PRNC. 160 PUERTO RICO NUCLEAR CENTER COMPUTER AIDED DECOMPOSITION OF GAMMA SPECTRA EMITTED BY CERTAIN RADIOACTIVE NUCLIDES By Aviva E. Gileadi and Nallagounder Kuppusamy OPERATED BY UNIVERSITY OF PUERTO RICO UNDER CONTRACT NO. AT (40-1-1833) FOR US ATOMIC ENERGY COMMISSION ---Page Break--- PRNC. 160 PUERTO RICO NUCLEAR CENTER COMPUTER AIDED DECOMPOSITION OF GAMMA SPECTRA EMITTED BY CERTAIN RADIOACTIVE NUCLIDES By Aviva E. Gileadi and Nallagounder Kuppusamy OPERATED BY UNIVERSITY OF PUERTO RICO UNDER CONTRACT NO. AT (4-1-1833) FOR US ATOMIC ENERGY COMMISSION ---Page Break--- University of Puerto Rico Mayaguez Campus COMPUTER AIDED DECOMPOSITION OF GAMMA SPECTRA EMITTED BY MIXTURES OF CERTAIN RADIOACTIVE NUCLIDES by Nallagounder Kuppusamy A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science (Nuclear Engineering) January 1973, Approved: _____ Chairman Graduate Committee ---Page Break--- ABSTRACT A computer code PRGA, written in FORTRAN IV, has been developed in order to perform decomposition of certain gamma spectra obtained by means of Ge(Li) diode equipped multichannel data acquisition system. The code uses spectra of the individual standards and those of the mixtures as input data and calculates the mixing factors pertinent to each component, using linear least squares fit techniques. PRGA is presently operative on both the IBM-360/40 and the PDP-DEC-10 computers at the Computer Center of the University of Puerto Rico, Mayaguez Campus. The code includes corrections designed to account for dead time losses, natural and spectral background, decay and counting statistics. Using source mixtures with premeasured mixing factors, specially prepared for the purpose of comparisons, it was found that the premeasured and PRGA computed mixing factors are in satisfactory agreement. ---Page Break--- ACKNOWLEDGEMENT It is the author's wish to express his gratitude and sincere thanks to those who helped him to complete this project: To DR. AVIVA E. GILEADI,

Professor, Nuclear Engineering Department, UPR-RUM, for suggesting the problem, for her dedicated guidance and competent supervision of the work, never sparing time nor effort. To DR. DONALD S. SASSCER, Head of the Nuclear Engineering Department, UPR-RUM, for his sincere interest in the author's work and especially for his efforts in securing the financial assistance needed for completion of this project. To DR. EDDIE ORTIZ, Senior Scientist, Nuclear Engineering Division PRNC, for his keen interest in the problem and for his valuable advice. To DR. XUD B. PEDERSEN, Associate Professor of Nuclear Engineering Department for his constructive criticism. To DR. ELWYN D. WOOD, Radioecology Division, PRNC, for his extreme generosity, for being always available for consultation and for contributing in a true academic spirit his most valuable time and expert advice on using the Ge(Li) detector system available in his department. To PROF. HIRAM D. A. CABASSA, Director, Computer Center, Mayaguez Campus for his knowledgeable advice and professional guidance in all the problems encountered while debugging and making it operative. ---Page Break--- To MISS MARIA LARA, Chemistry laboratory in charge, PRNC, for assisting to prepare the standards and mixtures of the Liquid sources used in this project. To the personnel of the Library and Reproduction office of the PRNC for their exemplary cooperation. ---Page Break--- TABLE OF CONTENTS ---Page Break--- LIST OF TABLES

factors for ten component simulated program. Comparison of premeasured and PRGA-computed mixing factors for

tuo component source mixtures. Comparison of premeasured and PRGA-computed mixing factors for three component source mixtures. Comparison of premeasured and PRGA-computed mixing factors for four component source mixtures. Comparison of premeasured and PRCA-computed mixing factors for five component source mixtures. Results quoted from reference (25) for ten component mixture. Results quoted from reference (8) for three component source mixtures. Results quoted from reference (6) for five component mixture. Page 42 4a aw 4s 46 7 ue 49 ---Page Break--- LIST OF FIGURES Figure No. Page 3.1 Data spectrum obtained with 2 lithium-drifted germanium detector. 20 3.2 Results of applying the correlation method to data obtained with a sodium iodide detector. a S.1 Block diagram of Ge(ui) detector and associated data acquisition system. 3H 5.3 Open-ended Coaxial Ge(Li) Detector. 38 5.2 Schematic representation of P-I-N structure in lithium drifted germanium detector. 36 5.4 Linearity check of data acquisition system, energy vs. channel number. 38 Gamma ray spectrum of radiation emitted by 25Mn°4 59 6.2 Gamma ray spectrum of radiation emitted by 58Cs!137 51. 6.3 Gamma ray spectrum of radiation emitted by 27Co87 52 6.4 Gamma ray spectrum of radiation emitted by 11Na 53 6.5 Gamma ray spectrum of radiation emitted by 2708 sy 6.6 Gamma ray spectrum of radiation emitted by those component source mixtures. Components: 11Na, 27Co87 and 25Mn°4 55 6.7 Gamma ray spectrum of radiation emitted by four component source mixtures. Components: 11Na, 27Co80, 25Mn°4 and 58Cs137 56 8.8 Gamma ray spectrum of radiation emitted by five component source mixtures. Components: 11Na, Freoeo, 2ohnee, Deine and SoeotsT 7 A,1 Arrangement of input card deck for PRGA-Code. 6s ---Page Break--- CHAPTER I INTRODUCTION During the last decade or so the development of lithium drifted germanium detectors requiring cryogenic techniques and associated low noise electronics and the use of such detectors with various sophisticated data acquisition systems,

featuring such items as multichannel analysers with large memories, often interfaced with digital data processors - made considerable impact on experimental photon spectrometry. Improvement of the experimental techniques resulted not only in higher accuracy and better resolution but also in an unprecedentedly large quantity of available gamma spectral data. In order to match the efficiency of data acquisition to that of converting these data into meaningful information, numerical techniques are required. Such techniques not only provide considerable savings in time but also significantly improve the accuracy of data analysis. Ideally, even the most complex spectra should be analyzable, qualitatively as well as quantitatively, with little or no man-machine interference. However, before such a rather ambitious objective could be achieved, several simpler partial programs need to be developed and checked out, each of them designed to perform a partial task in the framework of complete analysis. Once all the partial programs are operative, they are integrated into a complete system, capable of determining background, resolving and fitting complex peak groupings, determining the energies and intensities of the gamma rays as well as the amount of source nuclides within the analyzed mixture. The Nuclear Engineering Department of the University of Puerto Rico recently acquired a high-resolution gamma detecting system consisting of a lithium-drifted germanium detector (manufactured by Princeton Gamma-Tech) to be used in conjunction with a multichannel analyser (model No. 88-015 manufactured by Nuclear Data, Inc.). This system is to be used in a rather extensive neutron activation project planned by the Department. It is felt that a reliable and efficient computer code written especially for analyzing data acquired by the above-described Ge(Li) diode-equipped gamma spectrometer would be a welcome contribution to the departmental efforts in the field of neutron activation. With this general

Objective in mind, and as a first step towards it - in the present thesis a computer code PRGA was developed that is capable of decomposing gamma spectra emitted by certain source mixtures. PRGA is written in FORTRAN IV and is operational on the IBN-360/40 Computer at the University of Puerto Rico, Mayagüez Campus Computing Center. The code has been tested on gamma spectra emitted by several different premeasured source mixtures and its performance has been found satisfactory. All gamma spectra used in testing the PRGA code were acquired by means of the Ge(Li) diode equipped gamma ray detector system of the Radioecology Division of the Puerto Rico Nuclear Center, the description of which is given in Chapter V.

CHAPTER REVIEW OF LITERATURE

Gamma ray spectrometry is among the most versatile, most important and most frequently applied methods of modern science; accordingly, the professional literature pertinent to that subject cannot be exhaustively reviewed within the scope of the present thesis. An attempt is made, however, to briefly review a selected set of outstanding original papers on the subject of computerized decomposition techniques ("unscrambling") of gamma spectra. J. MILLS has developed a computer program AUTSPAN for the analysis of complex gamma spectra obtained with Ge(Li) detectors. The program contains options for data smoothing, peak location, and determination of peak parameters. G. D. ATKINSON Jr., J. B. WHITWORTH, and S. J. GAGE have written a code, NAA, which seeks out peaks, locates the peak maxima, predicts Compton knees, single and double escape peaks, and identifies the unknown nuclides present. The code is written in FORTRAN IV and is operational on the CDC-6600 computer. JEAN KERN, after a review of the most accurately known gamma calibration lines, presented a method of obtaining new secondary standards of similar precision, but extending to higher energies. Her method uses simultaneously pair peak method, energy combinations and

experimental non-linearity curves. W. C. WHITE, M. B. SHAPTRO and A. W. PRATT (4) applied linear programming to decompose spectra. J.T. ROUTTT and S. 6. PRUSSIN (5) have written a Fortran program which searches and fits the single and multiple peaks. In addition, their code performs the energy efficiency, line shape calibration, and error estimates. The program given by R. G. HELMER, R. L. HEATH, M. PUTNAM and D. H. GIPSON (6) computed the gamma ray energies and intensities and provided an estimate of uncertainty, by fitting the gamma ray peaks to a Gaussian and applying a correction for the nonlinearity of the electronic system, for the data obtained both by NaI(Tl) and Ge(Li) detector systems. R. GUNWINK and J.B. NIDAY (7) have constructed an elaborate program, GAMANAL, which determines the background, the energies and intensities of the gamma spectrum and the amounts of the source nuclides present in the mixture. Taking selected channels of data of pulse height distribution, F. D. KNIGHT (8) applied the method of simultaneous linear equations to find the abundance of the concerned nuclides present with the knowledge of the component spectra and the composite spectrum. The computer program, CAUSS-V, developed by R. G. HELMER and M. PUTNAM (9) locates the gamma ray peaks, determines the peak parameters, finds the gamma ray intensities and energies applying nonlinear least square curve fit for the pulse height distribution obtained with a Ge(Li) detector system. M. CIAMBI, L. DADDI and V. D. ANGELO (10) have fitted the gamma ray photo peaks to a Gaussian, using a maximum probability method and compared the results with those obtained by the least square method. W. W. BLACK (11) used correlation techniques to locate the photo peaks. He analyzed pulse height distributions obtained with Ge(Li), Si(Li), and NaI(T2) detectors. He also applied this method to data obtained by means of neutron time-of-flight analyzers. An early paper of

J. H. HUBBELL and N. E.

SCOFIELD (22) deals with “unscrambling" experimental gamma spectra using matrix techniques. WALTER F. BURRUS (13) used Fourier techniques to obtain the “unscrambled" spectrum and has assigned meaningful error estimates to the results. A. WEST Jr. and S. JOHNSON (24) discussed an unfolding code for the IBM 650. They described a procedure for removing scale and energy dependency. R. L. HEATH, R. G. HELMER, L. A. SCHMITTROTH, and G. A. CAZIER (15) used interpolation between experimental spectra to calculate pulse height distributions obtained by NaI(Tl) crystal system for sources emitting only one gamma ray. J. E. CLINE and R. L. HEATH (16) developed a method to determine both the relative detection efficiency and the linearity of the Ge(Li) detector system. G. HELMER, R. G. GREENWOOD, and R. J. GEHRKE (27) have measured the energies of gamma ray photons from 24 nuclides using a Ge(Li) detector and have applied corrections for the nonlinearity of the detector system and for the recoiling nucleus. MARTE PUTNAM, D. H. GIPSON, R. G. HELMER, and R. L. HEATH (18) developed a computer program that performs a nonlinear least squares fit to pulse height distributions obtained both from NaI(Tl) and Ge(Li) detector systems. Their program fits the data to their modified Gaussian functions and prints out the peak parameters. The program described by R. L. HEATH, R. G. HELMER, L. A. SCHMITTROTH, and G. A. CAZIER (19) smooths the gamma ray spectra, applies corrections to the gain shift of the detector system, and fits the data to Gaussians using linear least squares criterion. H. BABA, H. OKASHITA, S. BABA, T. SUZUKI, H. UMEZAWA, and H. NATSUME (20) constructed a program to analyze gamma ray spectra obtained by using a Ge(Li) detector. The analysis is based on the first derivative method associated with a number of peak shape tests. The effects of data smoothing and change in peak width were studied. K. LOW (71) attempted to find the contribution from known nuclides in a complex gamma ray spectrum, using

least squares method. ---Page Break--- FILIPPONE and F. J. MUNNO (22) discussed the influence of deadline losses on the magnitude and shape of the composite spectrum obtained by means of a multichannel analyser. They presented a relation including appropriate corrections. R. G. WAGGENER, L. F. ROGERS and P. ZANCA (23) Health Physics published a matrix method to correct for non-linear energy response of NaI(Tl) spectrometer systems. R. K. GILLETTE (24) has developed a computer program for the analysis of neutron activation data containing an option for smoothing gamma spectra. J. I. TROMBKA (25) developed a least squares fitting technique for the analysis of complex gamma ray pulse-height spectra, synthesizing the polyenergetic distribution from a series of monoenergetic components in the incident beam. H. P. YULE (26) published an exhaustive review paper on computation of experimental results in activation analysis. D. D. TUNNICLIFF and G. E. A. WYLD (27) have developed a code, based on linear least squares, that computes directly the weights of the components in a source mixture. ---Page Break--- CHAPTER TIT THEORETICAL BACKGROUND In the literature, numerous methods have been described for computer-aided analysis of gamma ray spectra obtained with Ge(Li) or NaI(Tl) detector systems. In most of these methods, the analysis is performed with the aid of calculated or measured response functions corresponding to monoenergetic photons or individual isotopic components of the sample. The physical and statistical phenomena determining the response of a semiconductor type detector to a monoenergetic gamma photon incident on it are quite complex, and the accurate fundamental calculation of peak shapes for the purpose of spectrum analysis is quite difficult. For this reason, and because the peak shape may be sensitive to small variations in experimental parameters, it is desirable to determine a mathematical representation of the composite spectra directly from measured data. In order to assign a suitable

functional representation, it is important to examine some of the factors that determine the peak shape. The primary factor determining the width of a photo peak is the statistical fluctuation in the division of the observed energy between ionization and heating of the crystal lattice. This gives rise to a Gaussian distribution in the width. The extent to which a small specified distribution is reflected upon the experimental data, taken with a particular system, is dependent on a number of factors. The material properties and the impurities in the detector affect the charge collection and the electronic noise associated with the leakage current. The combined effect of incomplete compensation of impurities and incomplete charge collection worsen the resolution and give rise to low energy tailing of the photo peak. At low energies, the contribution to the resolution from preamplifier noise is important, and at higher energies, the instabilities of the amplifier and the pulse-height analyser begin to affect the line width, especially when long counting times are involved. Although the use of the digital gain stabilizer can decrease the broadening, the stabilization may itself change the shape of the peak. Finally, random summing of pulses at high counting rates broadens the peaks and gives rise to tailing. The continuum under the peaks is due to Compton distribution from higher energy gamma rays and general counting background. Without detailed knowledge of the composition of the spectrum, we can only say that the continuum in the short interval under one peak on a cluster of peaks is, except for statistical fluctuations, a continuous smoothly varying function of energy. Such a function can be approximated with a polynomial. Among the several techniques used in computer-aided decomposition of complex gamma spectra, three major ones will be discussed briefly, following references. (a) Linear least squares technique (b) Non-linear least squares technique (c)

Correlation technique In the linear least squares technique, the pulse height spectrum due to a polyenergetic distribution of gamma rays is synthesized by using two series of normalized pulse height distributions, due to either monoenergetic components or to the pulse height distribution characteristic of various single nuclides in the source mixture. Each of these pulse height distributions is weighted so that their sum is a best fit based upon a least squares criterion to the experimentally determined polyenergetic pulse height distribution due to the source mixture under consideration. It is assumed that the data points in a portion of the experimental spectrum can be represented by a function which depends on a set of parameters p. The purpose of a least squares fit is to find the value of the parameters, which minimizes the sum of the squares of the deviations of the data from the function; that is, the residual is minimized. The y0 are experimental data points, the wy are the weights associated with the y0, and the y(p) are the values calculated from the function used to represent the data. The summation is over all the data points used in the fit. A necessary condition for R to be a minimum, as a function of the p, is that the set of equations are equal to zero for k = 1, 2, ..., Pj, (3.2) hold simultaneously for all values of k. If J is a linear function of the parameters p, the problem is a linear least squares problem, and expressions can be derived for the "best" value of the parameters. However, if the function is not linear in the parameters, no explicit solution of the equations exists. In this case, a method of "Linearization" may be used. One such method of Linearization is that of Cause. This method consists of linearizing the function with respect to a set of parameters by the use of a truncated Taylor series. Initial estimates, p0, of the parameters must be available in order to evaluate the derivatives in the expression; that is: on f(x) = f(p0) + f'(p0)(p - p0) + ...

HEH9) dim t ---Page Break --- 13 plus expressions containing higher derivatives, where the derivatives are evaluated at the initial values of the parameter. The function 9(p,) is a linear function of the p, if all derivatives beyond the first are neglected. This gives 2 Rn? = Sw [yy - 699) - SAY 3.3) > af: Hen sp Pk The conditions which now determine the minimum are given by aR/8C 3%) = 0 for

k = 1,2, 0.8 (3.4) this gives as many equations as there are parameters pj. The solution of this set of equations can be represented in a compact form by the use of matrix notation. Let the desired changes in the parameters be given by the vector ap = COP)s BPys bPy as) Let the vector B be defined as: 5 [Dao = P09 0; ~ IPC BIz/ apydene 8) ---Page Break --- Ww The coefficients of the gp, are represented by a symmetric matrix with the elements cn The set of equations can now be written caps p Where AP and P are column vectors. The solution is AP = A.8, where the matrix a = c7}, Since the higher derivatives have been neglected in equation (2.3) this process does not yield the solution of equation (3.2). Therefore, equation (3.u) is solved again with the af replaced by (oP + spy). This process is repeated in an iterative manner until all the jp, are less than some such that the iterations stop if py € ay for all i simultaneously. At this point the fitting process is concluded for this peak. In order to apply the non-linear least squares method to pulse height distributions obtained by means of a Ge(Li) detector system, the following should be considered: A gamma ray spectrum, obtained with a Ge(Li) detector, coupled to a multichannel analyser, consists primarily of a smooth continuous distribution on which is superimposed a series of peaks. Let a portion of this spectrum be represented by ---Page Break --- as 5+ Dy ty ro) 7 here ¥55 vo3ie*[1 # LGR + 2250; 5)?] G3) with Gay is a line which represents the continuous distributions In a complex peak the subscript j identifies the Gaussian in equation (3.9); the powers m, and

m, are predetermined, 2 even positive integers. The Gaussian parameters x (center of photo peak in channels), yo (count at peak or x), ¥ (full width of peak at half maximum in channels) can be determined in the fit. The parameters « and «, which represent the 2 "2 deviation of the photo peak from a Gaussian, can also be determined. The line parameters a (value at first channel in fit) and b (slope) can be determined in the fit. In some cases, the a, and a) terms have been used in fitting photo peaks from NaI(Tl) data, but a Gaussian function, i.e., zo a2. The correlation technique utilizes the cross correlation " c(r)=Lim 51 ff (terddt when T—» co 3.13: afew : : distribution of the complex spectrum). Assuming that a(t) = af (ten as) where a is a constant and n represents random noise and approximating f(t) and g(t) with a set of discrete values, the cross correlation function can be approximated as ce > f begs cas) where t and r are integers (e.g., channel numbers). For the purpose of discussion, f(t) is referred to as the search spectrum, a(t) the data spectrum, and C as the correlation spectrum. According to its definition, the cross correlation function is generated by forming the products of £, and g, keeping the search function sliding by one unit to the left each time it is incremented by one. Thus C will have a peak whenever the peak in the search spectrum overlaps itself in the data spectrum. This fact can be used to localize monoenergetic components in the polyenergetic spectrum. In order to do so successfully, it is necessary to find a method of enhancing the structure in the correlation spectrum; it is also desirable to remove all of the background not associated with the structure. Assuming that the data structure has a form of =f . G18) with b constant, it can be seen that flay, D0 if teem and Gan fee, to ar term where M is the number of points in the search spectrum f(t). This accomplishes both requirements, enhancement of the structure and suppression of

background. Therefore the expression of C may be modified to read: ---Page Break--- le c + Bete] A = Ss. When applying this method to actual data, certain modifications have to be introduced in order to take care of random fluctuations. It is clear that the term Seer will no longer vanish beyond the structure for data where A is fluctuating in a statistical manner. However, remembering that the computation of A, as given by equation (2.18), it can certainly be expected that fluctuations of one standard deviation or more would be smoothed out. Therefore the square root of A should be sufficient to suppress statistical fluctuations. With this in mind, the modified equation for C now reads: ce Ds: [ewe ve] @as When applying the cross-correlation method to the decomposition of

pulse height spectra, the search spectrum is a Gaussian, therefore Ylewras ove ---Page Break --- 19 where pam = abyint Qa. The only input parameters are the window width # and the Fut, Ng is @ constant. Figures 3.1 and 3.2 contain the pulse height distributions (data spectrum) and the pertinent cross-correlation functions obtained using appropriate search spectra, plotted on the same diagram. Figure (3.1) refers to a spectrum obtained by a Ge(Li) detector. Figure (3.2) refers to one obtained by a NaI(Tl) crystal. Both figures (quoted from reference 11) illustrate the effectiveness of the cross-correlation method in locating peaks. ---Page Break--- 1 aouasasas woss) We aunord ---Page Break--- (ut 92us49j94 oss) ze 3unoTd ---Page Break--- CHAPTER IV MATHEMATICAL BASIS OF THE PRGA-CODE ‘The PRCA code is based on a mathematical model using linear least squares techniques to calculate the mixing factors of a multicomponent spectrum. In its simplest form, the problem may be formulated in the following manner: Given the pulse height distribution spectrum of a source mixture, obtained by means of a certain gamma-ray detector system, as well as normalized pulse height distribution spectra of the individual components obtained by means of the

same gamma ray detector system, the mixing factors are to be determined. In order to obtain a numerical solution of the problem, the following mathematical model is used: Let S(I,K) denote the count rate in the K th channel due to the I th isotope, C(I) the T th mixing factor to be determined, T(K) the count rate in the K th channel due to mixture (given), T_L the total number of isotopes used in the mixture (given), K_K the total number of channels used (given). Under the assumption that T(K), the count rate in the K th channel due to the source mixture is produced by a linear combination of count rates corresponding to each component, T_C(K) may be expressed as:

C(I) * S(I,K)

In order to determine the optimal values of the C(I) mixing factors, a linear least squares fit is used, searching for a minimum of the function:

D = Σ |E - C(I) * S(I,K)|^2

with respect to the choice of the C(I) mixing factors. The minimizing C(I) values are determined by differentiating U with respect to each C(I) and setting the derivatives to zero. This leads to the system of linear equations of the following form:

A * C = B

for j = 1, 2, ... T

The solution of this system of equations yields the desired C(I) values. To execute the above computation of the C(I) values, a computer program PRGA was developed. The arrangement of the card deck and the listing of the program are presented in APPENDIX I. PRGA is written in FORTRAN IV, level 19, and is operative on the IBM 360/40 and on the DEC-PDP-10, both at the University of Puerto Rico, Mayaguez Campus, Computer Center. In order to facilitate the debugging procedure, the PRGA was tested on a simulated problem, which assumed a source mixture consisting of ten components and data from forty-one channels. After its performance on the simulated problem has been found excellent, PRGA.

was applied to actual experimental data, and the computed results were found to be in satisfactory

agreement with premeasured control data. ---Page Break--- 25 A brief description of the experimental equipment and procedures as well as a detailed comparison of the experimental mixing factors with those computed by the PRGA program are given in Chapters V and VI. The performance of the PRGA has been improved by the inclusion of several routines for various corrections. The mathematical basis of these routines is briefly presented below: a. Dead time correction was taken into account by first including the system dead time as an input parameter then correcting each raw count rate reading S in the following way: S (4.9) ms where S is the raw count rate per second and is the system dead time in seconds. Dead time values used in this paper were computed from the percent values automatically recorded by the counting system. No attempt was made to include channel and half-life dependent dead time correction such as advocated by W. FILIPPONE and F. J. MUNNO (see ref. 22) in the code at this stage of its development, primarily because all control data referred to sources with half-lives of several tens of days, thus the advocated correction would be negligible. ---Page Break--- 26 Correction for natural background is made simply by including the appropriate background count rates BB(K) as inputs in the program and by replacing S(ILK) with S(T, K) - BB(K) (4.20) for K = 2,2) 04. KK Corrections related to counting statistics. Due to the inherently random nature of radioactive disintegration, allowance had to be made for the statistical fluctuations in the count rates. This was accomplished by assigning a weight factor w to each value of u from the source modifying the function entering the least squares fit in the following manner: Correction for Compton scattering was made in a purely heuristic fashion, by deducting the pertinent ordinates of an appropriately chosen linear function from the

measured values. Assuming that the peak occurs at fo and the tangential points at K-M, the function to be deducted is resp. K, given by vei + EEO ysraay (wae), and the proper correction consists in replacing SCO =— 8(7,10-¥CK) for KS KM, KML, cess Kottt easy. Admittedly, the nonlinear method of fitting the individual peaks to the sum of a Gaussian and a linear function, as described in Chapter III, is better justified from the theoretical point of view. It should be observed, however, that even the above described simple linear routine is used by several authors (refs. 5, 9) and that its use in PRGA yielded satisfactory results. Decay corrections are necessary when the code is applied in neutron activation analysis involving short-lived isotopes. In order to understand how this correction has been applied, let us consider the time behaviour of a single isotope's activity assuming that 0 to ty - is the irradiation time, ty to t - is the cooling time, and ty to ty - is the counting interval. The activating flux is the decay constant of the i-th isotope, the activation (microscopic) cross section of the nuclide producing the i-th isotope, the time-dependent activity of the i-th isotope, the time-dependent number density of the i-th isotope, and the number density of the nuclide, the activation of which yields the i-th isotope. Under these assumptions, the following holds: Be dow agnpcer octet, ww = leading to Neo = Mgef. ost] o<tety was) during cooling, i.e. when ty < t < ty, and during counting, i.e., when t < ty. The activity of the sample at any instant of the counting interval is given by: t, t ty Ay CDE AN, (E)=NS a, (1-e™Nita eo“ (tty) (wae) Therefore, the count rate due to the i-th isotope will be proportional to: os S va Wait, | ast [sonaviiefer’ joe ee = , a ws) Peo b- 4] fewert oer] Hence in the case of a mixture consisting of short-lived isotopes, the mixing factors that will result.

from the least squares fit - described above - will depend upon ty, ty, tae ez» and ® and in order to get mixing factor characterizing the composition before irradiation, the following correction has to be applied: cect (4.20) ---Page Break--- 30 From the mixing factors, CC(I), of the unirradiated sample, the actual weights are computed by using the normalized activities and weights of the corresponding standard samples. In order to compute the weights of the individual components in the unirradiated mixture, the following basic equation has to be used: es mrittct) -aitets] [ayy = re 20

= @D Hara accare | oL % ap where: 100 = observed counts in channel K © = neutron flux WO) = weight of the J-th isotope in the sample AGG) = specific activity for radioisotope J at channel K i decay factor for radioisotope J. The validity of the above equation is subject to the following restrictions: (a) The number of counts observed for any component is directly proportional to the amount of the component present. (b) The spectra is additive. (c) The flux remains constant during irradiation. (d) The "dead time" of the data acquisition system does not change during any counting period. ---Page Break--- This results in a set of equations equal in number to the number of channels. If the specific activities A(x,s) have been determined by prior calibration, then this set of equations can be solved for the unknown weights WO) using least square techniques. a1 ---Page Break--- 32 CHAPTER V EXPERIMENTAL PROCEDURES AND EQUIPMENT The performance of the PRCA code was evaluated by comparing premeasured mixing factors with those computed by the code. Standard sources and source mixtures were prepared from a set of liquid reference sources manufactured by Atomic Development Corp.. The set included the following nuclides: nuclide | MOST PROBABLE ENERGIES | HALF LIFE MeV Na?2 0.511, 1.275 2.82 yr. nn 0.829 200 days co'? 0.122, 0.136 270 days co® 2.273, 1.392 5.2 yr. cs?87 0.662 30 yr. In order to ensure adequate accuracy self

Filling lambda pipettes were used for measuring radioactive liquids. Health Physics regulations and instructions referring to handling open sources were strictly observed. After receiving the reference sources, they were tested for leakage by the PRNC - Health Physics Division (see copy of leak test report). All operations involving liquid sources were performed under a hood, with the experimenter wearing protective gloves. Standards and mixtures were prepared at the same time in order to avoid errors due to decay. An aliquot of the reference liquid (e.g. S004) was pipetted on a planchet. A multiple of that aliquot was entered into the planchet that was designated to hold the mixture. Care was taken to deposit the liquid at the center of the planchet in order to preserve identical geometry as much as possible. All sources were dried under a lamp and after drying all were covered with thin plastic covers. All sources were counted on the Ge(Li) spectrometer of the PRNC Radioecology Division. A block diagram of the counting equipment is shown in Figure 5.1 and a list of the components is given below. Ge(Li) detector and associated data acquisition system components: HV - High voltage power supply, manufactured by Hewlett-Packard; model No. 3015. Ge(Li) - Lithium drifted germanium detector, manufactured by Canberra Industries Co.; model No. 7229-240; with cryostat model No. 7500. PRE AMP - Preamplifier, manufactured by Canberra Industries Co.; model No. 979. AMP - Main Amplifier, manufactured by Tennelec; model No. 70200. ADC - Analog to digital converter manufactured by Hewlett-Packard, model No. 160. MCA - Multichannel Analyzer, manufactured by Hewlett-Packard; model No. 45. TYPEWRITER - Manufactured by IBM; model No. 11-¢. X-Y PLOTTER - Manufactured by Hewlett-Packard; model No. 7890¢. The Ge(Li) detector used in this

system is of open-ended coaxial pin type. The starting material for the detector is P-type germanium (doped with gallium). Lithium, acting as a donor, is diffused at high temperature (400 °C) into the cylindrical ingot, creating a thin n-type layer on the surface. A bias voltage is used to cause the lithium ions to drift through the p-type material. During this process, an equilibrium condition is established where lithium ions pair with atoms of the doping material (gallium), creating a region with intrinsic properties. (See Figure 5.2). The term intrinsic implies that charge carriers will have a very long lifetime with all recombination processes reduced to a negligible level. Under reverse bias, the charge carriers can then be collected from this region, resulting in the production of a solid-state ionization chamber, schematically represented in Figure 5.2. Since the mobility of lithium ions in germanium is not negligible at room temperature, such devices, once fabricated,

must be maintained at low temperatures to preserve the structure. A liquid nitrogen-filled cryostat was used to maintain the required temperatures. Figure 5.2 indicates the configuration of the Ge(Li) detector actually used in this project. On average, only 2.8 eV is required to create an electron-hole pair in a Ge(Li) detector as compared to 30 eV in a gas-filled ionization chamber or to 500 eV required to produce a photoelectron at the photocathode of a scintillation detector system. It is this reduced energy requirement that improves the statistics and thereby the resolution of Ge(Li) detectors in comparison to gas-ionization chambers or scintillation detectors. The Figure 5. energy vs. channel number is plotted, indicating excellent linearity of the counting system used for data acquisition. Source mixtures and pertinent standards were counted within a few hours, thus reducing errors due to decay. Maximum counting

registered by the inbuilt dead-time counter were below 2%. Within each counting session the gain shift remained below observable. In order to ensure acceptable counting statistics, one-hour counts were taken. Count rate outputs were obtained both on an IBM typewriter and on an X-Y plotter. ---Page Break--- Lithium Diffused Junction N84 p-Type Core Open-ended Coaxial Ge(Li) Detector FIGURE 5.3 (from reference 28) ---Page Break--- ENERGY I ee SYSTEM, ENERGY V5. CHANNEL WBE 308 5300 —“eoe ‘OMANNEL NUMBER FIGURE 5.4 300) ‘00 ---Page Break--- 40 CHAPTER VI PRESENTATION AND DISCUSSION OF RESULTS PRCA computed results are presented in tabulated form side by side with premeasured mixing factors in order to facilitate comparison of the two. Entries in Table 6.1 refer to the ten-component simulated problem. Tables 6.2 through 6.5 contain results referring to two, three, four, and five component source mixtures respectively. Discrepancies of premeasured and PRCA computed mixing factors are indicated in percents. Figures 6.1 through 6.5 are samples of pulse height distribution spectra of standard sources and of source mixtures plotted from data obtained by the Ge(Li) detector equipped data acquisition system described in Chapter 7. The excellent agreement between assigned and PRCA computed mixing factors in Table 6.1 indicates that the performance of the PRCA code is essentially correct. When applied to experimentally acquired data, which by the nature of the acquisition are affected by such factors as gain shift, counting statistics, spectral background, etc., the discrepancy of premeasured and PRCA computed results - understandably enough - increases substantially. The PRCA computed results presented in Tables 6.2 through 6.8 include corrections intended to compensate for errors related to background, deadtime, Compton scattering, and ---Page Break--- 41 counting statistics. Comparable published results quoted from three references are presented in Tables 6.6 through 6.8. Based upon the results presented above, the

following can be concluded: (a) The code developed can determine mixing factors of source mixtures, using gamma spectrum of the composite source as well as those of the standard sources as input. (b) The PRGA-code is operative on the TBM/360-40 and the DEC-10 computer both at the Computer Center of the University of Puerto Rico, Mayaguez Campus. (c) PRGA's performance on a ten component simulated problem was found excellent. (d) PRGA computed mixing factors have been found in satisfactory agreement with premeasured values in a set of measurements performed on two, three, four and five component mixtures - especially prepared from reference source liquids for the purpose of this test. (e) As indicated by entry 3 in Table 6.3, PRGA gives a near-zero mixing factor for a standard absent from the composite spectrum. ---Page Break--- COMPARISON OF ASSIGNED AND PRGA-COMPUTED MIXING FACTORS TABLE 6.1 FOR TEN COMPONENT SIMULATED PROBLEM. 42 MIXING FACTORS component [Assigned | PRGA Computed Discrepancy | A 8.20 5.20 0.00 | B 7.30 7.19 1.82 | C 8.51 6.60 6.01 | D 20.60 10.62 9.08 | E 13.80 13.82 0.07 | F 9.00 0.86 0.88 1.6 | G 3.80 3.80 0.00 | H 0.05 0.05 0.00 ---Page Break--- TABLE 6.2 COMPARISON OF PREMEASURED AND PRGA-COMPUTED MIXING

FACTORS FOR TWO COMPONENT SOURCE MIXTURES 43 MIXING FACTORS SAMPLE DISCREPANCY NUMBER | component | PRGA-computed | premeasured | | 1 1.19 1.09 10-0 | 2 2.08 2.00 8.0 | 3 2.35 2.5 6.0 | 4 3.27 3.32 1.8 | 5 8.47 15.3 | 6 2.0 5.80 15.7 ---Page Break--- TABLE 6.3 COMPARISON OF PREMEASURED AND PRGA-COMPUTED MIXING FACTORS FOR THREE COMPONENT SOURCE MIXTURES 44 MIXING FACTORS SAMPLE DISCREPANCY NUMBER | component | premeasured | PRGA-computed | | 1 1.86 2.0 | 2 0.90 10.0 | 3 2.99 2.8 | 4 0.33 0.32 2.0 | 5 5.90 5.12 24 | 6 9.38 7 23.3 | 7 3.33 3.09 2.2 | 8 2.5 2.37 5.2 | 9 0.07 = ---Page Break--- TABLE 6.4 COMPARISON OF PREMEASURED AND PRGA-COMPUTED MIXING FACTORS FOR FOUR COMPONENT SOURCE MIXTURES MIXING FACTORS SAMPLE

DISCREPANCY numpex | component __| PRENEAS[PRCA=CORE| $ aina?? 2 1.62 13.0 2stins4 1 0.38 12.0 270089 2 1.95 2.5 sscs137 2 1.60 18.0 aina?? 2 Lieu 18.0 sa 2snins* 1 0.92 8.0, ° 27¢080 2 2.35 2.5 sscgi?? 2 2.61 23.5 * Computed with w= 1/TOD 8 computed with w= 1/SQRT(TCO) ---Page Break--- 46 TABLE 6.5 COMPARISON OF PREMEASURED AND PRGA-COMPUTED MIXING FACTORS ToR FIVE COMPONENT SOURCE MIXTURES > MIXING ACTORS SAMPLE DISCREPANCY numpex | compouewa| prewras.| pRca-coMP. 8 ana? L 0.92 8.00 7 27C087 1 0.76 24.00 oH 25th us 9.37 27C08° 1 2.03 3.00 sscs19)| 2 der 9.50 ana? a 0.93 7.90 aa 27¢087 2 0.79 22.00 2 25rinS* sé 1.7 8.20 27¢08 a 2.03 3.00 ssost37 2 277 22.50 * Computed with w= 1/TCK) ** Computed with uj = 1/SQRTCTCK) ---Page Break--- 4 TABLE 6.6 RESULTS QUOTED FROM REFERENCE FOR TEN COMPONENT MIXTURE ~ ~ “Quay PY 2s) quantity DISCREPANCY component | premeasures | compurep $ ae? 36-8 gm 20.0 ven 3.3 ask? 0.40 mgm 0.303 mgm 25.0 25Hn56 9.202 em 0.090%yem 20.4 zise® ay.2 22.2 yen aan aaas”® $.00 4.98 gem oe aan een 29cu%* 2.23 wen 211 yen 0.9 on so 5 2ucrSt 1.82 1.86 ym =34.0 g3x128 2.49 2.68 yen 2.6 s7iat¥ 2.19 3.02 wen 37.8 uana?? | 5.00 ug 17g suo | ---Page Break--- RESULTS QUOTED FROM REFERENCE TABLE 6.7 @ FOR THREE COMPONENT SOURCE MIXTURES 4B MIXING FACTORS DISCREPANCY coMpoNEnT. easureo | compurep 8 Sacer 1 1.03 2.92 5508137 5.2 5.31 2.07 27C08 5 5.22 2s ---Page Break--- TABLE 6.8 RESULTS QUOTED FROM REFERENCE (6) TOR FIVE COMPONENT MIXTURE 49 MIXING FACTORS DISCREPANCY component | premeasured | compurep 8 1 1 0.980 1.00 2 2 1.009 0.89 3 1 2.008 0.79 4 a 1.018 2.50 5 1 1.010 0.99 ---Page Break--- COUNT RATE PER HOUR 10,000 000 100 GAMMA RAY SPECTRUM OF 37 RADIATION EMITTED BY gac re) CHANNEL NUMBER FIGURE 6.2 E10 662 Mew 300 a8 ---Page Break--- COUNT RATE PER HOUR 10,000 GAMMA RAY SPECTRUM OF RADIATION EwiT TED BY C8 a a CHANNEL NUMBER FIGURE 6.3 720) ---Page Break--- 9 3yno14 waennn TaNNEHD sunset ed apn" 49 o3L4ma Kouviony 40 mows 3345 A¥Y YARD senisors 00% ‘now waa aava anno ---Page Break--- coe ows fom

aC om caries ono os. $79 3unoz4 waanw Tae 40 mnaioads Avw vaMvs ‘now wad 34¥¥ LNn09 ---Page Break--- 979 gangs w30nAN TaNNVHD coe ozs ons, 096 090 om 0m ooo on ETT 8 nam saziea sanzeto-3 ---Page Break--- “9 guns waenAW TaNNYHD 08 008 oz ov) os om oo een Woon 3 34¥ ANn02 a0 mnioaas Avy eMMYD san ss90r3 ran 29003, samo | ---Page Break--- 9 aunord w3ennw saNW¥HD 0% om oor cee ove om ow gotptpa “hase mais ane san 2990-3 san zziona now waa au¥y inn0> ---Page Break--- 58 Future plans include both increasing the accuracy and extending the scope of applicability of the PRGA-code. The accuracy is hoped to be increased by a) Establishing a library tape on which the spectra of individual standards, obtained with very good counting statistics, will be recorded. Whenever data on an additional standard spectrum becomes available, it will be entered into the library tape using an appropriate format. b) A baseline and gain shift routine will be added to the existing code. According to Parr and Lucas (31), even a gain shift

of one channel may change results considerably. The scope of applicability of PRCA is thought to be extended beyond the present one by (2) Including a routine based on cross-correlation techniques for locating peaks. (3) Including an option for locating peaks emitted by the same nuclide and assigning them the same intensity. (4) Applying nonlinear least squares fit techniques, i.e., to fit experimental points to the sum of a Gaussian and a linear function. ---Page Break--- 53 The ultimate objective in computer-aided spectral deconvolution, as indicated by several authors (28, 30), is to have a set of activation analysis data fed to the computer and have the computer determine the composition of the un-irradiated mixture with no further man-machine interference. Better yet, to have the computer continually monitor the output of the spectrometer, computing and evaluating while the counting is in progress, controlling the counting time, so that the sample is counted just long enough to get the desired statistical.

accuracy and then request the system to change samples. It is towards those very ambitious objectives that our future research efforts will be dedicated. ---Page Break--- Le 10. ni. 60 REFERENCES S.J. MILLS: A computer program for the automatic analysis of gamma ray spectra, Nucl. Instr. and Methods, pps 217-219; 81 (1970), G. D. ATKINSON Jr., J. B. WHITWORTH and S.J. GAGE: Computer-assisted analysis of gamma-ray spectra. Computer Physics Communications, pp. 40-46; 2 (1971)- JEAN KERN: Computer analysis of nuclear spectra and gamma energy standards. Nucl. Instr. and Methods, pp. 233-299; 78 (1970). WILLIAM C. WHITE, M. B. SHAPIRO and A. W. PRATT: Linear Programming applied to ultraviolet absorption spectroscopy, Communications of the ACM, March 1970. J.T. ROUTTI and S. G. PRUSSIN: Photo peak method for the computer analysis of gamma ray spectra from semiconductor detectors, Nucl. Instr. and Methods, pp. 128-142; 72 (1983). R. G. HELMER, L. HEATH, M. PUTNAM and D. H. GIPSON: Photopeak analysis program for photon energy and intensity determinations, Nucl. Instr. and Methods, pp. 56-573; 87 (1967). R. GUNNINK and J. B. NIDAY: Computerized quantitative analysis by gamma-ray spectrometry, Lawrence Livermore Laboratory, Report: UCRL-51061, March, 1972. F. D. KNIGHT: A system for the analysis of gamma-ray spectra by the method of simultaneous equations, E. I. Du Pont De Nemours and Company, Savannah River Laboratory, Report: DP-1171, November, 1968. R. G. HELMER and M. H. PUTNAM: A Computer program for the analysis of gamma-ray spectra from Ge(Li) spectrometers, Aerojet Nuclear Company, National Reactor Testing Station, Report: ANCR-1043; January 1972. M. CIAMBI, L. DADDI and V. D. ANGELO: Fitting of Gaussians to peaks by a maximum probability method, Nucl. Instr. and Methods, pp. 102-104; 66 (1968). W. W. BLACK: Application of correlation techniques to isolate structure in experimental data, Nucl. Instr. and Methods, pp. 317-327; 71 (1963). ---Page Break--- 1. as. qs. as. 16. uw. qe. as. 20. ae

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- bo 4B. 1e1s7- EN, Trt 35 Mensa teacrty SSBET AR) 00 46 181st, TEND Ttetero a6 ACD sacty T1s13T#10 EAUX(J) “ACI @ACITD XC =R TrCH>P1V)38,18,37 wolves 38 CONTINUE —i9. ~wSHSACITI 981) mattis - isist byes Tea Tens Bitvestficatt te - - ier — _ Hae —— 1H —__— yeken - - Net louzaaxrzens— 99.22 eeMstnin “xcept VeRO 22 Istew oe Ere eer 23 JSTRINAL) ahek 7 bo 25 Jin JSTEIST=Mad KeNehea=a . Pive1.007auxiK) 0: bk ee — weatkst) es ---Page Break--- AD-F6 “rae -Leuoststeyea Tayst D0 24 tetstp ten tie ke0.0 TF W=N729 27 6028 1813t, ENO 28 FeweBTTIeBCT) RETURN, Se LeReKea RETURN “Eno “V26T1 4) 29-Jane: 73 “ah ae

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