(KK.EQ.0) GO TO 31
DO 80 I=1,256
Y(N)=X(I)
80 N=N+1
IF(KK.NE.0) GO TO 10
31 N=N-1
ITIME=Y(1)
IF(ITIME.EQ.0) ITIME = 40000
PRINT*," ITIME = ",ITIME
PRINT 1010,M
IF(N.LE.MAX) GO TO 39
PRINT*," N GREATER THAN MAX, N = ",N
N=MAX
39 NN=(N/10)+1
DO 90 K=1,NN
IN=(K-1)*10
II=IN+1
IJ=IN+10
PRINT 1020,IN,(Y(J),J=II,IJ)
90 CONTINUE
RETURN
1010 FORMAT(1H0,T51,"TAGWORD NUMBER",5X,I5,5X,"READ")
1020 FORMAT(1X,I5,10F10.0)
END

```

```

SUBROUTINE RESULTS
DIMENSION FMT(6), WORD(20)
DIMENSION PEKERR(200), PKBACK(200), XSECTS(200), XSECEP(200),
1 QRELT(200), EX(200)
COMMON /A00/ VMM(562), IHOLD(20), NSSW1, NSSW2
COMMON/A01/STORZ(2102,10),S(2102),I7STRT(20),I7STOP(20),DUM(5538)
COMMON /A02/ SIGMA(20), ERRZ(20), PERSTO(21), STORHH(20),
1 XINTIS(20), INDX(20), INITAL(20), IFINAL(20), STORV1(2100),
2 RAWX(2100), ITIMES, NNX
COMMON/A03/ TITLE(20),PEKPOS(20),IFIXPK(20),BETA,GSTATE,
1 GSOVAL, NT, NCALC, IGS, LQ
COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
1 STOIPR, REFMAX, ID1, ID2, IDT, N3, NE, NREF
COMMON /A05/ BACK2(2100), DR(50), BACK(50), NJ, NBACK, NPKRD
COMMON /DATA/ DIST(2100), COUNTS(2100), RJNID, TODAY, FREQ, OFTEN,
1 NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR,MAXREF,MAXP2
DATA(FMT=8H(1XF9.4,, 7H3F10.2,, 14 , 5HF10.2, 5H/40X,, 5H 9F10.2))
DATA (WORD = 8H 9, 8H 10X, 3, 8H 20X, 7,
1 8H 30X, 6, 8H 40X, 5, 8H 50X, 4, 8H 60X, 3, 8H 70X, 2,
2 8H 80X, 1, 8H 9, 8H 10X, 3, 8H 20X, 7, 8H 30X, 6,
3 8H 40X, 5, 8H 50X, 4, 8H 60X, 3, 8H 70X, 2, 8H 30X, 1,
4 8H 9, 8H 10X, 2)
DATA (ISF=1HF), (IBLNK=1H )
C ...INITIALIZATION...
JQ = 0
JOB = 0
NNX = 1
MTP = 1
MTT = 1
NT1 = NT
C ...STORE INFORMATION AND GET READY TO CALL PREPAR...
50 DO 70 I=1,NT
J = NNX + I - 1
IHOLD(I) = IFIXPK(J)
70 PERSTO(I) = PEKPOS(J)
80 DELTA1 = DELTA1/OFTEN
DELTA2 = DELTA2/OFTEN
CALL PREPAR
DO 140 I=1,NT
J = NNX + I - 1
140 IFIXPK(J) = IHOLD(I)
NNX = NNX + NT
IF (NSSW2.GT.0) WRITE(C,9042)
9042 FORMAT(10H0 DISTANCE,2X8HRAW DATA,2X10HBACKGROUND,2X9HCOMPOSITE,4X
116HRESOLVED SPECTRA)
C ... CALCULATE AREAS AND ERRORS FOR THIS GROUP...
DO 91 I=1,NT
XINTIS(I) = 0.
DO 3005 J=1,MAXP2
3005 XINTIS(I) = XINTIS(I) + STORZ(J,I)
JQ=JQ+1
PEKPOS (JQ)=PERSTO (I)
PEKERR (JQ)=SIGMA(I)
PKBACK(JQ) = 0.0
XSECTS(JQ)=XINTIS(I)
91 XSECEP(JQ)= XSECTS(JQ)*ERRZ(I)
C ...ADD BACKGROUNDS AND PRINT THE RESOLVED AND COMPOSITE SPECTRA

```

```

JPP = 0
DO3300 I=1,ITIMES
MQP = JPP + 1
JPP=MQP+INDEX(I)-1
MZZ=INITAL (I)
MMX=IFINAL(I)
IF (NSSW2.EQ.0) GO TO 1530
IF (MZZ-MIT) 2011,2011,2010
2010 MZP = MZZ - 1
DO 2012 L = MTT,47P
2012 WRITE(6,FMT) DIST(L),COUNTS(L),BACK2(L)
2011 WRITE(6,9032) (PERSTO (JP),JP=MQP,JPP)
9032 FORMAT(40X,9F10.2)
1530 DO 3010 J=MZZ,MMX
      K1 = 0
      K2 = 0
      M = J - MZZ + 1
      STORV1(J) = BACK2(J)
      DO 1310 JP = MQP,JPP
      J2 = JP
      IF ((M.GE.IZSTRT(JP)).AND.(M.LE.IZSTOP(JP))) GO TO 1320
1310 K1 = K1 + 1
      IF (NSSW2.EQ.0) GO TO 3010
      WRITE(6,FMT) DIST(J),COUNTS(J),BACK2(J)
      GO TO 3010
1320 DO 1330 JP = J2,JPP
      IF ((M.LT.IZSTRT(JP)).OR.(M.GT.IZSTOP(JP))) GO TO 1340
      JB = JQB + JP
      PKBACK(JB) = PKBACK(JB) + BACK2(J)
1325 K2 = K2 + 1
      ITT = M - IZSTRT(JP) + 1
      STORV1(J) = STORV1(J) + STORZ(ITT,JP)
      STORZ(ITT,JP) = STORZ(ITT,JP) + BACK2(J)
1330 S(K2) = STORZ(ITT,JP)
1340 FMT(3) = WORD(K1 + 1)
      IF (NSSW2.EQ.0) GO TO 3010
3009 WRITE(6,FMT) (DIST(J),COUNTS(J),BACK2(J),STORV1(J),(S(K),K=1,K2))
3010 CONTINUE
      MTT = MMX + 1
3300 CONTINUE
      JQB = JQB + NT
      32 IF (NSSW2.EQ.0) GO TO 3401
      DO3400 I=MTT,NCHANN
3400 WRITE(6,FMT) DIST(I),COUNTS(I),BACK2(I)
C      ...PRINT HEADINGS...
3401 WRITE(6,85) (TITLE(I),I=1,8 ),TODAY
      WRITE(6,200)
550 DO 560 I=1,JC
      IPF = IBLNK
      IF (IFIXPK(I).GT.0) IPF = ISF
      AREA = XSECTS(I)+PKBACK(I)
      STXERR = 0.
      IF (AREA.GT.0.) STXERR = SORT(AREA)
      WRITE(6,212) PEKPOS(I),IPF,PEKERR(I),XSECTS(I),XSECEK(I),
1      PKBACK(I),STXERR
560 CONTINUE
      DEVST=DEVSQ=C.0

```

```

AUNK=ARES=0.0
DO 5000 IJK=1,MAXREF
AUNK=AUNK+COUNTS(IJK)
ARES=ARES+STORV1(IJK)
DEVSQ=DEVSQ+(COUNTS(IJK)-STORV1(IJK))**2
5010 CONTINUE
DEVST=SQRT(DEVSQ)
PRINT*," AREA UNKNOWN = ",AUNK," AREA RESOLVED = ",ARES," RMS ERR
COR = ",DEVST
RETURN
85  FORMAT(1H1,1X,8A10,10X,A10)
200  FORMAT(/6X+HPEAK,23X3H      ,19X5HNJ43.,35X4HEST./4X8HPOSITION,5X7H
1     ,6X6H      ,5X5HERROR,7X6HCOJUNTS,12X5HERRDR,13X10HBACKGROUND
2,6X5HEKROK/)
201  FORMAT(3XF9.3,1XA1,3XF9.4,4XF8.4,4XF8.2,5XF9.2,3(4XF9.2))
202  FORMAT(F9.+,1X,2F10.4,2F10.2,F9.2,F9.1,3XA6,F9.1)
221  FORMAT(3XF9.3,1XA1,3XF9.4,16XF6.2,5XF9.2,3(4XF9.2))
222  FORMAT(F9.4,1XF10.4,10X,2F10.2,F9.2,F9.1,3XA6,F9.1)
212  FORMAT(3XF9.3,1XA1,26XF6.2,5XF12.2,3(4XF11.2))
215  FORMAT(F9.+,21X,2F10.2,F9.2,F9.1,3XA6,F9.1)
230  FORMAT(2H-1)
END

```

```

SUBROUTINE SPECTRM
C ...READS THE SPECTRUM CARDS AND SETS THE DISTANCE AND COUNT ARRAYS
DIMENSION YSAV(10)
COMMON/DATE4/X(2100),Y(2100),RUNID,TODAY,FREQ,DELX,NOFTEN,
1 N,II,IJ,ISPECT,IFMT,IERR,MAXREF,MAXP2
COMMON /OPTN/ KEPREF,KEPDAT
C ..... INITIALIZE COUNTS ARRAY TO ZERO
DO 100 I=1,2100
100 Y(I)=0.0
N=10
DELX = 1.0
PRINT*," ENTERED SPECTRUM, CALLING RDSPEC"
CALL RDSPEC(Y,N,NTAG,MAXREF)
IF(N.GT.2100) GO TO 235
D1=0.0
GO TO 250
235 WRITE(6,2) N
245 IERR=1
GO TO 300
C .... SET THE DISTANCE VALUES ....
250 X(1)=D1
DO 260 I=2,N
260 X(I)=D1 + FLOAT(I-1)*DELX
300 RETURN
30  FORMAT(F8.0,9F7.0,8XF3.0)
1  FORMAT(6H0 D = ,F9.3,16H LESS THAN 01 = ,F9.3)
2  FORMAT(11H0 NCHANN = ,I5,19H GREATER THAN 2100)
5  FORMAT(F5.0/10(F8.0,2X))
END

```

```

SUBROUTINE REFPEK
C   DETERMINES THE PARAMETERS OF THE REFERENCE PEAK
COMMON /A02/ DUMANS(161), STORV1(2100), RAWX(2100), ITIMES, MNX
COMMON /A03/ SKIP(55),LO
COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
1   STOIPR, REFMAX, ID1, ID2, IDT, N1, NE, NREF
COMMON /A05/ BACK2(2100), DB(50), BACK(50), NJ, NBACK, NPKRO
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
1   NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IFRR, MAXREF, MAXP2
COMMON /OPTN/ KEFREF, KFPDAT
IF (LO) 10,30,10
10 IF (NREF) 300,200,300
30 IF (NREF) 100,200,80
C   SELECT REFSHAPE FROM INTERNAL DATA
90 DO90 I=1,20
30 STOREF(I) = INTREF(I,NREF)
C   FIND LOWER EDGE OF PEAK
100 DO110 I=1,MAXREF
IF (STOREF(I)) 110,110,120
110 CONTINUE
120 IMIN = I
IF (I.GT.1) IMIN = I - 1
C   FIND UPPER EDGE OF PEAK
I = MAXREF
130 IF (STOREF(I)) 140,140,150
140 I=I-1
GO TO 130
170 IMAX = I
IF (I.LT.MAXREF) IMAX = I+1
C   FIND TOP OF PEAK
REFMAX=0.0
DO 170 I=IMIN,IMAX
IF (REFMAX-STOREF(I)) 160,170,170
150 REFMAX = STOREF(I)
ITOP=I
170 CONTINUE
SREF = .001* REFMAX
C   FINDS THIRD HEIGHT
REFTHD = REFMAX/3.
DO 180 I=ITOP,IMAX
IF (STOREF(I)-REFTHD) 190,180,180
180 CONTINUE
180 RI=I
OFFSET = (REFTHD-STOREF(I))/(STOREF(I-1)-STOREF(I))
RTHPOS=RI-OFFSET
DELTA1 = (FLOAT(IMAX)-RTHPOS)*OFTEN
DELTA2 = (RTHPOS-FLOAT(IMIN))*OFTEN
DELTA3 = (RTHPOS-FLOAT(ITOP))*OFTEN
RTHPOS = (RTHPOS-1.0)*OFTEN
STORE = 0.0
210 IDT=(DELTA2+DELTA1)/OFTEN + 1.1
ID1=(DELTA1+DELTA3)/OFTEN +0.1
ID2=(DELTA2-DELTA3)/OFTEN +.1
NE = NCHANN - ID1
N9 = ID2 + 1
IF (NREF) 230,210,230
C   SELECT REFSHAPE FROM RAW SPECTRUM

```

```

210 KU = (STOIPR-DIST(1))/OFTEN + 0.1
    IID = KU - ID2
    IMIN = 1
    IMAX = IMIN + IDT - 1
    STORE = OFTEM*FLOAT(IID) + DIST(1)
    RTHPCS = STOIPR + DELTA3
    DO 220 IR=1, IDT
220 STOREF(IR)=RAWX(IID+IR)
230 IF (LQ) 240, 240, 300
240 DO 250 I=IMIN, IMAX
250 STOREF(I-IMIN+1) = STOREF(I)
    DO 255 IM=ITOP, IMAX
255 IF(STOREF(IM).LT.SREF)STOREF(IM)=0.0
    IM=IMAX-IMIN+2
    DO 260 I=IM, MAXREF
260 STOREF(I)=0.0
    IF (NNX) 400, 400, 300
300 WRITE(6, 310) DELTA1, DELTA2, DELTA3
310 FORMAT(11H0 DELTA1 = ,F9.2, 8X9HDELTA2 = ,F9.2, 8X9HDELTA3 = ,F9.2)
    PRINT*, " IDT = ", IDT, " ID1 = ", ID1, " ID2 = ", ID2
    WRITE(6, 350) RTHPOS
350 FORMAT(32H REFERENCE PEAK THIRD HEIGHT = ,F9.4)
400 RETURN
    END

```

```

1 FUNCTION PPOISS(NOBS, AVERAG)
    PPOISS=((AVERAG**NOBS)/FACTOR(NOBS))*EXP(-AVERAG)
    RETURN
    END

```

```

SUBROUTINE OUTPUT(X, NMAX)
    DIMENSION X(1)
    IMAX=NMAX/10
    DO 100 K=1, IMAX
        I1=K*10
        I0=I1-9
100 PRINT 200, (X(I), I=I0, I1)
200 FORMAT(5X, 10(E9.3, 2X))
    RETURN
    END

```

```

SUBROUTINE PGRND
C ...CALCULATES THE BACKGROUNDS...
COMMON /A02/ DE(32), RHO2(32), W(50), X(10), A(10,10), DUMMY(-099)
COMMON /A03/ TITLE(20), PEAK(20), BLNK(23), NPEAK, NCALC, IGS, LQ
COMMON /A04/ INTREF(20,10), STOREF(2100), DELTA1, DELTA2, DELTA3,
1 STOIPR, REFMAX, ID1, ID2, IDT, N3, NE, NREF
COMMON /A05/ BACK2(2100), DB(50), BACK(50), NJ, NBACK, NPKRD
COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
1 NOFTEN, NCHANN, SKIP(5), MAXREF, MAXP2
QQ = DIST(1)
IF (NBACK-1) 10,700,900
C ...AUTOMATIC BACKGROUND SELECTION...
10 NP = NPEAK + 1
IJ = 0
NJ = 1
RHO2(NJ) = 1.E10
DO 200 JJ=1,NP
IJ = IJ + 1
IF(IJ-NP) 20,30,400
20 LOCPK = (PEAK(IJ)-DELTA3-QQ)/OFTEN + 1.1
IF(IJ-1) 40,40,60
40 NDEL = LOCPK - ID2 - 1
MA = 0
GO TO 100
50 NDEL = IFIX((PEAK(IJ)-PEAK(IJ-1))/OFTEN + 0.1) - IDT
MA = LOCPK - ID2 - NDEL - 1
GO TO 100
30 LOCPK = (PEAK(IJ-1)-DELTA3-QQ)/OFTEN + 1.1
NDEL = NCHANNEL - LOCPK - ID1
MA = LOCPK + ID1
100 IF(NDEL-10) 200,120,120
120 JBACK = FLOAT(NDEL)/10.0 + 0.2
JP = NDEL/JBACK
SHIFT = FLOAT(JP)/2.
DO 160 I=1,JBACK
NJ = NJ + 1
B = 0.0
DO 140 IP=1,JP
140 B = B + COUNTS(MA+IP)
RHO2(NJ) = B/FLOAT(JP)
BACK(NJ) = RHO2(NJ)
CHECK = RHO2(NJ-1) + 2.*SQRT(RHO2(NJ-1)+1.)
IF (RHO2(NJ)-CHECK) 160,160,150
150 NJ = NJ - 1
GO TO 170
150 DE(NJ) = DIST(MA+1) + OFTEN*SHIFT
DB(NJ) = DE(NJ)
C ...TEST FOR LIMIT OF 50 POINTS AND TAKE APPROPRIATE ACTION...
170 IF (NJ-49) 180,175,+00
175 IF (IJ.GE.NP) GO TO 400
IJ = NP
GO TO 80
130 MA = MA + JP
200 CONTINUE
400 IF (NJ-5) +10,420,420
410 M = NJ - 1
GO TO 430

```

```

420 M = 4
430 N = NJ
500 MM = M + 1
    DO 510 I=1,N
510 W(I) = 1.0
    CALL LSQPOL(N,MM)
    DO 540 I=1,NCHANN
    BACK2(I) = X(I)
    DO 520 IP=1,M
520 BACK2(I) = BACK2(I) + X(IP+1)*DIST(I)**IP
    IF(BACK2(I)) 530,540,540
530 BACK2(I) = 0.0
540 CONTINUE
    GO TO 800
C    ...INTERPOLATE THE BACKGROUND THROUGH THE POINTS READ IN...
700 JC1=0
    JC2=0
    IF(DB(1)-DIST(1)) 710,710,705
705 JC1=1
    DE(1) = DIST(1)
    RHO2(1)=BACK(1)
710 IF(DB(NJ)-DIST(NCHANN)) 715,750,750
715 JC2=1
    DE(NJ+JC1+1) = DIST(NCHANN)
    RHO2(NJ+JC1+1)=BACK(NJ)
750 DO 755 I=1,NJ
    DE(I+JC1)=DB(I)
755 RHO2(I+JC1)=BACK(I)
    N=NJ+JC1+JC2
    IF (N.LT.3) GO TO 900
    J=2
    DO 790 I=1,NCHANN
    DIX = DIST(I)
770 IF(DIX-DE(J+1)) 750,775,775
775 J=J+1
    IF (J.GE.N) J= J - 1
780 DEM1=(DE(J-1)-DE(J))*(DE(J-1)-DE(J+1))
    DEM2=(DE(J)-DE(J-1))*(DE(J)-DE(J+1))
    DEM3=(DE(J+1)-DE(J-1))*(DE(J+1)-DE(J))
    BACK2(I)=(DIX-DE(J))*(DIX-DE(J+1))/DEM1*RHO2(J-1)
    1 + (DIX-DE(J-1))*(DIX-DE(J+1))/DEM2*RHO2(J)
    2 + (DIX-DE(J-1))*(DIX-DE(J))/DEM3*RHO2(J+1)
    IF(BACK2(I).LT.0.0) BACK2(I)=0.0
790 CONTINUE
800 WRITE(6,310) (DE(I),RHO2(I),I=1,N)
810 FORMAT(26H0POINTS USED BY BACKGROUND)/(2F12.3)
    GO TO 1000
C    ...CALCULATE THE BACKGROUND INTERVALS...
900 IJ = 2
    DB(1) = DIST(1)
    IF (NJ.EQ.1) DB(2) = DIST(NCHANN) + DBTEN
    DO 920 I=1,NCHANN
    IF (DIST(I).GE.DB(IJ)) IJ = IJ + 1
    IF (IJ.EQ.NJ) DB(NJ+1) = DIST(NCHANN) + DBTEN
920 BACK2(I) = BACK(IJ-1)
    WRITE(6,930)
930 FORMAT(13H0    DISTANCE,17X11H BACKGROUND)

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```

DO 940 I=1,NJ
DIX = DB(I+1) - CTFN
940 WRITE(6,950) (DB(I),DIX,BACK(I))
950 FORMAT(F9.3,1H-,F9.3,14XF6.2)
1000 RETURN
END

```

```

C      SUBROUTINE LSQPOL(NSUB,MSUB)
C      LEAST SQUARE POLYNOMIAL FIT
C      COMMON /A02/ X(52), Y(52), W(50), B(10), A(10,10), XPOWER(50),
1     DUMMY(4049)
      N=NSUB
      M=MSUB
      M1=M+1
      M3=M+M+M
      M31=M3-1
      M41=M31+1

```

```

C      FORMATION AND INVERSION OF SYSTEM OF NORMAL EQUATIONS
C
C

```

```

DO 100 K2=M1,M41
XPOWER(K2)=0.0
100 CONTINUE
DO 200 K1=1,N
TERM=W(K1)
DO 200 K2=M1,M31
XPOWER(K2)=TERM+XPOWER(K2)
TERM=X(K1)*TERM
200 CONTINUE
DO 300 I=1,M
DO 300 J=1,M
K2=I+J+M-1
A(I,J)=XPOWER(K2)
300 CONTINUE
DO 400 K=1,N
TERM=W(K)+Y(K)
DO 400 K2=M3,M41
XPOWER(K2)=TERM+XPOWER(K2)
TERM=X(K)*TERM
400 CONTINUE
DO 500 I=1,M
K2=I+M31
B(I)=XPOWER(K2)
500 CONTINUE
CALL MATINV(A, M, B, 1, DETERM, 10)
700 CONTINUE
RETURN
END

```

```

SUBROUTINE PREFAR
C   ...CONVERTS DATA TO CHANNEL NUMBERS AND PREPARES IT FOR THE
C   VARIABLE-METRIC PACKAGE...
REAL LPF
COMMON /A00/ HH(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
1  GB(20),F9,GS,E,SL,FP,GSP,TO,ZZZ,AA,SSS,FO,GTP,FB,GTT,GSR,
2  DELTA,EE,LT,MS,IT,L,THOLD(20),NSSW1,NSSW2
COMMON/A01/ Z(2102,10),SS(2102),IZSTR(20),IZSTOP(20),R(2102),
1  X(2100),W(2100),E(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2  REP, F, FBEST, LPF(22), LP(22), IRS, IPR, IPRE, I1C, ITC, IOFF
COMMON /A02/ SIGMA(20), ERRZ(20), PERSTO(21), STORMH(20),
1  XINTIS(20), INDEX(20), INITAL(20), IFINAL(20), STORV1(2100),
2  RAWX(2100), ITIMES, MNX
COMMON /A03/ DUMMY(53),NT,NCALC,IGS,LQ
COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
1  STOIPR, REFMAX, ID1, ID2, IDT, V3, NE, VREF
COMMON /DATA/ DIST(2100), COUNTS(2100), RJNID, TODAY, FREQ, OFTEN,
1  SKIP(7),MAXREF,MAXP2
DEL = 0.1
QQ = DIST(1)
C   ...CONVERT ALL UNITS TO CHANNEL NUMBER...
DO 1060 I=1,NT
PERSTO(I)=(PERSTO(I)-QQ)/OFTEN + 1.0
1060 STORH(I) = 1.0
PERSTO (NT+1)=3000.0
DEL3 =AINT(DELTA1+DELTA2+0.1)
IPR=(2.0+DELTA2)
IPRE=((2.0+DELTA2)-FLOAT(IPR))*10.0
DO 1061 I = 1,MAXP2
1061 R(I)=0.0
DO 1065 I=1,IDT
1065 R(I+1) = STOREF(I)
IRS = IDT + 1
I1C=1
ITIMES=0
III = 1
C   III = (NUMBER OF PEAKS ALREADY ANALYZED) + 1
2000 IOFF = III - 1
C   ...DIVIDE GROUP OF PEAKS INTO NON-OVERLAPPING SUBGROUPS...
MS=0
LT=0
IF(III-NT)2001,2001,3000
C   I1CSS = (FIRST CHANNEL NUMBER OF FIRST PEAK IN SUBGROUP) - 1
2001 I1CSS = PERSTO(III) - DELTA2 + 0.1
IF(I1CSS.GT.1) I1CSS = I1CSS - 1
DO 2015 JJ=1,20
LT=LT+1
IF(PERSTO (III+JJ)-PERSTO (III+JJ-1)- DEL3) 2015,2015,2020
2015 CONTINUE
2020 XXX = PERSTO(III)
C   ITC = TOTAL NUMBER OF CHANNELS IN THE SUBGROUP
ITC = PERSTO(LT+IOFF) - XXX + DELTA1 + DELTA2 + 3.1
C   ...SETUP INITIAL MATRIX, DATA, WEIGHTS, AND PARAMETERS...
DO 2025 I=1,LT
DO 2025 J=1,LT
2025 HH(I,J)=0.0
DELTA=1.0

```

```

DO 2030 I=1,LT
IM = IOFF + I
PER(I) = PERSTO(IM) - XXX + DELTA2 + 2.
HH(I,I)=STORHH (IM)**2
IF (IHOLD(IM)) 2028,2028,2027
2027 HH(I,I) = 0.0
GO TO 2030
2028 DELTA = DELTA*HH(I,I)
2030 CONTINUE
DO 2035 I=IIC,ITC
JJ = I + IICSS - 1
X(I)=RAWX(JJ)
2035 W(I)=1.0/SQRT(X(I)+10.0)
EE = FLOAT(ITC-LT)*0.05
CALL DAVIDN
ITIMES=ITIMES+1
C      INDEX = NUMBER OF PEAKS IN SUBGROUP
C      INITIAL = STARTING CHANNEL NUMBER IN SUBGROUP
C      IFINAL = FINAL CHANNEL NUMBER FOR SUBGROUP
INDEX(ITIMES)=LT
INITIAL(ITIMES) = IICSS
IFINAL(ITIMES) = IICSS + ITC - 1
Q3 = ITC - LT
C      ...CALC. ERRORS IN POSITIONS AND COMPUTE NORMALIZED INDIV. PEAKS
DO 2042 I=1,LT
IM = IOFF + I
PERSTO (IM)=(PER(I)+XXX-DELTA2-3.0)*OFTEN + Q3
STORHH(IM)=HH(I,I)
SIGMA(IM)=SQRT (ABS ((2.0*STORHH (IM)*FREST)/Q3))*OFTEN
IF(A(I)) 2115,2110,2115
2110 ERR7(IM) = 0.0
GO TO 2120
2115 ERR7(IM)=ERR(I) /A(I)
2120 DO 2040 J=1,MAXP2
2040 Z(J,IM) = Z(J,IM)*A(I)
2042 CONTINUE
IF (IT.GE.25) WRITE(6,1001) (PERSTO(I),I=1,LT)
III = III + LT
GO TO 2000
3000 RETURN
1001 FORMAT(51H) EPSILON TOO SMALL - CANNOT CONVERGE FOR PEAKS AT ,5F10
1.2/(10F10.2)
END

```

```

SUBROUTINE FCN(LLTT,SP,F9,PER,M1)
C ...SETS UP THE LINEAR EQUATIONS AND OBTAINS RELATIVE PEAK HEIGHTS.
REAL LPF
DIMENSION PFR(20),GR(20)
COMMON/A01/Z(2102,10),SS(2102),I7STRT(20),IZSTOP(20),R(2102),
1 X(2100),W(2100),E(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2 REF,F,FBEST,LPF(22),LP(22),IRS,IPR,IPRE,I1C,ITC,I0FF
COMMON /DATA/ DIST(2100),COUNTS(2100),RJND,TODAY,FREQ,OFTEN,
1 NOFTEN,NCHANN,II,IJ,ISPECT,IFMT,IERR,MAXREF,MAXP2
LT=LLTT
IF(M1.EQ.1) FBEST = 1.0E10
4006 DO 91 L=1,LT
LP(L) = PER(L)
LPF(L) = (PER(L)-FLOAT(LP(L)))*10.0
91 CALL SHIFT(L)
PRINT*," IF M1 = 3 = ",M1," WILL CALL FUN FROM FCN "
205 IF (M1-3) 222,219,222
C DUMMY CALL TO FUN TO FORM THE ARRAY E
219 CALL FUN(LT)
DO 220 I=I1C,ITC
220 W(I) = 1.0/SQRT(ABS(E(I))+10.)
222 DO 210 M=1,LT
MM = M + I0FF
DO 210 L = 1,M
LL = L + I0FF
C(M,L) = 0.0
DO 200 I=I1C,ITC
IF ((I.LT.IZSTRT(LL)).OR.(I.GT.IZSTOP(LL))) GO TO 200
IF ((I.LT.IZSTRT(MM)).OR.(I.GT.IZSTOP(MM))) GO TO 200
IL = I - IZSTRT(LL) + 1
IM = I - IZSTRT(MM) + 1
C(M,L) = C(M,L) + W(I)*W(I)*Z(IL,LL)*Z(IM,MM)
200 CONTINUE
210 C(L,M) = C(M,L)
DO 201 M=1,LT
MM = M + I0FF
A(M) = 0.0
DO 201 I=I1C,ITC
IF ((I.LT.IZSTRT(MM)).OR.(I.GT.IZSTOP(MM))) GO TO 201
IM = I - IZSTRT(MM) + 1
A(M) = A(M) + W(I)*W(I)*X(I)*Z(IM,MM)
201 CONTINUE
CALL MATINV(C,LT,A,1,DETERM,5)
CALL DERIVP(LT,PER)
DO 1000 L=1,LT
1600 GR(L) = G(L)
PRINT*," CALLING FUN FROM FCN, F = ",F," GR=G= ",G
CALL FUN(LT)
IF(M1-3) 206,1011,206
1011 F7 = F/(ITC-I1C-LT)
DO 1006 L=1,LT
REP = F7*C(L,L)
1006 ERR(L) = SQRT(ABS(REP))
206 F9 = F
IF (F9.LT.FBEST) FBEST = F9
RETURN
END

```

```

SUBROUTINE DERIVP(LLTT,PER)
C   ...CALCULATES DERIVATIVES OF FUNCTION F(FUN) WITH CHANGE
C   IN POSITION
REAL LPF,LOPE
DIMENSION PER(20)
COMMON/A01/Z(2102,10),SS(2102),IZSTRT(20),IZSTOP(20),R(2102),
1  X(2100),W(2100),E(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2  REP,F,FBEST,LPF(22),LP(22),IRS,IPR,IPRE,IIC,ITC,IOFF
COMMON /DATA/ DIST(2100),COUNTS(2100),RJNID,TODAY,FREQ,OFTEN,
1  NOFTEN,NCHANN,II,IJ,ISPECT,I=MT,IERR,MAXREF,MAXP2
LT=LLTT
DO 94 L=1,LT
LL=L+IOFF
DO 94 I=1,MAXP2
34 SS(I)=Z(I,LL)
ISAV1=IZSTRT(LL)
ISAV2=IZSTOP(LL)
LOP=LP(L)
LOPE=LPF(L)
Y=PEF(L)+DEL
LP(21)=Y
LPF(21)=(Y-FLOAT(LP(21)))*10.0
Y=PER(L)-DEL
LP(22)=Y
LPF(22)=(Y-FLOAT(LP(22)))*10.0
LP(L)=LP(21)
LPF(L)=LPF(21)
CALL SHIFT(L)
PRINT*," CALLING FUN FROM DERIVP, L = ",L," F = ",F
CALL FUN(LT)
FP=F
LP(L)=LP(22)
LPF(L)=LPF(22)
CALL SHIFT(L)
PRINT*," CALLING FUN FROM DERIVP, F = ",F
CALL FUN(LT)
G(L)=(FP-F)/(2.0*DEL)
DO 95 I=1,MAXP2
95 Z(I,LL)=SS(I)
IZSTRT(LL)=ISAV1
IZSTOP(LL)=ISAV2
LP(L)=LOP
36 LPF(L)=LOPE
RETURN
END

```

```

SUBROUTINE SHIFT(.0)
C   ...CONTROLS INTERPOLATION OF FRF. PEAK FOR SHIFTING FRACTIONS
C   OF CHANNELS
C   ...CONTROLS INTERPOLATION OF REF. PEAK FOR SHIFTING FRACTIONS OF C
REAL LPF
COMMON/A01/Z (2102,10),SS (2102),IZSTRT (20),IZSTOP (20),R (2102),
1  X (2100),W (2100),E (2100),C (20,20), A (20), G (20), ERR (20), DEL,
2  REP, F, FREST, LPF (22), LP (22), IRS, IPR, IPRE, IIC, ITC, IOFF
COMMON /DATA/ DIST (2100), COUNTS (2100), RUNID, TODAY, FREQ, OFTEN,
1  NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
L=LD
LL = L + IOFF
C1=LP (L)
C2=LPF (L)
U=C1+C2/10.0
B8=IFR
P9=IFRE
DO 100 J=1,MAXP2
100 Z (J,LL) = J.0
B1=B8+P9/10.0
IF (B1-U) 300,19,3
C   SUBROUTINE SHIFTL L LESS THAN R
9   J=1
IZSTRT (LL) = 1
IF (IPRE-LPF (L)) 10,11,12
10  F = 10+IPRE-LPF (L)
I = IPR-LP (L)
GO TO 14
11  F=0.0
GO TO 13
12  F = IPRE-LPF (L)
13  I = IPR-LP (L)+1
14  F1 = F/10.0
15  Z (J,LL) = R (I) + F1*(R (I+1)-R (I))
I=I+1
J=J+1
IF (I-IRS) 16,16,17
16  IF (J-ITC) 15,15,17
17  IZSTOP (LL) = J - 1
GO TO 23
C   SUBROUTINE SHIFTO L EQUAL R
18  DO 20 J=1,IRS
20  Z (J,LL) = R (J)
IZSTRT (LL) = 1
IZSTOP (LL) = IRS
GO TO 23
C   SUBROUTINE SHIFTR R LESS THAN L
300 I=1
IF (IPRE-LPF (L)) 1,2,3
1  F = 10+IPRE-LPF (L)
K = LP (L)-IPR+2
GO TO 5
2  F=0.0
GO TO 4
3  F = IPRE-LPF (L)
4  K =LP (L)-IPR+1
5  F1 = F/10.0

```

```

      IZSTRT(LL) = K
      J = 1
6     Z(J,LL) = R(I) + F1*(R(I+1)-R(I))
      I=I+1
      J=J+1
      K = K + 1
      IF (I-IRS) 7,7,3
7     IF (K-ITC) 5,6,8
8     IZSTOP(LL) = K - 1
23    RETURN
      END

```

```

C     SUBROUTINE FUN(LT)
      ...CALCULATES THE FUNCTION F WHICH IS BEING MINIMIZED...
      REAL LPF
      COMMON/A01/Z(2102,1),SS(2102),I7STRT(20),I7STOP(20),R(2102),
1     X(2100),W(2100),F(2100),C(20,20),A(20),G(20),ERR(20),DEL,
2     REP,F,FBEST,LPF(22),LP(22),IRS,IPR,IPRE,I10,ITC,I0FF
      COMMON /DATA/ DIST(2100),COUNTS(2100),RUNID,TODAY,FREQ,OFTEN,
1     NOFTEN,NCHANN,II,IJ,ISPECT,IFMT,IERR,MAXREF,MAXP2
      F=0.0
      DO 60 I=1,ITC
50    E(I) = 0.0
      DO 70 L=1,LT
      I1 = IZSTRT(L+I0FF)
      I2 = I7STOP(L+I0FF)
      DO 80 I=I1,I2
      J = I - I1 + 1
70    E(I) = E(I) + A(L)*Z(J,L+I0FF)
      DO 80 I=I1,ITC
      F1 = (X(I)-E(I))*W(I)
80    F = F + F1*F1
      RETURN
      END

```

```

C     SUBROUTINE ARYODR(A,B,N,L)
      OPDERS THE ARRAY A, AND MAKES SAME ORDERING TO B IF L=2.
      INTEGER B
      DIMENSION A(1),B(1)
      NP = N - 1
      DO 50 I=1,NP
      K = I + 1
      DO 50 J = K,N
      IF (A(I)-A(J)) 50,50,20
20    IF (L-1) 40,40,30
30    ISAV = B(I)
      B(I) = B(J)
      B(J) = ISAV
40    SAVE = A(I)
      A(I) = A(J)
      A(J) = SAVE
50    CONTINUE
      RETURN
      END

```

```

SUBROUTINE MATINV(A, NSUB, B, MSUB, JET, NMAX)
C
DIMENSION A(NMAX, NSUB), B(NMAX, MSUB)
DIMENSION PIVOT(100), INDEX(100), IPIVOT(100)
EQUIVALENCE (PIVOT, INDEX, IPIVOT), (AMAX, T), (IROW, I1, IRC),
1 (TEMP, SWAP)
DATA (ISHIFT=4096), (MASK=0000000077777777B)
C
N=NSUB
M=MSUB
C
C INITIALIZATION
C
DETERM=1.0
DO 20 I=1, N
IPIVOT(I)=0
20 CONTINUE
DO 500 I=1, N
C
C SEARCH FOR PIVOT ELEMENT
C
AMAX=0.
DO 105 J=1, N
TEMP=IPIVOT(J).AND..NOT.MASK
IF(TEMP) 105, 60.
60 DO 100 K=1, N
TEMP=IPIVOT(K).AND..NOT.MASK
IF(TEMP) 100, 80
30 TEMP=ABS (A(J, K))
IF(TEMP-AMAX) 100, 85, 85
35 IROW=J
ICOLUM=K
AMAX=TEMP
100 CONTINUE
105 CONTINUE
INDEX(I)=INDEX(I)+(ISHIFT*IROW+ICOLUM)
J=IROW
AMAX=A(J, ICOLUM)
DETERM=AMAX*DETERM
C
C MATRIX SINGULAR
C
IF(DETERM) 110, 500
C
110 PIVOT(ICOLUM)=INDEX(ICOLUM).OR.AMAX.AND..NOT.MASK
C
C INTERCHANGE ROWS
C
IF(IROW-ICOLUM) 1+0, 260
140 DETERM=-DETERM
DO 200 K=1, N
SWAP = A(J, K)
A(J, K)=A(ICOLUM, K)
A(ICOLUM, K)=SWAP
200 CONTINUE
DO 250 K=1, M
SWAP=B(J, K)

```

```

      B(J,K)=B(ICOLUM,K)
      B(ICOLUM,K)=SWAP
250  CONTINUE
C
C   DIVIDE PIVOT ROW
C
250  K=ICCLUM
      A(ICOLUM,K)=1.0
      DO 350 K=1,N
        A(ICCLUM,K)=A(ICCLUM,K)/AMAX
350  CONTINUE
      DO 370 K=1,M
        B(ICCLUM,K)=B(ICCLUM,K)/AMAX
370  CONTINUE
C
C   REDUCE
C
      DO 550 J=1,N
        IF(J-ICOLUM) 400,550
400  T=A(J,ICOLUM)
        A(J,ICOLUM)=0.0
        DO 450 K=1,N
          A(J,K)=A(J,K)-A(ICOLUM,K)*T
450  CONTINUE
        DO 500 K=1,M
          B(J,K)=B(J,K)-B(ICOLUM,K)*T
500  CONTINUE
550  CONTINUE
C
C   INTERCHANGE
C
600  DO 710 I=1,N
      I1=N+1-I
      IRC=INDEX(I1).AND.MASK
      K=IRC/ISHIFT
      ICOLUM=IRC-K*ISHIFT
      IF(K-ICOLUM) 650,710
650  DO 705 J=1,N
        SWAP=A(J,K)
        A(J,K)=A(J,ICOLUM)
        A(J,ICOLUM)=SWAP
705  CONTINUE
710  CONTINUE
C
740  DET=DETERM
C   RETURN
      ENTRY OMATINV
      RETURN
      END

```

```

SUBROUTINE DAVIDN
C   ...THIS IS THE CONTROL ROUTINE FOR THE VARIABLE-METRIC PACKAGE...
COMMON /A00/ H(20,20),Y(20),G(20),S(20),XP(20),GP(20),T(20),
1  GB(20),F,GS,EL,SL,FP,GSP,T0,Z,0,A,SSS,F0,GTP,FB,GTI,GSB,
2  DELTA,E,N,MS,IF,L,IHOLD(20),NSSW1,NSSW2
15  M1=1
    IT = 0
    F=0.0
    CALL FCN(N,G,F,X,M1)
    IF(NSSW1)20,25,20
20  WRITE(6,3) IT,MS,F
    GO TO 840
120 M1=2
200 CALL READY
    PRINT*,"          CALLED READY      L= ",L
    GO TO (800,300,500,500), L
300 CALL AIM
    PRINT*,"          CALLED AIM        L= ",L
    GO TO (400,500,500,500), L
400 CALL FIRE
    GO TO (500,500,300,300), L
500 CALL DRESS
    IF (IT-25) 120,550,550
550 M1 = 3
    GO TO 900
900 M1=3
    IF(NSSW1)22,25,22
    22 WRITE(6,11)
810 DO 820 II=1,N
820 WRITE(6,7) (H(II,JJ),JJ=1,N)
830 WRITE(6,12) DELTA,F,GS
840 IF(NSSW1)24,25,24
    24 WRITE(6,10) (X(I),I=1,N)
    GO TO (850,850,850), M1
850 WRITE(6,13) (G(I),I=1,N)
860 WRITE(6,9)
    25 GO TO (120,120,900), M1
900 IF (N.GT.1) CALL ORDER
    CALL FCN(N,G,F,X,M1)
30  RETURN
    3  FORMAT(6E12.5)
    7  FORMAT(1H08E14.5)
    8  FORMAT(4H0IT I4,7H STEP I4,4H F=E14.5)
    9  FORMAT(20H0- - - - -)
   10  FORMAT(3H0X=3E14.5/(3H0 8E14.5))
   11  FORMAT(13H0FINAL VALUES/13H0ERROR MATRIX)
   12  FORMAT(7H0DELTA=E14.5,4H F=E14.5,5H GS=E14.5)
   13  FORMAT(3H0G=8E14.5/(3H0 8E14.5))
    END
  
```

```

SUBROUTINE READY
COMMON /A00/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
1 GB(20),F,GS,EL,SL,FP,GSP,T0,Z,I,A,GSS,F0,GTP,FB,GTT,GSR,
2 DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
200 L=1
CALL MATMPY(N,N,H,G,S)
DO 205 I=1,N
205 S(I)=-S(I)
CALL MATMPY(1,N,S,G,GS)
IF (GS+E) 210,240,240
210 L=2
EL=2.0
T0=EL*F/GS
IF (T0+EL) 213, 213, 212
212 EL=-T0
213 SL=-GS
DO 215 I=1,N
215 XP(I)=X(I)+EL*S(I)
CALL FCN(N,GP,FP,XP,I)
CALL MATMPY(1,N,S,G,GSP)
IF (-GSP) 240,240,220
220 IF (F-FP) 240,240,225
225 L=3
IF(NSSW1) 100,101,100
100 WRITE(6,1)
101 FB=FP
DO 230 I=1,N
GB(I)=GP(I)
T(I)=XP(I)
230 CONTINUE
IF (EL-2.0) 240,235,240
235 L=4
DELTA=DELTA+DELTA
T0=1.0/SL
240 RETURN
1 FORMAT(10HOUNDERSHOT)
END

```

```

SUBROUTINE MATMPY(M,N,H,G,S)
DIMENSION H(20,20),G(20),S(20)
700 DO 720 II=1,M
S(II)=0.0
DO 720 JJ=1,N
720 S(II)=H(JJ,II)*G(JJ)+S(II)
740 RETURN
END

```

```

SUBROUTINE A14
COMMON /A00/ H(20,20),Y(20),G(20),S(20),XP(20),GP(20),T(20),
1 GR(20),F,GS,EL,SL,FP,GSP,T0,Z,?,A,GSS,F0,GTP,FP,GTF,GSR,
2 DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
300 L=1
Z=3.0/EL*(F-FP)+GS+GSP
Q=ABS (Z*SQRT (1.0-(GS/Z)*(GSP/Z)))
A=(Q-Z+GSP)/(Q+Q-GS+GSP)
T0=EL/3.0*(Q+Q+Z+GS)*A*A
F0=FP-T0
CALL MATMPY(N,N,H,GP,T)
DO 305 I=1,N
305 T(I)=(GSP/SL)*S(I)-T(I)
CALL MATMPY(1,N,T,GP,GTP)
IF (T0+T0+GTF) 315,310,310
310 DO 312 I=1,N
312 T(I)=XP(I)+A*(X(I)-XP(I))
GO TO 340
315 IF (F+F+GTP) 310,320,320
320 DO 322 I=1,N
322 T(I)=T(I)+XP(I)
CALL FCN(N,G3,FB,T,?)
IF (F0-F9) 310,325,325
325 L=3
IF(NSSW1)100,101,100
100 WRITE(6,1)
101 DO 327 I=1,N
327 S(I)=T(I)-XP(I)
CALL MATMPY(1,N,S,G3,GTT)
GTT=GTT-GTP
IF (GTT) 340,330,330
330 L=2
GSS=GTT
SL=-GTP
EL=1.0
340 RETURN
1 FORMAT(9H0RICOCHET)
END

```

```

SUBROUTINE FIRE
COMMON /A00/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
1 GB(20),F,GS,EL,SL,FP,GSP,T0,Z,0,A,GSS,F0,GTP,FB,GTT,GSB,
2 DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
EQUIVALENCE (TEMP,GTT)
400 L=1
TEMP=A/(1.0-A)
CALL FCN(N,GB,FB,T,2)
CALL MATMPY(1,N,S,G3,GSR)
T0=F
IF (T0-FP) 403, 403, 402
402 T0=FF
403 IF (T0-FB+E) 415, 405, 405
405 GSS=C+0
T0=GSB*(TEMP-1.0/TEMP)
IF (ABS (T0)-0) 430,410,410
410 L=2
GO TO 440
415 L=3
IF(FP-F) 425,420,+20
420 IF(NSSW1)100,101,100
100 WRITE(6,1)
101 EL=(1.0-A)*EL
FP=FB
GSP=GSR
DO 422 I=1,N
XP(I)=T(I)
GP(I)=GB(I)
422 CONTINUE
GO TO 440
425 IF(NSSW1)200,201,200
200 WRITE(6,2)
201 EL=EL*A
F=FB
GS=GSB
DO 427 I=1,N
X(I)=T(I)
G(I)=GP(I)
427 CONTINUE
GO TO 440
430 GSS=GSS+T0
DO 435 I=1,N
435 G(I)=(GB(I)-G(I))*TEMP+(GP(I)-G3(I))/TEMP
440 RETURN
1 FORMAT(10H0MOVE LEFT)
2 FORMAT(11H0MCVE RIGHT)
END

```

```

SUBROUTINE DRESS
COMMON /A00/ H(20,20),Y(20),G(20),S(20),XP(20),GP(20),T(20),
1 GB(20),F,GS,EL,SL,FP,GSP,T0,Z,A,GSS,F0,GTP,FB,GTT,GSB,
2 DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
500 GO TO (505,520,530,525), L
505 CALL MATMPY(N,N,H,G,X)
CALL MATMPY(1,N,X,G,T0)
IF (T0-GSS**2/SL-E) 510,510,510
510 DO 512 II=1,N
DO 512 JJ=1,N
512 H(II,JJ)=H(II,JJ)-X(II)*X(JJ)/T0
DELTA=DELTA*(EL*GSS/T0)
T0=EL/GSS
GO TO 525
515 IF(NSSW1)200,520,200
200 WRITE(6,1)
520 DELTA=DELTA*(EL*SL/GSS)
T0=EL/GSS-1.0/SL
525 DO 527 II=1,N
DO 527 JJ=1,N
527 H(II,JJ)=H(II,JJ)+T0*S(II)*S(JJ)
530 IT=IT+1
F=FB
IF(NSSW1)100,101,100
100 WRITE(6,+) IT,MS,F,GS
101 DO 532 I=1,N
G(I)=GB(I)
X(I)=T(I)
532 CONTINUE
IF(NSSW1)535,540,535
535 WRITE(6,2) (X(I),I=1,N)
WRITE(6,3) DELTA
540 RETURN
1 FORMAT(9H0COLINEAR)
2 FORMAT(3H0X=,8E14.5/(3H0 ,8E14.5))
3 FORMAT(7H0DELTA=,E14.5/20H0- - - - -)
4 FORMAT(4H0IT ,I4,7H STEP ,I4,4H F=,E14.5,5H GS=,E14.5)
END

```

```

SUBROUTINE ORDER
COMMON /A0J/ HH(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
1 GB(20),F,GS,EL,SL,FP,GSP,T0,Z,A,GSS,F0,GTP,FB,GTT,GSB,
2 DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
JC = N - 1
DO 100 I=1,JC
K = I + 1
DO 100 J=K,N
IF (PER(I)-PER(J)) 100,100,60
50 SAVE = PER(I)
PER(I) = PER(J)
PER(J) = SAVE
SAVE = HH(I,I)
HH(I,I) = HH(J,J)
HH(J,J) = SAVE
ISAV = IHOLD(I)
IHOLD(I) = IHOLD(J)
IHOLD(J) = ISAV
100 CONTINUE
RETURN
END

```

Appendix I

Miscellaneous Plots

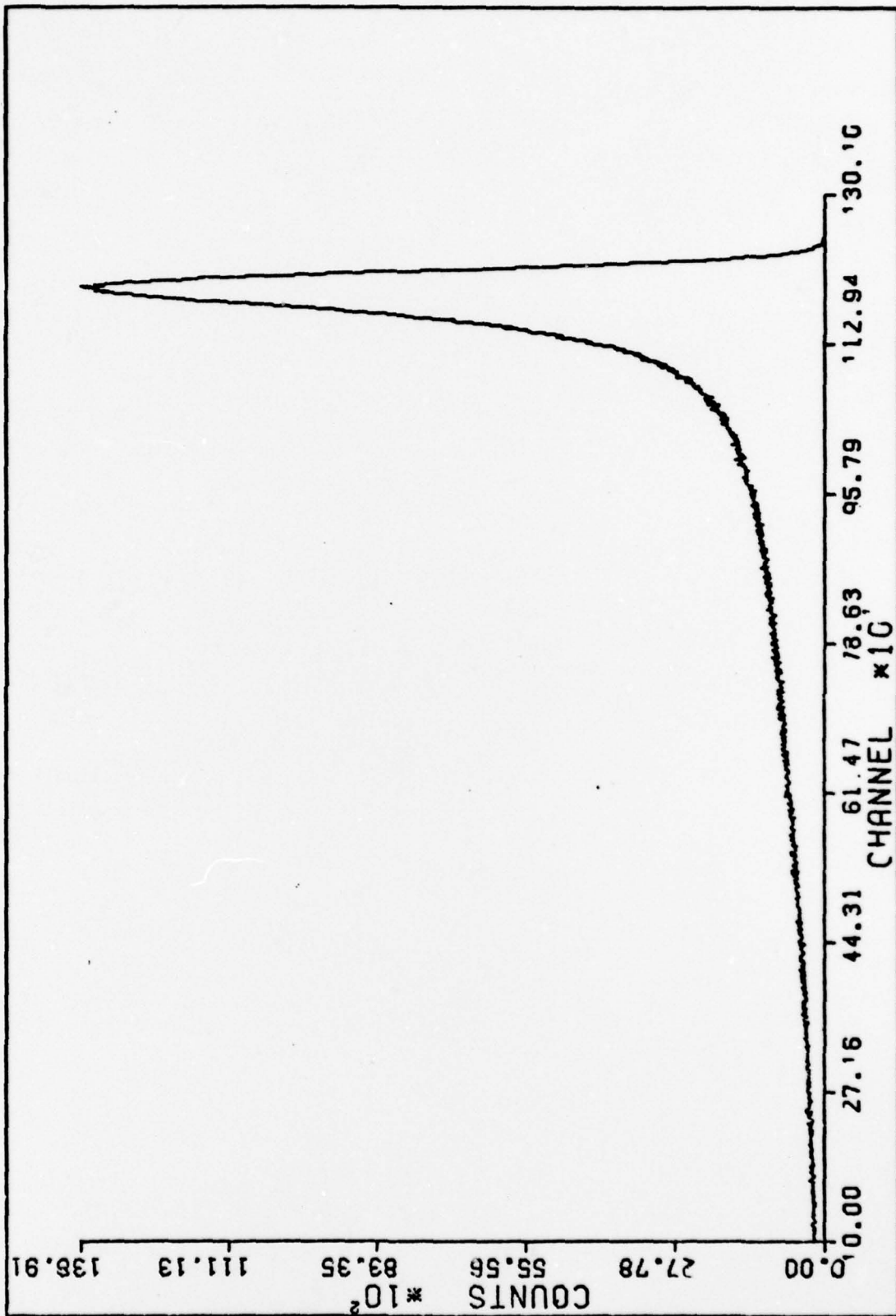


FIG 25. RA DEF # 11 (UNOXIDIZED) 0.6 KEV/CHANNEL 40.000 SEC.

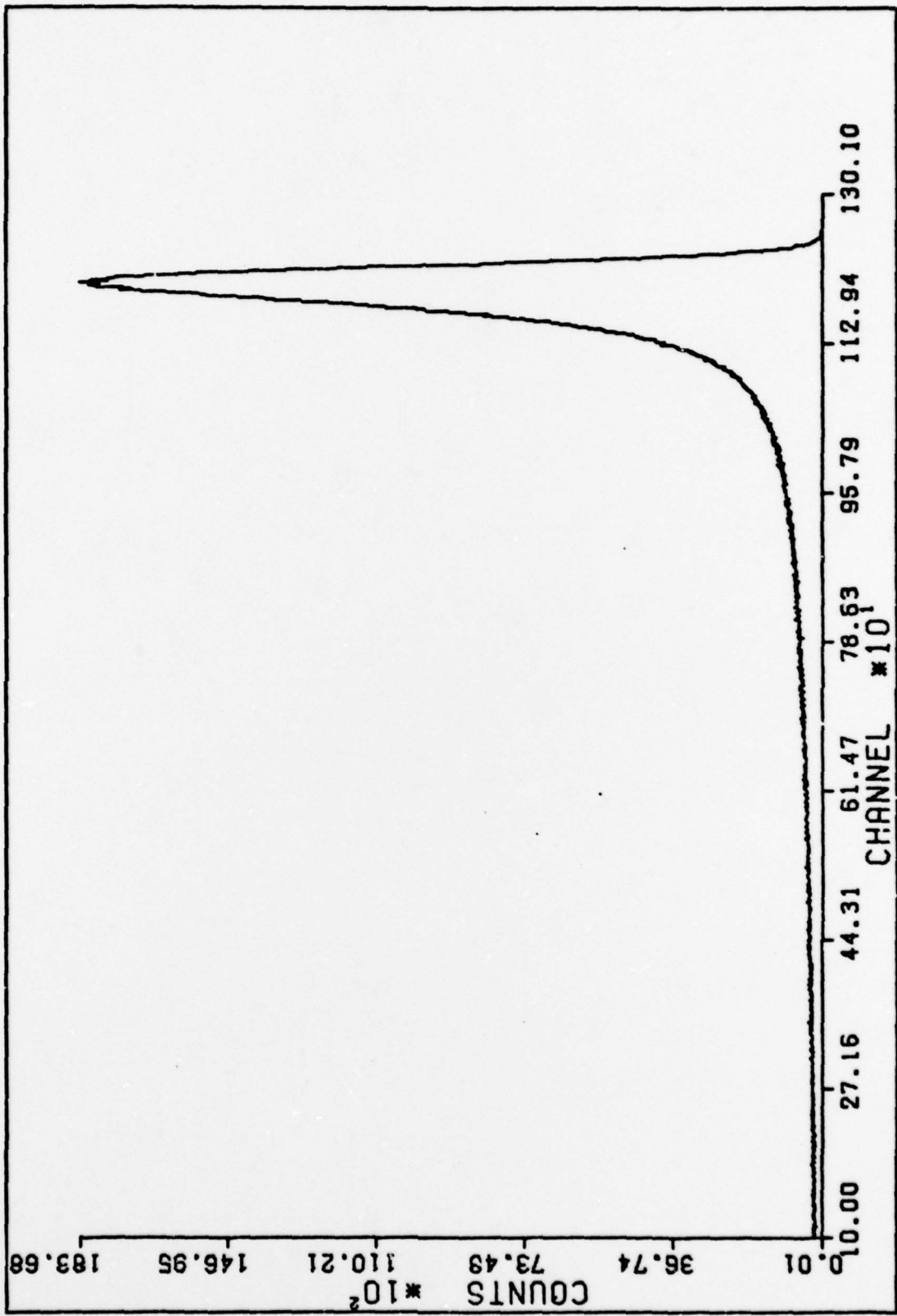


FIG 26. RR DEF # 12 (UNOXIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

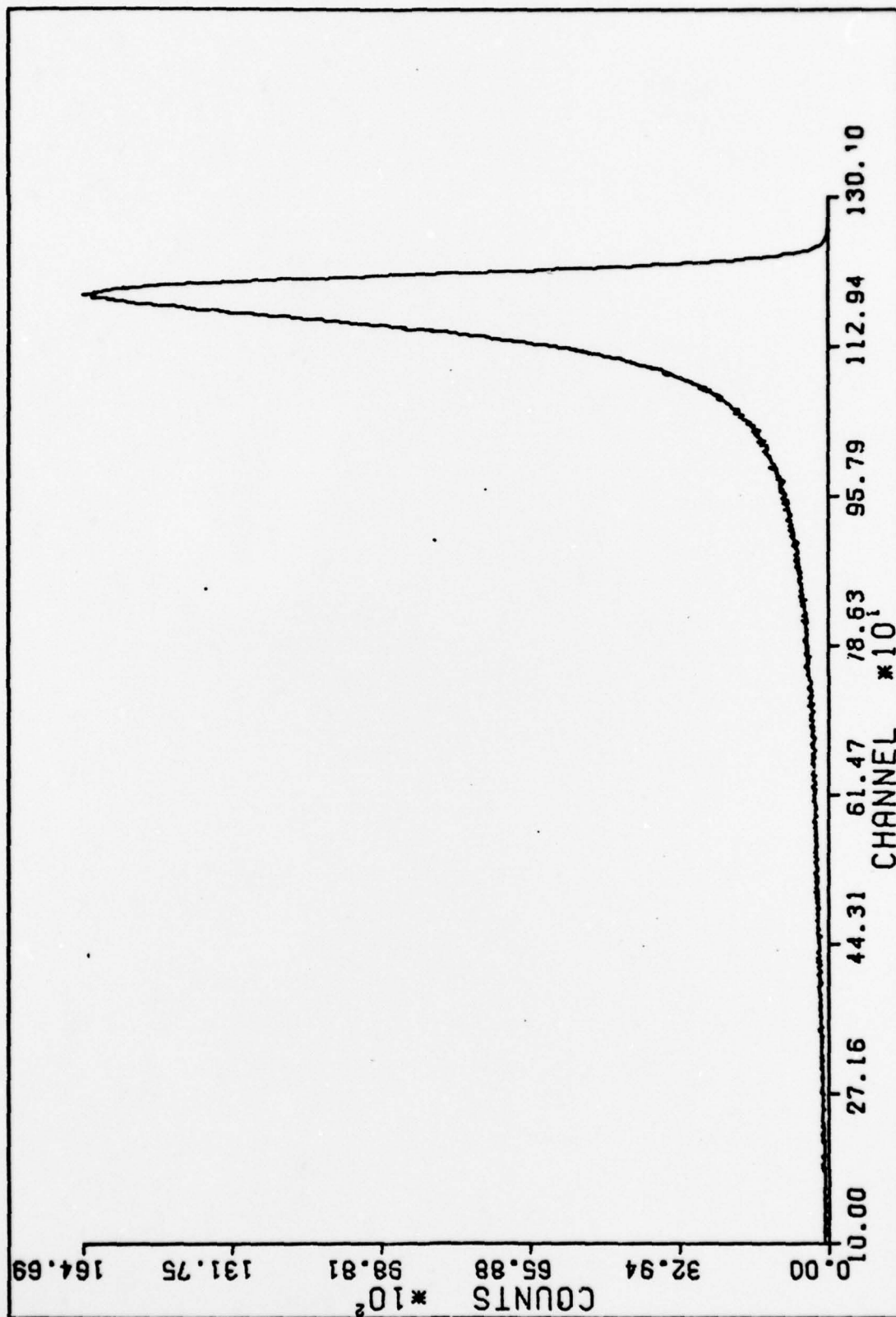


FIG 27. RA DEF # 13 (UNOXIDIZED) 0.6 KEV/CHANNEL 40.000 SEC.

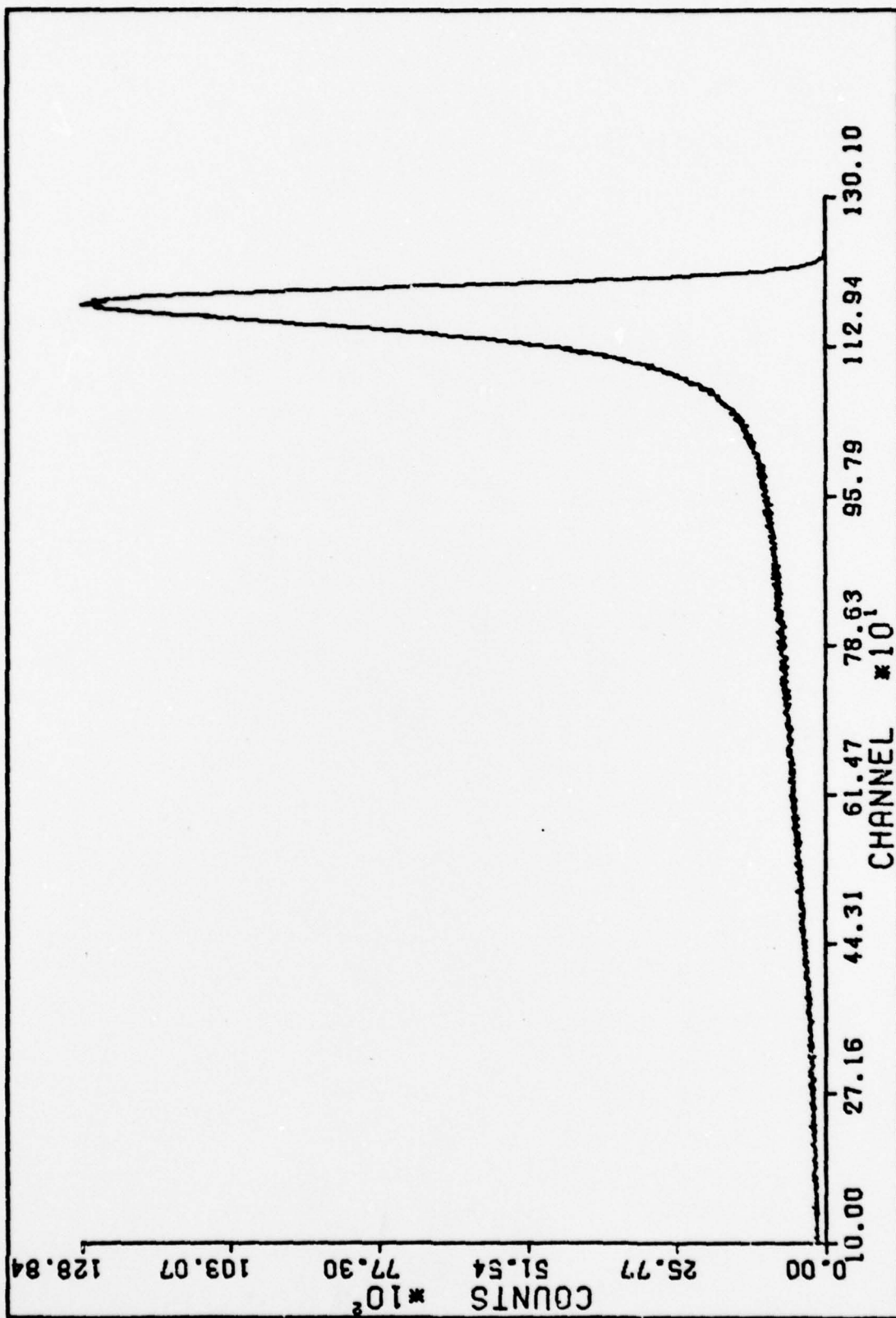


FIG 28. RA DEF # 14 (UNOXIDIZED) 0.6 KEV/CHANNEL 40.000 SEC.

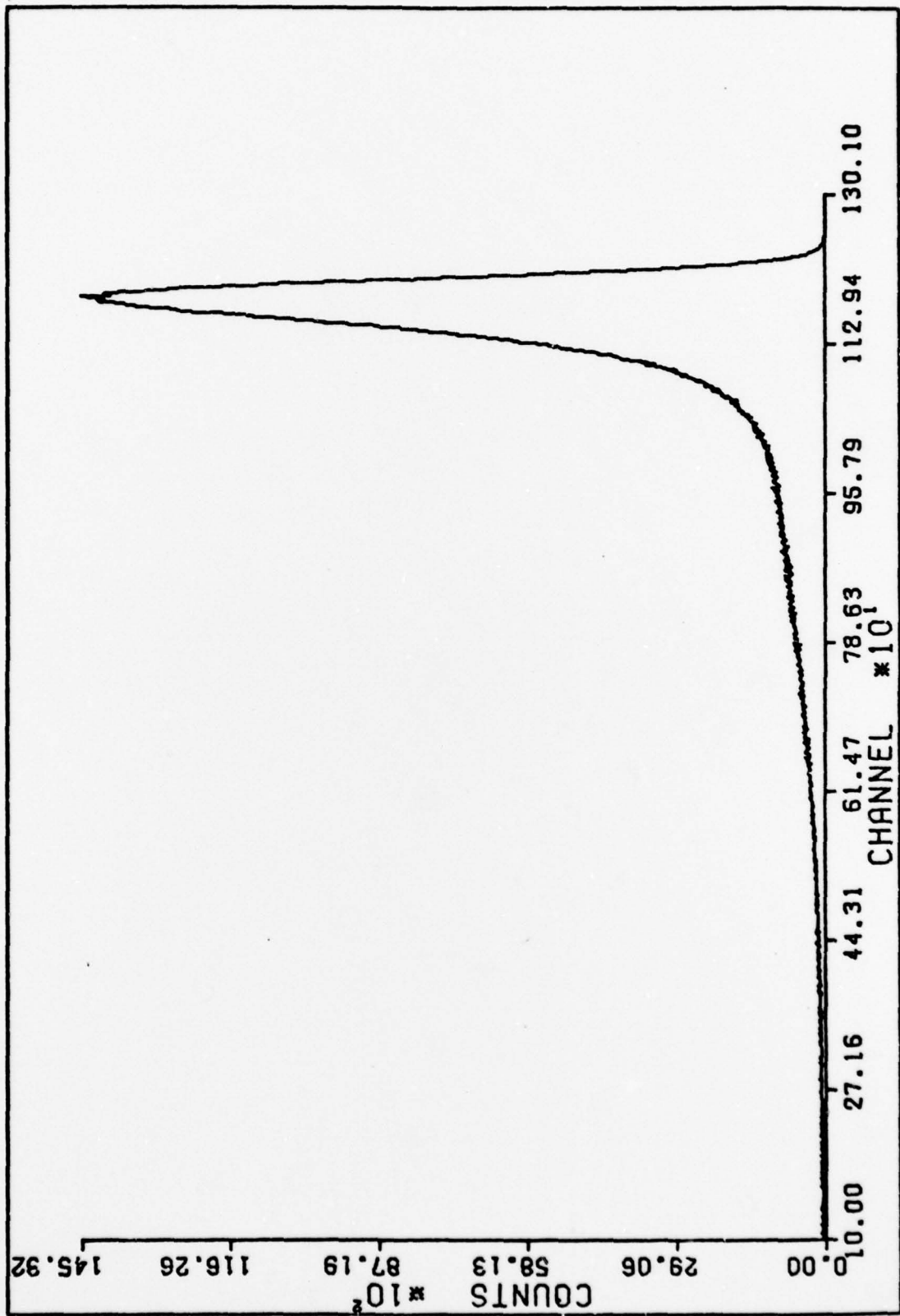


FIG 29 RA DEF # 15 (UNOXIDIZED) 0.6 KEV/CHANNEL 40000 SEC.

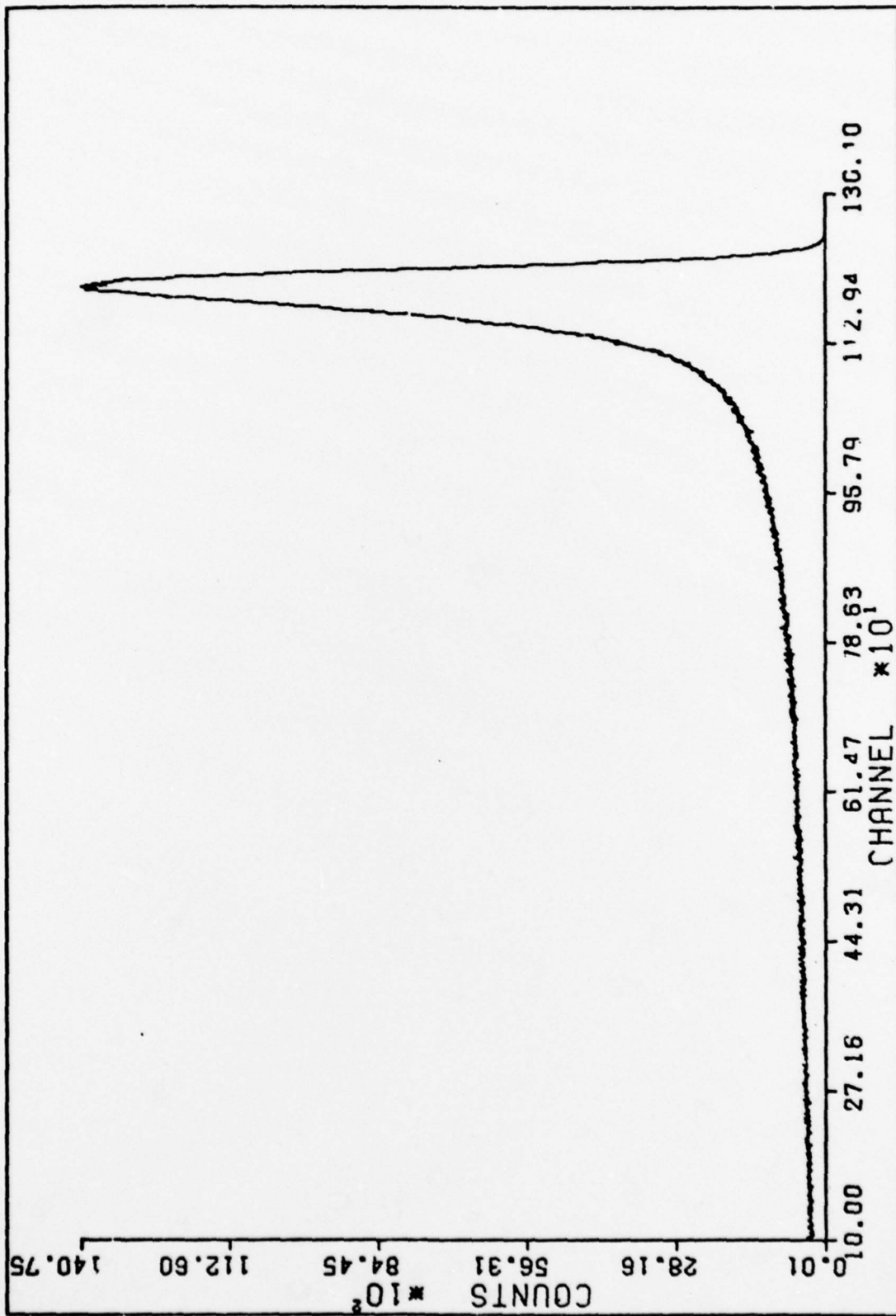


FIG 30. RA DEF # 16 (UNOXIDIZED) 0.6 KEV/CHANNEL 40.000 SEC.

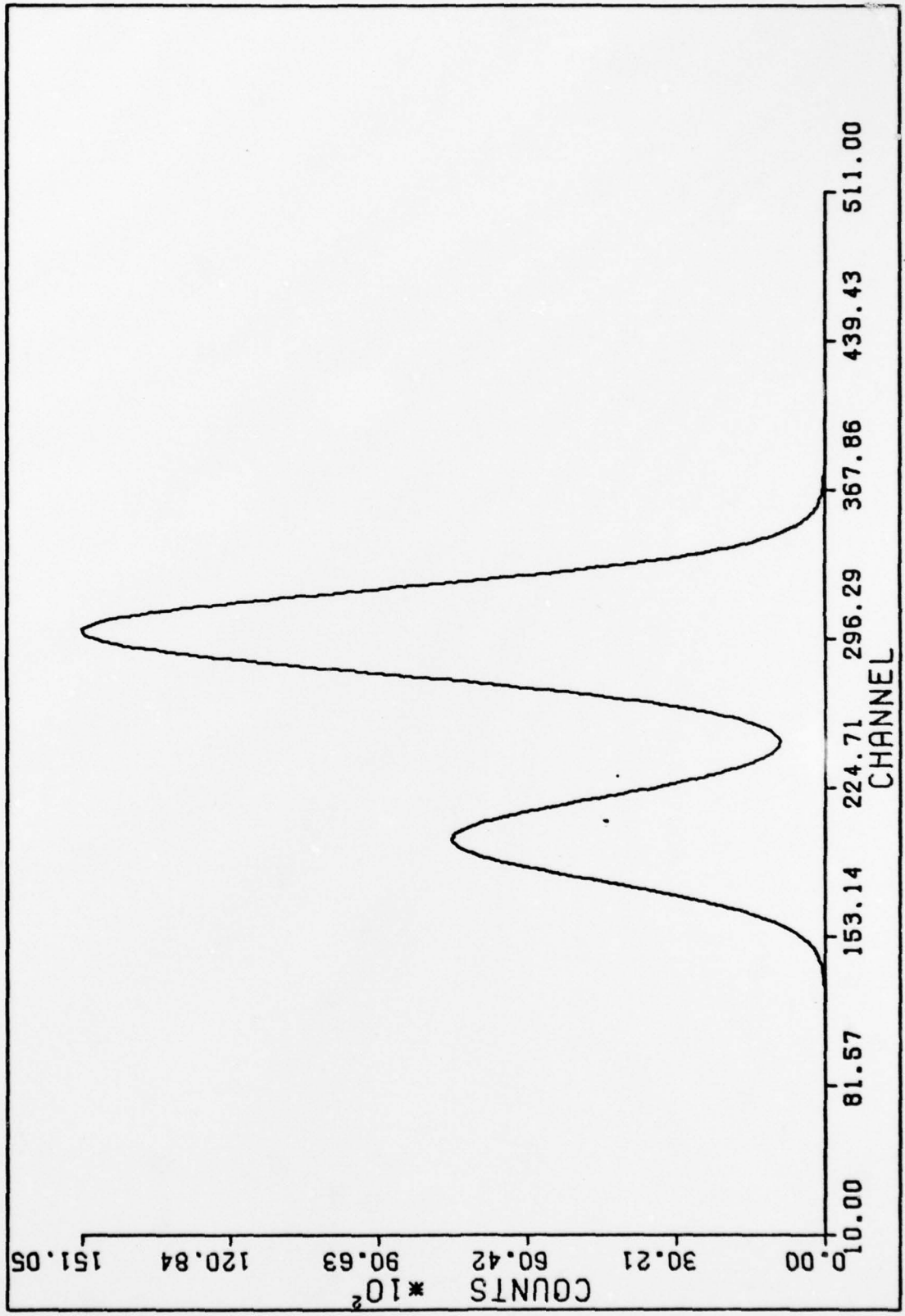


Fig. 31. Randomized Gaussian Peaks. Separation = 100 Channels. Heights are 10000, 20000.

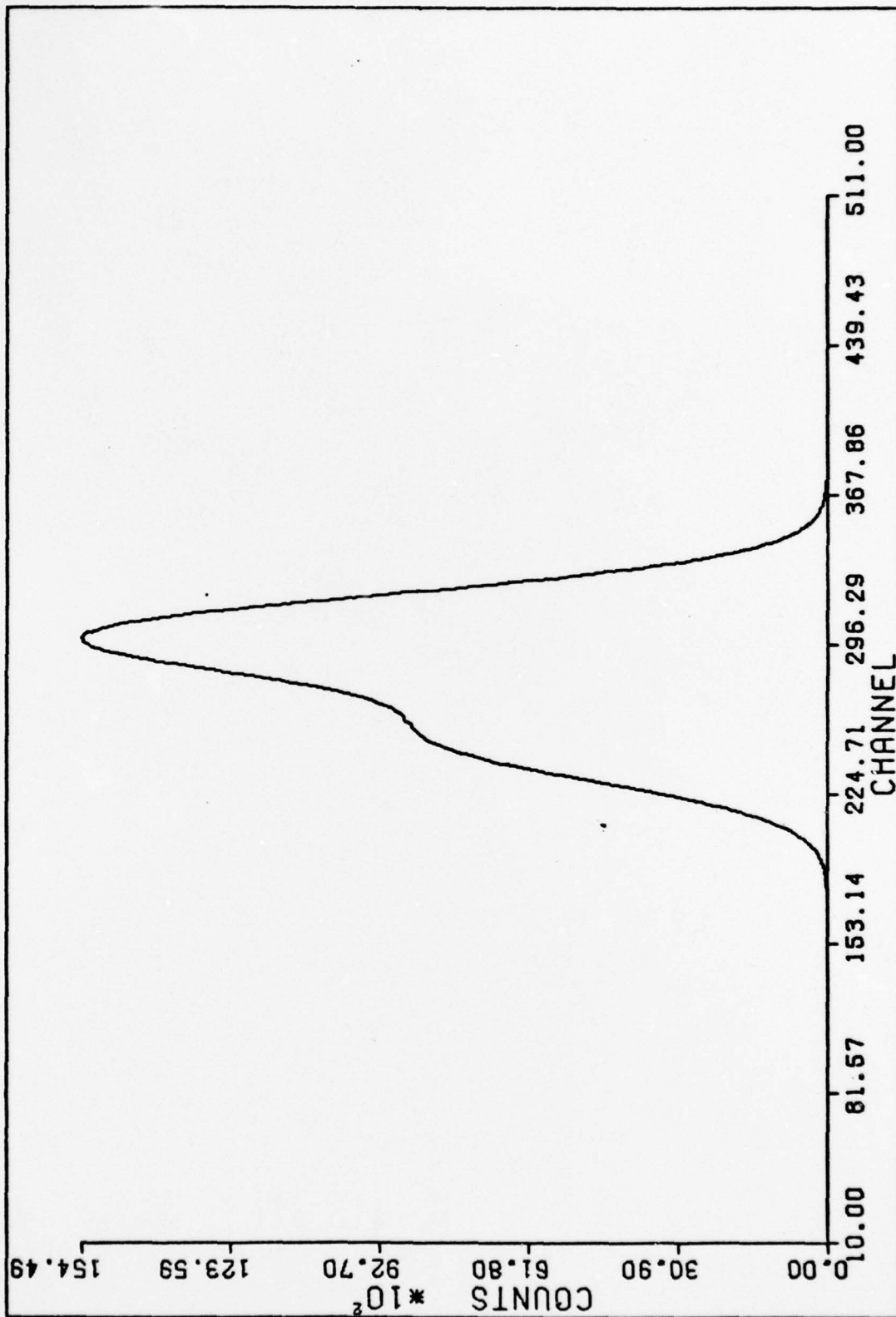


Fig. 32. Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 10000, 20000.

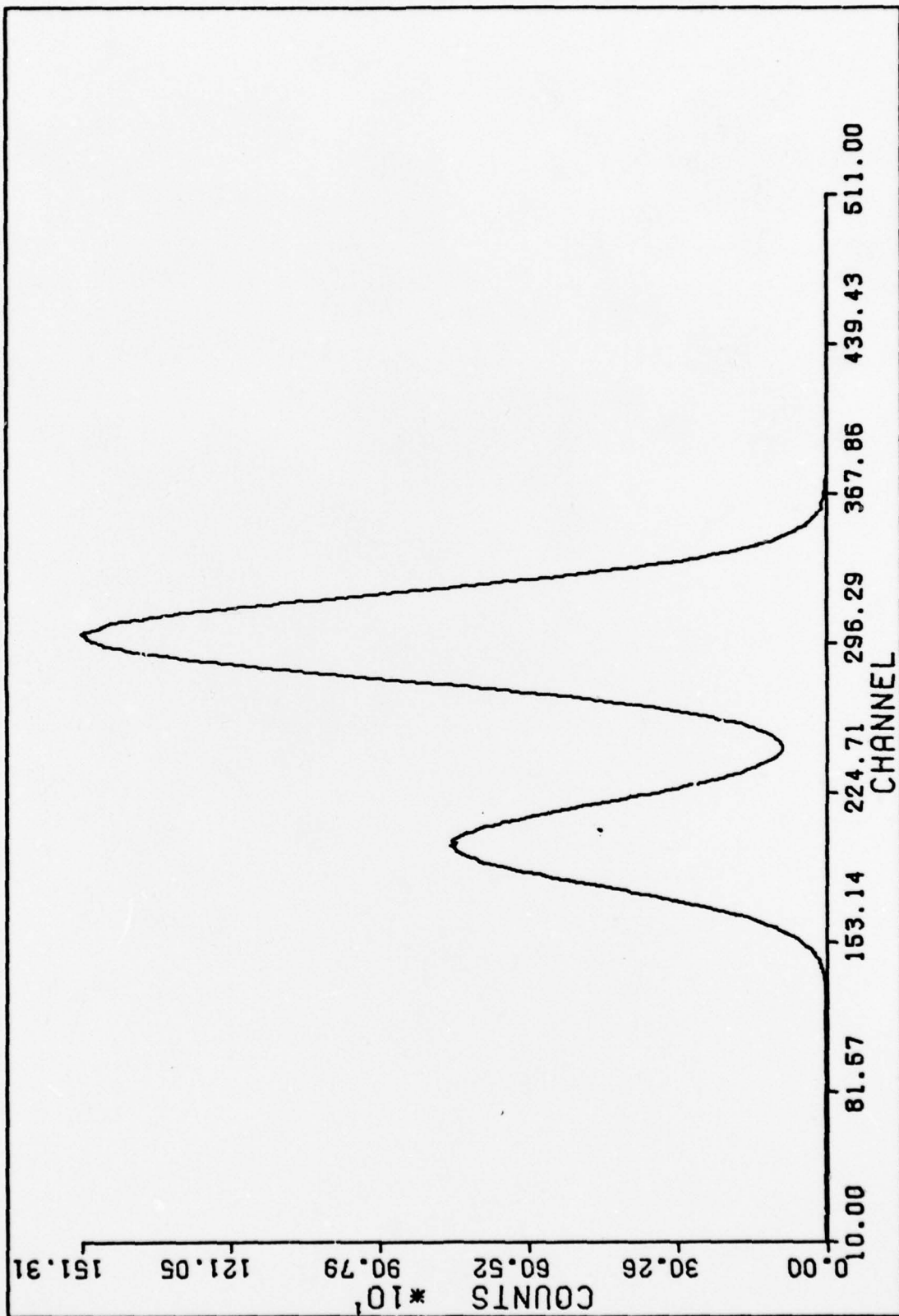


Fig. 33. Randomized Gaussian Peaks. Separation = 100 Channels.
 Heights are 1000, 2000.

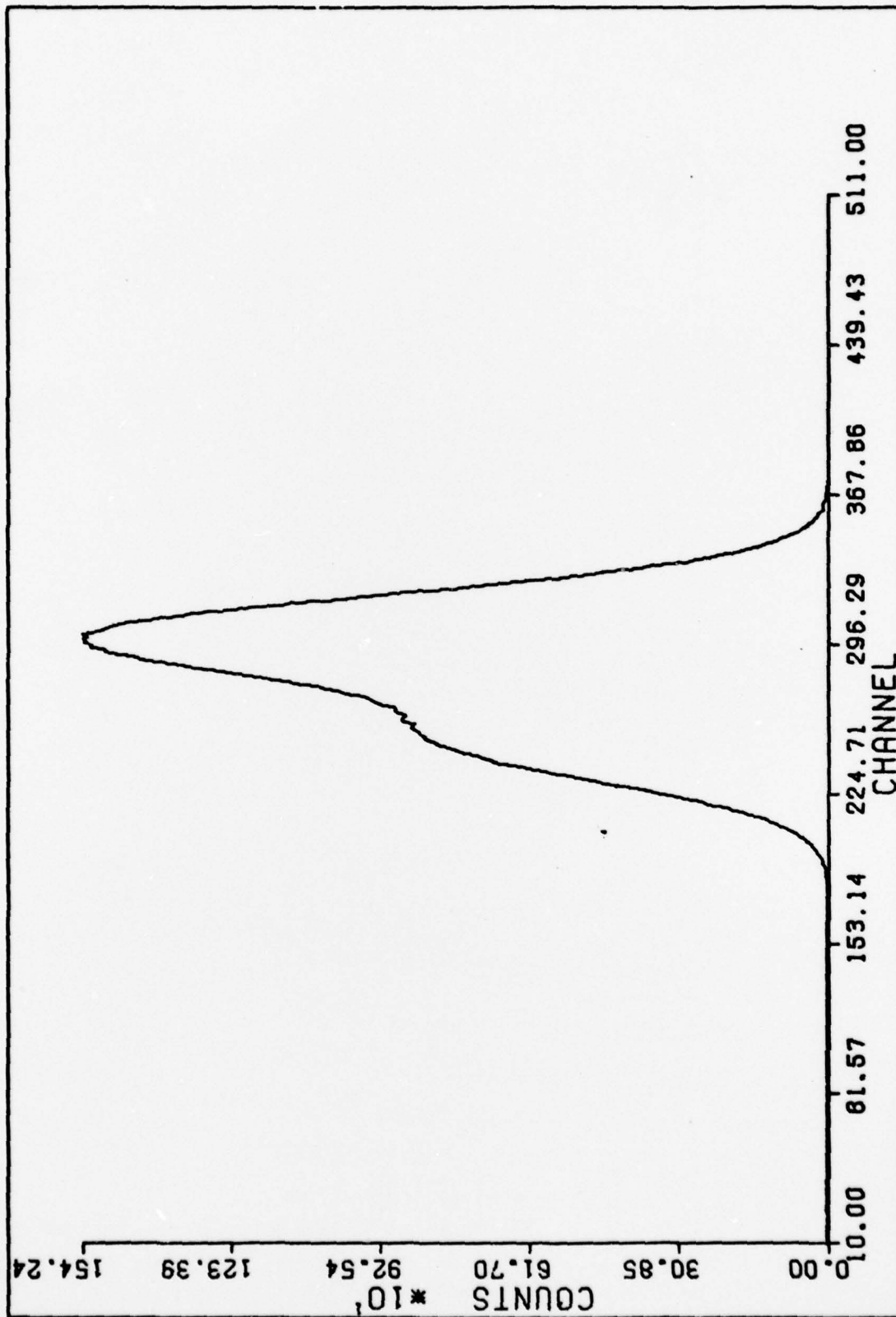


Fig. 34. Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 1000, 2000.

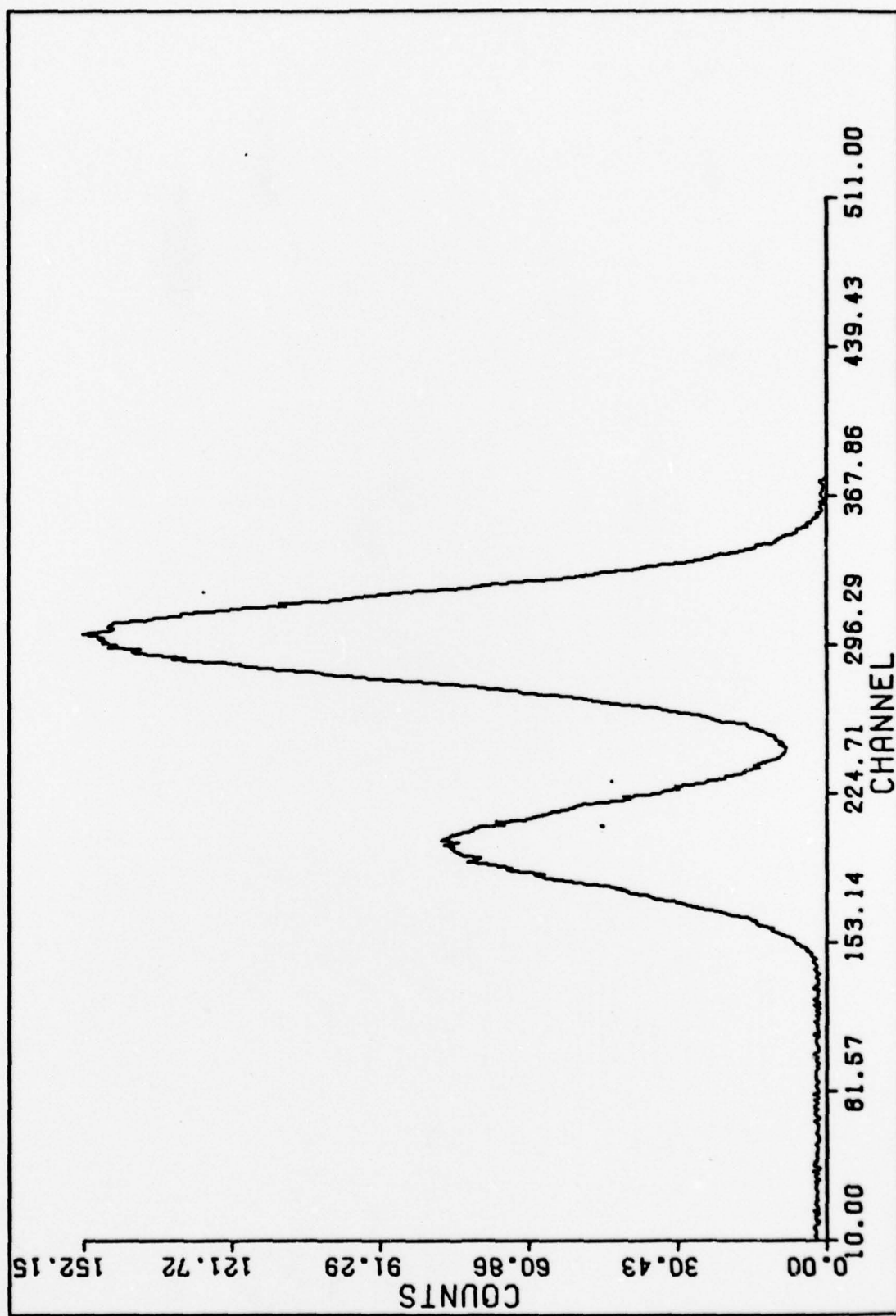


Fig. 35. Randomized Gaussian Peaks. Separation = 100 Channels. Heights are 100, 200.

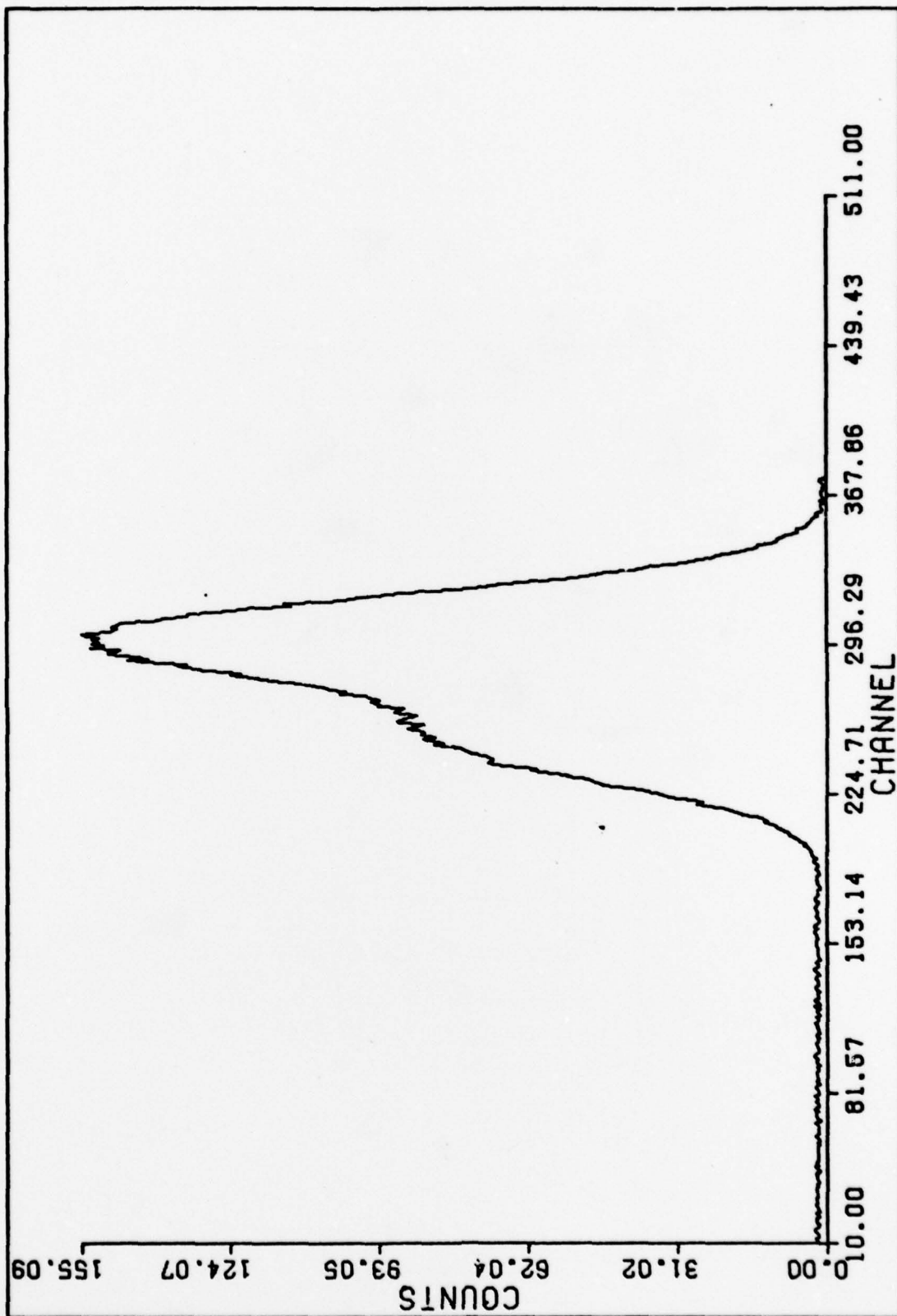


Fig. 36. Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 100, 200.

Vita

John Robert Harstine was born on 14 February 1950 in Tulsa, Oklahoma. He graduated from El Dorado High School in El Dorado, Kansas, in 1968 and attended the Lyman Briggs College of Michigan State University from which he received the degree of Bachelor of Science in Physics in 1972. He received a commission in the United States Air Force through the ROTC program and began active duty in November of 1972. After receiving technical training at Sheppard Air Force Base, Texas, and Vandenberg Air Force Base, California, he served as a missile launch officer in the Titan II ICBM at Davis-Monthan Air Force Base, Arizona. He entered the School of Engineering, Air Force Institute of Technology, in August of 1977.

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