ornl

ORNL
Master Copy

ORNL/RSIC-57

**OAK RIDGE
NATIONAL
LABORATORY**

LOCKHEED MARTIN

**Abstracts of Computer Programs
and Data Libraries Pertaining to
Photon Production Data**

RECEIVED

AUG 21 1998

OSTI

John E. White
Jennifer B. Manneschildt
Sheila Y. Finch
J. Kirk Dickens

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MANAGED AND OPERATED BY
LOCKHEED MARTIN ENERGY RESEARCH CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

ORNL-27 (3-98)

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P. O. Box 62, Oak Ridge, TN 37831; prices available from (423) 576-8401, FTS 626-8401.

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161.

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

**Portions of this document may be illegible
electronic image products. Images are
produced from the best available original
document.**

Computational Physics and Engineering Division

ABSTRACTS OF COMPUTER PROGRAMS AND DATA LIBRARIES PERTAINING TO PHOTON PRODUCTION DATA

**John E. White, Jennifer B. Manneschildt,
Sheila Y. Finch
Radiation Safety Information Computational Center
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, Tennessee, USA 37831-6362**

and

**J. Kirk Dickens
Joint Institute for Heavy Ion Research
Holifield Radioactive Ion Beam Facility
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, Tennessee, USA 37831-4740**

Prepared by the
OAK RIDGE NATIONAL LABORATORY
managed by
LOCKHEED MARTIN ENERGY RESEARCH, INC.
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-96OR22464

CONTENTS

ABSTRACT	1
SECTION 1	
INTRODUCTION	3
SECTION 2	
PEAK ANALYSIS CODES	5
<u>ACTIVE-PC</u>	7
<u>AMUSE</u>	9
<u>ANA</u>	11
<u>BOB-7 SERIES</u>	13
<u>CERPI-CEREL</u>	15
<u>GAMAN</u>	17
<u>GAMANAL</u>	19
<u>GAMX1</u>	27
<u>GASPAN-ZKD</u>	29
<u>GAUSS</u>	33
<u>GAUSS6</u>	35
<u>GRETEL</u>	39
<u>GRPANL</u>	41
<u>HYPERMET</u>	43
<u>JADSPE</u>	45
<u>RICKI</u>	49
<u>SAMPO-LRC</u>	55
<u>SAMPO80</u>	57
<u>SKEWGAUS</u>	59
<u>TPASS</u>	61
SECTION 3	
UNFOLDING ANALYSIS CODES	63
<u>ALPHA-M</u>	65
<u>CONFOLD</u>	67
<u>CUPED</u>	69
<u>DOMUS</u>	71
<u>FERDO/FERD</u>	73
<u>FERD-PC</u>	75
<u>NAISAP</u>	77
<u>RADAK</u>	79
<u>UNSPEC</u>	83
<u>UPEAK</u>	85
SECTION 4	
MODEL PREDICTIONS OF PHOTON YIELDS	87

<u>ALICE-91</u>	<u>89</u>
<u>CASTHY</u>	<u>93</u>
<u>EMPIRE</u>	<u>95</u>
<u>ERINNI</u>	<u>97</u>
<u>EXIFON-GAMMA</u>	<u>99</u>
<u>GNASH-FKK</u>	<u>101</u>
<u>PEGAS</u>	<u>103</u>
<u>PEOAG-2</u>	<u>105</u>
<u>TNG1</u>	<u>107</u>

SECTION 5

<u>MISCELLANEOUS PROGRAMS</u>	<u>109</u>
<u>BOMJ</u>	<u>111</u>
<u>COINC</u>	<u>113</u>
<u>CURVE.LSFIT</u>	<u>117</u>
<u>DIMEN</u>	<u>121</u>
<u>GABAS</u>	<u>123</u>
<u>GASS</u>	<u>125</u>
<u>GRAP</u>	<u>127</u>
<u>MARTHA</u>	<u>131</u>
<u>MGA</u>	<u>135</u>
<u>PAPER 1</u>	<u>139</u>
<u>XRAY_AAC</u>	<u>141</u>

SECTION 6

<u>DATA LIBRARIES</u>	<u>143</u>
<u>GAMDAT-78</u>	<u>145</u>
<u>GAMTAB</u>	<u>147</u>
<u>GAMTOT78</u>	<u>149</u>
<u>NFCLIST</u>	<u>151</u>
<u>NUCDECAY</u>	<u>153</u>
<u>RADDECAY 4.02</u>	<u>155</u>
<u>TPASGAM85</u>	<u>157</u>
<u>XG-IAEA</u>	<u>159</u>

<u>ACKNOWLEDGMENTS</u>	<u>161</u>
------------------------------	------------

ABSTRACT

Abstracts, or descriptions, of computer programs and data libraries pertaining to Photon Production Data (Measurements, Evaluations and Calculations) maintained in the collections of the Radiation Safety Information Computational Center, Oak Ridge, Tennessee USA and at the OECD/NEA Data Bank, Paris, are collected in this document.

SECTION 1

INTRODUCTION

In 1994 the International Atomic Energy Agency authorized a Coordinated Research Programme (CRP) for the purpose of addressing open problems in photon production, focusing on neutron-induced reactions in the standard energy range. Two meetings of the CRP have been held: the first in November 1994 held in Bologna, Italy; the second in May 1996 held in Vienna. One of the goals of the CRP was to provide methods for handling photon data, and it was considered important to provide a list of existing codes available in the documentation centers. At the second CRP meeting the following *Action* was placed on one of us (Dickens; USA): "A tabulation will be made of general codes important for photon production currently available at the Radiation Safety Information Computational Center at ORNL, Oak Ridge, and at OECD/NEA Data Bank, Paris. This should be supplemented by comments and assessments of the codes."

This document contains abstracts or descriptions of 50 codes and 8 photon data libraries available from the respective specialized information analysis centers. These 50 codes are separated into four categories, namely experimental data reduction by (a) photon peak analysis, or by (b) unfolding; (c) model predictions; and (d) miscellaneous. A fifth category presents information on the data libraries.

SECTION 2

PEAK ANALYSIS CODES

These are programs designed to analyze gamma-ray spectra obtained with high-resolution Ge or Si detectors. A program identifies peaks in the spectrum, determines the net yield in counts in a given peak, and then, depending upon the design of the code identifies the centroid of the peak with a photon energy and the yield with the number of detected photons. The computer codes use different methods for defining peaks, backgrounds, identifications, and (when included in the program) determination of the responsible radionuclide(s).

Comments and assessments: the computer codes are written by scientists usually to accommodate a research activity, an activity which may involve a specific computer environment and/or a specific programming language. This observation is one reason that the compilers do not make a recommendation for choice of code to use. The second reason relates to a study done by Parr, Houtermans, and Schaerf¹ who, in 1978, did a study involving 47 users of 4 different codes; the major conclusion of these authors was:

"Perhaps rather surprisingly each of these four programs produced results covering a wide range of performance, demonstrating once again that it is the user rather than the program who plays the major role in determining the quality of the results."

Two of the tested codes, GAMANL and SAMPO, have since been improved and are included in the present compilation. However, the compilers suggest that the above conclusion remains valid for all but rote applications; certainly for fundamental studies user interpretation of computer-program results is a necessity.

REFERENCE

1. R. M. Parr, H. Houtermans, and K. Schaerf, in "Computers in Activation Analysis and Gamma-Ray Spectroscopy," Proc. of the Am. Nucl. Soc. Topical Conf. at Mayaguez, P. R., April 30 - May 4, 1978, eds B. S. Carpenter, M. D. D'Agostino and H. P. Yule (Tech. Information Center, U. S. Department of Energy, Washington, 1979), p 544.

**RSICC CODE PACKAGE PSR-287
NEA CODE PACKAGE IAEA0960**

1. NAME AND TITLE

ACTIVE-PC: A Program to Process Gamma or X-ray spectra.

2. CONTRIBUTOR

Joint Institute of Nuclear Research, Dubna, USSR, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; all IBM PC's.

4. NATURE OF PROBLEM SOLVED

ACTIV analyzes gamma-ray spectra measured by various types of detectors and under a large variety of conditions.

5. METHOD OF SOLUTION

ACTIV performs calibration of the measurement apparatus. It deletes outliers from the spectrum. It also creates peak models with the use of histograms. The spectrum is divided into several intervals and peak search is performed in each of these intervals. A least squares estimator is used to determine peak positions and areas.

6. RESTRICTIONS OR LIMITATIONS

A maximum of 20 peaks in the spectrum interval can be handled.

7. TYPICAL RUNNING TIME

At the NEA Data Bank, the sample problem took about 343 seconds on an IBM PC/AT with a math co-processor. AT RSICC, the same problem took about 590 seconds on an IBM PC/XT with a math co-processor; compilation of all Fortran sources took about 60 minutes and linking took 12 minutes.

8. COMPUTER HARDWARE REQUIREMENTS

IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77 and uses RM Fortran Version 4.0 or higher compiler. The PLINK86 overlay linker is also necessary.

10. REFERENCE

"The Long Write Up of the Program ACTIV," informal notes by V. B. Zlokazov, JINR, Dubna, USSR.

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/DD (360 K) 5.25 inch diskette.

12. DATE OF ABSTRACT

November 1990.

KEYWORDS: MICROCOMPUTER; GAMMA-RAY SPECTRUM ANALYSIS;
INTERACTIVE, ON-LINE

RSICC CODE PACKAGE PSR-028

1. NAME AND TITLE

AMUSE: Gamma-Ray Spectra Unfolding Code.

2. CONTRIBUTOR

Los Alamos National Laboratory, Los Alamos, New Mexico.

3. CODING LANGUAGE AND COMPUTER

Fortran 63; CDC-6600.

4. NATURE OF PROBLEM SOLVED

AMUSE unfolds complex gamma-ray spectra obtained with Ge(Li) detectors. It will analyze 20 independent regions in a spectrum with up to 350 data points and 11 full-energy lines in each region. Gaussian and exponential functions represent the data analytically. The best least-squares values of the energy, area, and width can be obtained for each full-energy peak.

5. METHOD OF SOLUTION

AMUSE determines the number of counts in the full-energy peaks of complex gamma-ray spectra. A sequence of related spectra is recorded on magnetic tape, along with identification information. For unfolding, the first spectrum in the series is divided into regions that contain the peaks to be analyzed. Estimates of certain parameters are made and then each region is analyzed separately. If subsequent spectra use the same regional divisions, it is possible to use the results of one spectrum as the estimates for parameters in the following spectrum.

A Gaussian function with two exponential tails on its low-energy side is fitted to each full-energy peak. A single exponential function is then fitted to the entire region to represent contributions from higher-energy lines and background. The sign and magnitude of each parameter are checked after each iteration to prevent the least-squares analysis from diverging.

Spectra are taken in sequence from different positions on the element. Then a preparatory program is used to edit the data from the analyzer and to rewrite them into a format compatible with the CDC-6600 computer. This computer is used for the spectral unfolding code. Finally, another program is used to extract data from the sequence of unfolded spectra to infer the spatial distributions of selected radionuclides.

6. RESTRICTIONS AND LIMITATIONS

Analyses of spectra by this code are not influenced by the source geometry and no library of spectra is required. However, it is necessary to apply attenuation corrections to the results. These corrections are normally applied by other codes after the results of this code have been obtained.

AMUSE can analyze up to 220 peaks in a single pass through one spectrum.

7. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for AMUSE.

8. COMPUTER HARDWARE REQUIREMENTS

AMUSE is operable on the CDC 6600 computer.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran 63 compiler is required.

10. REFERENCE

W. M. Sanders and D. M. Holm, "An Analytical Method for Unfolding Gamma-Ray Spectra,"
LA-4030 (July 1968).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code
and sample problem input written in BCD card images; total records 1450.

12. DATE OF ABSTRACT

November 1983.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING

RSICC CODE PACKAGE PSR-356

1. NAME AND TITLE

ANA: Code System for Gamma-Ray Spectra Analyses.

AUXILIARY ROUTINES:

KATOK: A Program for Resolving of Multiplets and Calculation of Peak Position, Net Area, FWHM and Their Uncertainty.

RM: A Utility for Displaying Text Files

2. CONTRIBUTORS

Institute of Nuclear Research and Nuclear Energy, Sofia, Bulgaria, and International Atomic Energy Agency, Vienna, Austria.

3. CODING LANGUAGE AND COMPUTER

Borland C/C++ v3.1 and 8088 Assembler language; IBM PC's and compatibles (P00356/IBMPC/00).

4. NATURE OF PROBLEM SOLVED

ANA (ANALysis of gamma-ray spectra) covers identification of radionuclides and quantitative spectra analysis. Calculation of elemental concentration using comparative Neutron Activation Analyses (NAA). Isotope identification and calculation of specific activities. Spectrum data reduction with precise calculation of essential peak parameters.

5. METHOD OF SOLUTION

Energy calibration - line or parabolic approximation.

FWHM calibration - parabolic approximation; automatic peak search (based on first derivative method); calculation of first derivative using orthonormal polynomial approximation of the raw or smoothed spectrum.

Manual peak search - gives the experienced user the ability to correct the results of automatic peak search; resolving of multiplets and calculation of peak parameters (Gaussian peak shape, polynomial background approximation, normalized Gauss, Newton approximation method (KATOK)).

Calculation of results for NAA - calculation of concentration of elements of interest in the sample and its uncertainty and/or calculation of LLD; background and dead time correction of required.

Efficiency calibration - spline method and polynomial approximation based on orthonormal polynomials.

Isotope identification - isotope library, user defined separation of analytical and additional isotope lines, background correction, calculation of LLD and MDC.

6. RESTRICTIONS OR LIMITATIONS

Spectra formats supported - ORTEC, CANBERRA s-100, ACCUSPEC, IAEA ASCII format 'GANAAS'.

Spectrum length - from 512 to 8192 channels.

Energy calibration - from 2 to 20 peaks.

Efficiency calibration - from 3 to 20 peaks.
Maximum length of a single ROI - 500 channels. Maximum number of peaks in a ROI -20,
maximum degree of background polynomial 4.
Number of ROIs in a spectrum is unlimited.
Efficiency calibration - from 2 to 20 peaks.

7. TYPICAL RUNNING TIME

The time for calculation of peak parameters depends on complexity of the spectrum and specific PC hardware. On a 386 based machine with a math coprocessor a spectrum containing 140 peaks has been reduced to 25 seconds.

8. COMPUTER HARDWARE REQUIREMENTS

ANA runs on an IBM PC or compatible with a 286 or greater processor. A math coprocessor is recommended but not required. At least 1.5 MB of disk space is required. An EGA or VGA graphics adapter is required and a color monitor is recommended.

9. COMPUTER SOFTWARE REQUIREMENTS

Borland C/C++ v3.1 was used to compile the source code and create the executable included in the package.

10. REFERENCE

P. Mishev, "ANA User's Manual," Institute of Nuclear Research and Nuclear Energy (1993).

11. CONTENTS OF CODE PACKAGE

The referenced document and 1 DS/HD 3.5" (1.44 MB) DOS diskette containing a self-extracting archive file are included. The archived file contains C source files, executables, sample input and output, and an information file.

12. DATE OF ABSTRACT

July 1995.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; PLOTTING; MICROCOMPUTER

RSICC CODE PACKAGE PSR-084
NEA CODE PACKAGE NEA-0660

1. NAME AND TITLE

BOB-7 SERIES: Theory and Use of Gamma-Ray Spectrum Analysis Codes for Ge(Li) Detectors.

2. CONTRIBUTOR

Japan Atomic Energy Research Institute, Tokai Research Establishment, Ibaraki-ken, Japan.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; FACOM 230-60.

4. NATURE OF PROBLEM SOLVED

BOB-7 SERIES analyzes the Ge(Li) gamma-ray spectrum and other types of spectra to determine the energies and intensities of the peaks detected. The spectrum is plotted in option.

5. METHOD OF SOLUTION

The analysis is carried out by the photopeak method. The peak search is based on the first derivative method associated with various peak shape tests. The usual least squares method is adopted for resolving the complex of peaks. The line shape function as the basis of the fit is an asymmetric Gaussian with a tail; the asymmetry is realized with two half-Gaussian of different widths combined at the top. The shape of the base line under the peak can be selected out of the linear, exponential, and various stepwise functions.

6. RESTRICTIONS OR LIMITATIONS

BOB-7 SERIES accepts a spectrum containing up to 200 peaks. The preferable spectrum size is 4100 or less, though larger data sizes are acceptable. The multiplicity of the complex of peaks should not exceed 18 in the case of "with tail" or 19 in the case of "without tail," and the fitting range must be less than 200 channels.

The pile-up effect appearing in the measurement at a high counting rate causes attenuation of the peak area. Correction for the effect is not considered in BOB-7 SERIES. The channel shift during the measurement is not corrected, either. BOB-7 SERIES does not require the accurate FWHM value as an input datum; a rough measure of the peak width is, however, still necessary.

7. TYPICAL RUNNING TIME

The running time for BOB-7 SERIES depends upon the complexity of the spectrum rather than on the spectrum size. The analysis of a spectrum containing about 50 peaks with medium complexity (the maximum multiplicity among the complexes is about 5) requires approximately 10 seconds.

8. COMPUTER HARDWARE REQUIREMENTS

BOB-7 SERIES is operable on the FACOM 230-60 computer. A 103 K word memory is required. A CALCOMP plotter, one or two magnetic tape units or a card puncher are optional.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

Hiroshi Baba, "Usage of the BOB7-Series Programs for the Analysis of Ge(Li) Gamma-Ray Spectra," JAERI-M 7017 (March 1977).

Hiroshi Baba, Toshiaki Sekine, Sumiko Baba, and Hiroshi Okashita, "A Method of the Gamma-Ray Spectrum Analysis: Fortran IV Programs 'BOB 73' for Ge(Li) Detectors and 'NAISAP' for NaI(Tl) Detectors," JAERI 1227 (June 1973).

Hiroshi Baba, Hiroshi Okashita, Sumiko Baba, Toshio Suzuki, Hirokazu Umezawa, and Haruo Natsume, "Fast Computer Analysis of the Gamma Spectrum from Ge(Li) Detectors," *J. Nucl. Sci. Technol.*, Vol. 8, No. 12 (December 1971) 41-50.

Sumiko Baba, Hiroshi Baba, and Hiroshi Okashita, "BOB70: Program Code for the Analysis of Gamma Ray Spectra from a Ge(Li) Detector," ORNL-tr-2939/JAERI 1216 (April 1971).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 17,119.

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING

RSICC CODE PACKAGE PSR-147

1. NAME AND TITLE

CERPI-CEREL: Code Systems for Automatic Analysis of Gamma-Ray Spectra Obtained with Ge(Li) Detectors.

2. CONTRIBUTORS

Institute of Physics, University of Rome, Rome, Italy.

Comitato Nazionale per l'Energia Nucleare, Centro di Studi Nucleari della Casaccia, Roma, Italia.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 360/370.

4. NATURE OF PROBLEM SOLVED

CERPI and CEREL are automatic analyzers of gamma-ray spectra obtained with Ge(Li) detectors. CERPI analyzes experimental gamma-ray spectra in order to find the photopeak positions and areas. CEREL looks for those elements or nuclides which are potential emitters of the gamma-lines. It is possible to search by elements or nuclides, depending on the input parameter.

CERPI-CEREL contains features such as determination of peak energies and intensities, nuclide identification, and mass computation.

5. METHOD OF SOLUTION

CERPI detects the significant peaks in the spectrum by observing the behavior of the second derivative function after random variations in counts per channel have been minimized by the application of a smoothing filter function. Once the peaks have been identified, CERPI determines their mass centers, areas and corresponding errors with a least-squares fit. Each significant peak is fitted with a Gaussian function superimposed on a linear or quadratic background. The determination of the minimum of the X^2 function is accomplished by a variant of the gradient method.

CEREL does automatic isotope identification on the basis of gamma-ray energy comparison. It contains features such as determination of peak energies and intensities, nuclide identification, and mass computation. The energy calibration curve is determined starting from some known energy lines and by means of a fitting procedure with orthogonal polynomials using the F test for the automatic determination of the polynomial order. The single and double escape peaks are used for a more careful determination of the photopeak intensities and then removed from the observed spectrum. Pagden's isotope catalog is used for both nuclide identification and mass calculation.

6. RESTRICTIONS OR LIMITATIONS

The high precision and sensitivity of CERPI-CEREL make it very suitable to very complex spectrum analyses where many peaks overlap each other. This high sensitivity may imply the introduction of some spurious peaks. The higher the number of peaks identified, especially the number of spurious ones, the higher is the probability of introducing fictitious elements and the more complicated is the resolution of the mass matrix.

Particular care must also be taken in the choice of the input parameters because the fitting procedure is affected by this choice.

7. TYPICAL RUNNING TIME

The running times of CERPI-CEREL depend strongly on the complexity of the spectrum and the number of channels in a typical peak. On an IBM 360/75 system, the analysis of a 4096-channel spectrum requires approximately 4 min of CPU processor time if about 250 peaks are printed on the final table.

8. COMPUTER HARDWARE REQUIREMENTS

CERPI-CEREL is operable on the IBM 360/370 computers.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

M. Giannini, P. R. Oliva, and C. Ramorino, "CERPI and CEREL, Two Computer Codes for the Automatic Identification and Determination of Gamma Emitters in Thermal Neutron Activated Samples," RT/FI(78)5 (May 1978).

M. Giannini, P. R. Oliva, and M. C. Ramorino, "Automatic Element Analysis in Thermal Neutron Activated Samples," RT/FI(78)15 (October 1978).

M. Giannini, P. R. Oliva, and M. C. Ramorino, "Automatic Peak Identification in the Analysis of Gamma-Ray Spectra Obtained with Ge(Li) Detectors," RT/FI(72)14 (April 1972).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input, the isotope catalogue and the array listings written in EBCDIC card images, plus output from the sample problems written in list format; total records 12,333.

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: ACTIVATION SPECTRA ANALYSIS; DATA PROCESSING, SPECTRA;
GAMMA-RAY SPECTRUM ANALYSIS; GERMANIUM (Ge(Li))
DETECTOR; UNFOLDING

RSICC COMPUTER CODE PSR-083

1. NAME AND TITLE

GAMAN: Qualitative and Quantitative Evaluation of Ge(Li) Gamma-Ray Spectra.

2. CONTRIBUTOR

Whiteshell Nuclear Research Establishment, Pinawa, Manitoba, Canada.

3. CODING LANGUAGE AND COMPUTER

Fortran IV and Assembler Language; PDP-10.

4. NATURE OF PROBLEM SOLVED

GAMAN does qualitative and quantitative analyses of gamma-ray spectra from Ge(Li) detectors.

5. METHOD OF SOLUTION

GAMAN "smooths" the spectral data by fitting 5 channel groups of data to a polynomial. The derivative is calculated at the midpoint of each group. A change of sign in the derivative indicates the beginning of a peak. The maximum and minimum values of the derivative are used to check on whether the peak height is statistically significant.

The significant peaks are fitted to a modified Gaussian function using a non-linear least squares procedure. This results in the calculation of the area and centroid of each peak and, by addition of calibration data, the gamma emission rates and energies are calculated and listed.

The listed energies are compared with gamma-ray energies in a library of isotopes and the isotopes present are identified.

The gamma-ray emission rate for each isotope is corrected for gamma-ray abundance and the disintegration rate is calculated.

6. RESTRICTIONS OR LIMITATIONS

None noted.

7. TYPICAL RUNNING TIME

GAMAN runs in < 120 seconds for 30 peaks.

8. COMPUTER HARDWARE REQUIREMENTS

GAMAN is operable on the PDP-10 computer. It requires 64 K of core memory.

9. COMPUTER SOFTWARE REQUIREMENTS

Fortran IV and Assembler Language compilers are required.

10. REFERENCES

"User's Guide for GAMAN 5," Informal Notes.

L. T. Felawka, J. G. Molnar, J. D. Chen and D. G. Boase, "GAMAN - A Computer Program for the Qualitative and Quantitative Evaluation of Ge(Li) Gamma-Ray Spectra," AECL-4217 (January 1973).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in ASCII, plus output from the sample problem; total records 2550.

12. DATE OF ABSTRACT

February 1975.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS;
UNFOLDING

NEA CODE PACKAGE NESC9654/01

NESC9654 GAMANAL,RADIOACTIVE SPECIES MIX BY GAMMA SPECTRA ANAL 890116

1. NAME OR DESIGNATION OF PROGRAM - GAMANAL.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
GAMANAL	NESC9654/01	DEC VAX 11/750	DEC VAX 11/780	T

3. DESCRIPTION OF PROGRAM OR FUNCTION

GAMANAL provides a complete qualitative and quantitative analysis of mixtures of radioactive species such as fission products by computer interpretation of high-resolution gamma-ray spectra. The program first determines and removes the background or Compton continuum under the peaks in a spectrum to locate the peak regions. This is done by examining the pulse-height spectrum data for background and peak regions and then fitting these data with the proper shape functions. When determining the photon emission rate, corrections are made for the effects of geometry, attenuation, and detector efficiency. Nonlinearities in the equipment are taken into account in setting up the energy scale. The total intensities and gamma-ray energies are listed and plotted and, if no further reduction of the spectral data is requested, the program repeats this process with the next spectrum. Otherwise, a library of decay scheme information is searched to make a tentative identification of each of the peaks. These proposed nuclides are examined for interferences between their photopeaks to determine which isotope is responsible for the peak in question. A matrix of the probable nuclides and the identified peaks is constructed and is then divided into sets of nuclides which interfere with each other. These independent sets are combined to form a working matrix. A least-squares solution of the corresponding set of simultaneous equations is made to determine the amounts of the various component nuclides present and their estimated errors.

4. METHOD OF SOLUTION

Peaks are located by a point-by-point examination of the first and second derivatives within the bounds of identified peak regions using statistically-weighted tests. Peak shapes are characterized by a shape analysis functions, which is the sum of a Gaussian and a tailing term.

The data points in an overlapping peak multiplet are considered to be linear combinations of the contributions from each peak. A detailed analysis of each peak region is done by keeping some shape parameters fixed and obtaining the best least-squares value for all free parameters using the Newton-Raphson (Gauss) iterative technique. A Taylor expansion about trial values is used to linearize the equations. A matrix of linear equations that describe the spectral intensities is formed to correct for unresolved peak interferences. A Gaussian function is used to determine how well the component nuclide's gamma-ray energy agrees with the energy of the peak in question.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

6. TYPICAL RUNNING TIME

NESC9654/01: NEA-DB ran the test case on a VAX-11/780 computer with the VERSAPLOT o/p plotter in 71 seconds of CPU time.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

LIBETP, an auxiliary program which is used to generate a GAMANAL decay-scheme library, is included. Graphic output is provided by DIGLIB and DIGRAPH, which are included. DIGLIB is a collection of FORTRAN-callable subroutines for two-dimensional plots. DIGRAPH acts as a shell for the GKS graphics routines.

9. STATUS

NESC9654/01 : Known to NEADB
 : Offered to NEADB
 : Requested by NEADB
 : Arrived at NEADB
 : in preparation
 : Tested at NEADB

10. REFERENCES

- NESC9654/01 :
- NEA Data Bank:
 Note Concerning Documentation of GAMANAL.
 NEADB Note (February 1988)
 - C. Yuelys-Miksis:
 GAMANAL Tape Directory
 NESC Note 86-35 (April 15, 1986)
 - R. Gunnink and J.B. Niday:
 Computerized Quantitative Analysis by Gamma-Ray Spectrometry.
 Volume 1. Description of the GAMANAL Program.,
 UCRL-51061, Vol. I (March 1, 1972)
 - J.B. Niday and R. Gunnink:
 Computerized Quantitative Analysis by Gamma-Ray Spectrometry.
 Volume III. A User's Guide to GAMANAL.
 UCRL-51061, Vol. III (July 8, 1971)
 - R. Gunnink and J.B. Niday:
 Computerized Quantitative Analysis by Gamma-Ray Spectrometry.
 Volume IV. Auxiliary Programs for GAMANAL.
 UCRL-51061, Vol. IV (June 1, 1972)

11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

NESC9654/01 : FORTRAN-77

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

VMS 4.2 (DEC VAX11/750), VMS 4.4 (DEC VAX11/780).

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

R. Gunnink
Lawrence Livermore National Laboratory
Livermore, California, U.S.A.

16. MATERIAL AVAILABLE

NESC9654/01 :
GAMANAL Source Code
DIGLIB Source Code
DIGRAPH Source Code
HELP File
Command Procedures
Sample Problem Input Data
Report: Machine Readable Documentation
GAMANAL Sample Output
NESC Note 86-35 (April 15, 1986)
NEADB Note (February 1988)
Report: UCRL-51061, Vol. 1 (March 1, 1972)
Report: UCRL-51061, Vol. 3 (July 8, 1971)
Report: UCRL-51061, Vol. 4 (June 1, 1972)

INFORMATION FILE	330 records
COMMAND FILE TO RESTORE ORIGINAL FILENAMES	230 records
HELP FILE	248 records
LIBRARY PROGRAM FORTRAN SOURCE	533 records
LIBRARY PROGRAM INPUT DATA	563 records
PERIODIC TABLE SYMBOLS	5 records
LIBRARY PROGRAM PRINTED OUTPUT LISTING	1586 records
COMMAND FILE TO CREATE OBJECT LIBRARY	64 records
COMMON STATEMENTS FORTRAN SOURCE	229 records
BGGPM.FOR	FORTRAN SOURCE
BKGRD.FOR	FORTRAN SOURCE
CALCMU.FOR	FORTRAN SOURCE
	32 records
	509 records
	128 records

CALEFF.FOR	FORTRAN SOURCE	19 records
CALGPM.FOR	FORTRAN SOURCE	129 records
CPUTIME.FOR	FORTRAN SOURCE	24 records
ENDIT.FOR	FORTRAN SOURCE	114 records
EVAL.FOR	FORTRAN SOURCE	496 records
FINDE.FOR	FORTRAN SOURCE	273 records
FIT.FOR	FORTRAN SOURCE	625 records
FSLOT.FOR	FORTRAN SOURCE	22 records
GRAPH.FOR	FORTRAN SOURCE	382 records
IDENTIFY.FOR	FORTRAN SOURCE	554 records
INTAKE.FOR	FORTRAN SOURCE	1300 records
LDMATX.FOR	FORTRAN SOURCE	334 records
LIMIT.FOR	FORTRAN SOURCE	53 records
LSLOT.FOR	FORTRAN SOURCE	23 records
MAIN.FOR	FORTRAN SOURCE	439 records
MLR.FOR	FORTRAN SOURCE	332 records
MLRERR.FOR	FORTRAN SOURCE	135 records
NEXTSEED.FOR	FORTRAN SOURCE	87 records
OUTGO.FOR	FORTRAN SOURCE	329 records
PAUSE.FOR	FORTRAN SOURCE	14 records
PKSCH.FOR	FORTRAN SOURCE	321 records
RDLIBE.FOR	FORTRAN SOURCE	51 records
REDOBG.FOR	FORTRAN SOURCE	34 records
REPORT.FOR	FORTRAN SOURCE	62 records
SHAPE.FOR	FORTRAN SOURCE	144 records
SMOOTH.FOR	FORTRAN SOURCE	126 records
TIMCHK.FOR	FORTRAN SOURCE	157 records
XLODBG.FOR	FORTRAN SOURCE	123 records
GAMCARDS.PGM	FORTRAN SOURCE	664 records
GAMANAL INPUT DATA FILE		433 records
BACKGROUND DATA LIBRARY FILE		142 records
SEED FOR PUNFIL NAME		1 record
GAMANAL TEST CASE OUTPUT LISTING		870 records
DIGRAPH USERS GUIDE		1566 records
COMMAND FILE TO CREATE OBJECT LIBRARY		72 records
ALINAX.FOR	FORTRAN SOURCE	99 records
BLKSCR.FOR	FORTRAN SOURCE	60 records
DEVCHR.FOR	FORTRAN SOURCE	79 records
GAXIS.FOR	FORTRAN SOURCE	628 records
GBEGIN.FOR	FORTRAN SOURCE	71 records
GBOX.FOR	FORTRAN SOURCE	18 records
GCLOSE.FOR	FORTRAN SOURCE	59 records
GEND.FOR	FORTRAN SOURCE	72 records
GERROR.FOR	FORTRAN SOURCE	141 records
GFONT.FOR	FORTRAN SOURCE	63 records
GIERROR.FOR	FORTRAN SOURCE	137 records
GILOT.FOR	FORTRAN SOURCE	118 records

GITRACE.FOR	FORTRAN SOURCE	124 records
GLEGEND.FOR	FORTRAN SOURCE	105 records
GLIMIT.FOR	FORTRAN SOURCE	79 records
GLINE.FOR	FORTRAN SOURCE	99 records
GOPEN.FOR	FORTRAN SOURCE	121 records
GPLOT.FOR	FORTRAN SOURCE	105 records
GSCALE.FOR	FORTRAN SOURCE	20 records
GTAG.FOR	FORTRAN SOURCE	78 records
GTEXT.FOR	FORTRAN SOURCE	98 records
GTITLE.FOR	FORTRAN SOURCE	83 records
GTRACE.FOR	FORTRAN SOURCE	132 records
GWCLPR.FOR	FORTRAN SOURCE	70 records
GWCLPS.FOR	FORTRAN SOURCE	82 records
GWINDW.FOR	FORTRAN SOURCE	134 records
GWNDWR.FOR	FORTRAN SOURCE	96 records
LINAX.FOR	FORTRAN SOURCE	100 records
NDIGITS.FOR	FORTRAN SOURCE	14 records
PAUSE.FOR	FORTRAN SOURCE	14 records
PCURSOR.FOR	FORTRAN SOURCE	12 records
REALSTR.FOR	FORTRAN SOURCE	99 records
RLAB.FOR	FORTRAN SOURCE	41 records
SAXIS.FOR	FORTRAN SOURCE	54 records
SCALE1.FOR	FORTRAN SOURCE	58 records
DAYPRM.PRM	FORTRAN INCLUDE FILE	2 records
DEVLST.PRM	FORTRAN INCLUDE FILE	8 records
DGRAPH.PRM	FORTRAN INCLUDE FILE	8 records
GCAPOS.PRM	FORTRAN INCLUDE FILE	1 record
GCCFNT.PRM	FORTRAN INCLUDE FILE	3196 records
GCCIDX.PRM	FORTRAN INCLUDE FILE	2 records
GCCLIP.PRM	FORTRAN INCLUDE FILE	1 record
GCCOFF.PRM	FORTRAN INCLUDE FILE	1 record
GCCPAR.PRM	FORTRAN INCLUDE FILE	1 record
GCCRROT.PRM	FORTRAN INCLUDE FILE	3 records
GCCTBL.PRM	FORTRAN INCLUDE FILE	4 records
GCCTBL1.PRM	FORTRAN INCLUDE FILE	3388 records
GCDCHR.PRM	FORTRAN INCLUDE FILE	2 records
GCDPRM.PRM	FORTRAN INCLUDE FILE	1 record
GCDSEL.PRM	FORTRAN INCLUDE FILE	1 record
GCFNT.PRM	FORTRAN INCLUDE FILE	1 record
GCFNTL.PRM	FORTRAN INCLUDE FILE	2 records
GCLTYP.PRM	FORTRAN INCLUDE FILE	2 records
GCVPOS.PRM	FORTRAN INCLUDE FILE	2 records
POIDF.PRM	FORTRAN INCLUDE FILE	1 record
PLTCLP.PRM	FORTRAN INCLUDE FILE	1 record
PLTCOM.PRM	FORTRAN INCLUDE FILE	2 records
PLTPRM.PRM	FORTRAN INCLUDE FILE	1 record
PLTSIZ.PRM	FORTRAN INCLUDE FILE	1 record

DIGLIB USERS GUIDE		3220 records
COMMAND FILE TO CREATE OBJECT LIBRARY		150 records
AXIS.FOR	FORTTRAN SOURCE	278 records
BGNPLT.FOR	FORTTRAN SOURCE	67 records
CLLINE.FOR	FORTTRAN SOURCE	210 records
CONCAT.FOR	FORTTRAN SOURCE	8 records
CSZMAP.FOR	FORTTRAN SOURCE	8 records
CURSOR.FOR	FORTTRAN SOURCE	22 records
CURVE.FOR	FORTTRAN SOURCE	60 records
CURVEY.FOR	FORTTRAN SOURCE	57 records
DAYCOM.FOR	FORTTRAN SOURCE	68 records
DAYEND.FOR	FORTTRAN SOURCE	73 records
DAYOPT.FOR	FORTTRAN SOURCE	99 records
DEVSEL.FOR	FORTTRAN SOURCE	148 records
ENDPLT.FOR	FORTTRAN SOURCE	17 records
FNTLD.FOR	FORTTRAN SOURCE	109 records
FNTRPL.FOR	FORTTRAN SOURCE	152 records
FNTSEL.FOR	FORTTRAN SOURCE	97 records
FULMAP.FOR	FORTTRAN SOURCE	26 records
GD2623.FOR	FORTTRAN SOURCE	188 records
GD2648.FOR	FORTTRAN SOURCE	188 records
GD2648CON.FOR	FORTTRAN SOURCE	11 records
GD4010.FOR	FORTTRAN SOURCE	168 records
GD4010CON.FOR	FORTTRAN SOURCE	130 records
GD4012.FOR	FORTTRAN SOURCE	168 records
GD4014.FOR	FORTTRAN SOURCE	168 records
GD4014REM.FOR	FORTTRAN SOURCE	168 records
GD4025.FOR	FORTTRAN SOURCE	199 records
GD4027MAP.FOR	FORTTRAN SOURCE	12 records
GD4027MIX.FOR	FORTTRAN SOURCE	12 records
GD4105.FOR	FORTTRAN SOURCE	321 records
GD9400.FOR	FORTTRAN SOURCE	254 records
GD9400LUT.FOR	FORTTRAN SOURCE	349 records
GDAIDS.FOR	FORTTRAN SOURCE	12 records
GDDG460.FOR	FORTTRAN SOURCE	251 records
GDDM800.FOR	FORTTRAN SOURCE	221 records
GDHP150.FOR	FORTTRAN SOURCE	242 records
GDHRZ100.FOR	FORTTRAN SOURCE	180 records
GDIO.FOR	FORTTRAN SOURCE	234 records
GDLASER.FOR	FORTTRAN SOURCE	136 records
GDLEX.FOR	FORTTRAN SOURCE	261 records
GDP600BD.FOR	FORTTRAN SOURCE	348 records
GDP600BS.FOR	FORTTRAN SOURCE	305 records
GDP600LD.FOR	FORTTRAN SOURCE	355 records
GDP600LS.FOR	FORTTRAN SOURCE	311 records
GDRTRO.FOR	FORTTRAN SOURCE	176 records
GDVERS.FOR	FORTTRAN SOURCE	115 records

GDVT125.FOR	FORTTRAN SOURCE	471 records
GDVX128.FOR	FORTTRAN SOURCE	154 records
GDVX384.FOR	FORTTRAN SOURCE	175 records
GDWAIT.FOR	FORTTRAN SOURCE	16 records
GETSTR.FOR	FORTTRAN SOURCE	7 records
GOODCS.FOR	FORTTRAN SOURCE	36 records
GSCCLC.FOR	FORTTRAN SOURCE	13 records
GSCCMP.FOR	FORTTRAN SOURCE	19 records
GSCGET.FOR	FORTTRAN SOURCE	107 records
GSCHIT.FOR	FORTTRAN SOURCE	13 records
GSCOLR.FOR	FORTTRAN SOURCE	51 records
GSCWID.FOR	FORTTRAN SOURCE	13 records
GSDRAW.FOR	FORTTRAN SOURCE	79 records
GSDRGB.FOR	FORTTRAN SOURCE	30 records
GSDRVR.FOR	FORTTRAN SOURCE	91 records
GSDRW1.FOR	FORTTRAN SOURCE	24 records
GSDRW2.FOR	FORTTRAN SOURCE	83 records
GSETDP.FOR	FORTTRAN SOURCE	35 records
GSFILL.FOR	FORTTRAN SOURCE	171 records
GSGIN.FOR	FORTTRAN SOURCE	36 records
GSIRST.FOR	FORTTRAN SOURCE	15 records
GSIVIS.FOR	FORTTRAN SOURCE	13 records
GSLENS.FOR	FORTTRAN SOURCE	13 records
GSLTYP.FOR	FORTTRAN SOURCE	27 records
GSMOV1.FOR	FORTTRAN SOURCE	16 records
GSMOVE.FOR	FORTTRAN SOURCE	27 records
GSPOLY.FOR	FORTTRAN SOURCE	11 records
GSPSTR.FOR	FORTTRAN SOURCE	46 records
GSRCLP.FOR	FORTTRAN SOURCE	14 records
GSRST.FOR	FORTTRAN SOURCE	28 records
GSSCLP.FOR	FORTTRAN SOURCE	24 records
GSSETC.FOR	FORTTRAN SOURCE	32 records
GSSTRK.FOR	FORTTRAN SOURCE	120 records
GSWNDO.FOR	FORTTRAN SOURCE	21 records
HATCH.FOR	FORTTRAN SOURCE	267 records
LAXIS.FOR	FORTTRAN SOURCE	26 records
LEN.FOR	FORTTRAN SOURCE	9 records
LINLAB.FOR	FORTTRAN SOURCE	43 records
LOGLAB.FOR	FORTTRAN SOURCE	17 records
MAPIT.FOR	FORTTRAN SOURCE	283 records
MAPPRM.FOR	FORTTRAN SOURCE	34 records
MAPSET.FOR	FORTTRAN SOURCE	24 records
MAPSIZ.FOR	FORTTRAN SOURCE	32 records
MAPSML.FOR	FORTTRAN SOURCE	305 records
MAPSZ2.FOR	FORTTRAN SOURCE	32 records
MINMAX.FOR	FORTTRAN SOURCE	12 records
NUMSTR.FOR	FORTTRAN SOURCE	15 records

PLTBOX.FOR	FORTTRAN SOURCE	21 records
PLTBX2.FOR	FORTTRAN SOURCE	21 records
POINTC.FOR	FORTTRAN SOURCE	33 records
POINTS.FOR	FORTTRAN SOURCE	27 records
POINTY.FOR	FORTTRAN SOURCE	27 records
PURJOY.FOR	FORTTRAN SOURCE	899 records
PUTSTR.FOR	FORTTRAN SOURCE	6 records
RASTER/FILE 1	FORTTRAN SOURCE	12 records
RASTER/FILE 2	FORTTRAN SOURCE	12 records
RASTER/FILE 3	FORTTRAN SOURCE	224 records
RASTER/FILE 4	FORTTRAN SOURCE	181 records
RLSDEV.FOR	FORTTRAN SOURCE	28 records
RSTMAP.FOR	FORTTRAN SOURCE	36 records
SAVMAP.FOR	FORTTRAN SOURCE	38 records
SCALE.FOR	FORTTRAN SOURCE	20 records
SCOPY.FOR	FORTTRAN SOURCE	7 records
STRPBL.FOR	FORTTRAN SOURCE	13 records
SYAXIS.FOR	FORTTRAN SOURCE	158 records
SYMBOL.FOR	FORTTRAN SOURCE	160 records
TRACCY.FOR	FORTTRAN SOURCE	39 records
TRACE.FOR	FORTTRAN SOURCE	30 records
TRACEC.FOR	FORTTRAN SOURCE	36 records
TRACEY.FOR	FORTTRAN SOURCE	33 records
GBCOMMON.CMN	FORTTRAN SOURCE	6 records
FNTDAT.PGM	FORTTRAN SOURCE	67 records
FNTTST.PGM	FORTTRAN SOURCE	93 records
TRNSFNT.PGM	FORTTRAN SOURCE	156 records
TRNSLATE.PGM	FORTTRAN SOURCE	178 records
DINTERP2.PGM	FORTTRAN SOURCE	102 records
LOOKUP2.FOR	FORTTRAN SOURCE	488 records

17. CATEGORY = 0 ,

KEYWORDS Gauss function
Li-drifted Ge detectors
emission spectra
gamma spectra
isotopes
spectra unfolding

**RSICC CODE PACKAGE PSR-209
NEA CODE PACKAGE IAEA0832**

1. NAME AND TITLE

GAMX1: A Computer Code System for Evaluating Spectra Peak Areas.

2. CONTRIBUTOR

Atomic Energy Board, Pelindaba, Pretoria, Republic of South Africa, through the NEA Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER

Fortran; IBM 360/370.

4. NATURE OF PROBLEM SOLVED

GAMX1 evaluates accurate peak areas of gamma-ray and X-ray spectra generated by Ge(Li) and Si(Li) spectrometers. It renders accurate estimates of peak heights, position of centroids, and the backgrounds in the vicinity of the photopeaks being analyzed. However, it is intended to analyze spectra containing isolated peaks of known energy only; no facilities for peak location, energy calibration, or the analysis of doublets are included.

5. METHOD OF SOLUTION

Photopeaks are analytically represented by a function composed of two Gaussians and an arc tangent superimposed upon a cubic polynomial background, thus ensuring the flexibility required for an authentic reproduction of X-ray and gamma-ray line shapes. This analytic peak function is applied to experimental spectra by virtue of the iterative Newton-Raphson non-linear least-squares fitting technique and the resulting set of equations is solved by pivotal condensation with back substitution. The empirical energy dependence of certain peak parameters is derived to enable the characteristics of the detection and measuring system to be quantified in terms of the energy dependence of the detector response before general spectra are analyzed. The quality of the fit to the photopeaks allows the uncertainty in each parameter and in the peak area to be computed. The error computed for the area of each individual peak is typically of the order of twice the uncertainty to be expected purely from statistics.

6. RESTRICTIONS OR LIMITATIONS

Twelve previously analyzed GAMX1 peaks are employed in the present study, the energy of each photopeak (MeV) is 10F7.3, the parametric data pertaining to each photopeak is a set format, and the number of constants in each empirical equation is 411. The coefficients of the empirical parametric energy equations is a set format, the energy dependence of each parametric function in the sequence is 411, the number of peaks to be analyzed is 13, and a maximum of 200 data points exist for each spectrum.

7. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for GAMX1.

8. COMPUTER HARDWARE REQUIREMENTS

GAMX1 is operable on the IBM 360/370 computers.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran compiler is required.

10. REFERENCE

J. White, "GAMX—A Computer Program for the Evaluation of Gamma-Ray and X-Ray Peak Areas from Spectra Generated by Semiconductor Detectors," PEL-255 (November 1976).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 2079.

12. DATE OF ABSTRACT

November 1984.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; DETECTOR RESPONSE

NEA CODE PACKAGE IAEA0877

IAEA0877 GASPAN -ZKD,GE(LI) DETECTOR & MULTICHANNEL_ANALYSER
GAMMA_SPECTRA UNFOLDING 830809

1. NAME OR DESIGNATION OF PROGRAM. GASPAN-ZKD.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
GASPAN-ZKD	IAEA0877/01	IBM 370/168	IBM 370/168	T

3. NATURE OF PHYSICAL PROBLEM SOLVED.

Analysis of gamma ray spectra obtained by a Ge(Li) detector and a multichannel pulse-height analyser to determine energy and intensity of gamma-lines.

4. METHOD OF SOLUTION.

After smoothing the spectral data (approximation to a power function by least squares method) domains with significant negative second differences are determined which mark the position of the peaks. A Gaussian function plus a quadratic function is fitted to each peak. The program allows identifying unresolved multiple peaks. It is possible to fit simultaneously up to 5 peaks.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.

Limited to spectra with 4096 channels and 100 peaks.

6. TYPICAL RUNNING TIME.

The running time depends on the number of channels and peaks and the demanded precision. The calculation for a spectrum with 1700 channels and 42 peaks requires 250 seconds of CPU-time. NEA-DB executed the test case on IBM 370/168 in 5 CPU seconds.

7. UNUSUAL FEATURES OF THE PROGRAM.

The programme uses an overly structure.

8. RELATED AND AUXILIARY PROGRAMS.

Random transfer system 'REX'.

9. STATUS

IAEA0877/01 : Arrived at NEADB

: in preparation
: Tested at NEADB

10. REFERENCES.

- H.P. Yule: "Mathematical Smoothing of Gamma Ray Spectra," Nuclear Instruments and Methods, Vol. 54, 1967, no.1, pp. 61-65
- S.J. Mills: "'AUTSPAN' - A Computer Program for the Automatic Analysis of Gamma Ray Spectra," CSIR Research Report 289, National Physical Research Laboratory, Pretoria (1969)
- M.A. Mariscotti: "A Method for Automatic Identification of Peaks in the Presence of Background and Its Applications to Spectrum Analysis," Nuclear Instruments and Methods, Vol. 50, 1967, pp. 309-320
- B. Lindemann and M. Geisler: "GASPAN - A program for automatic evaluation of gamma spectra with the help of photo peak analysis," (in German) (December 1972)

11. MACHINE REQUIREMENTS.

400K bytes of main storage on IBM 370/168.

12. PROGRAMMING LANGUAGE USED

IAEA0877/01 : FORTRAN-IV

13. OPERATING SYSTEM OR MONITOR UNDER WHICH PROGRAM IS EXECUTED.

OS370/081 using the FORTRAN-H-EXTENDED compiler.

14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.

Input of the spectral data by perforated tape.

15. NAME AND ESTABLISHMENT OF AUTHOR.

B.Lindemann, M.Geisler
Zentralinstitut fuer Isotopen und Strahlenforschung
DDR 705 Leipzig
Permoserstrasse 15.

16. MATERIAL AVAILABLE

source program mag tape
test-case data mag tape
test-case output mag tape
Report: Report on GASPAN (in German) (Dec. 1972)
GASPAN-ZKD INFORMATION FILE 41 records
GASPAN-ZKD SOURCE (FORTRAN-4) 45 records

GASPAN-ZKD JCL 23 records
GASPAN-ZKD INPUT FOR TEST CASE 214 records
GASPAN-ZKD OUTPUT OF TEST CASE 38 records

17. CATEGORY = O ,

KEYWORDS Gauss function
Li-drifted Ge detectors
gamma detectors
gamma spectra
least square fit
multi-channel analysers
radiation detectors

RSICC CODE PACKAGE PSR-045
NEA CODE PACKAGE NESC0605

1. NAME AND TITLE

GAUSS: A Code system for Analysis of Gamma-Ray Spectra from Ge(Li) Spectrometers.

GAUSS V (PSR-45A) was the original GAUSS package in the RSICC collection and was written for the IBM 360/75 computer. This original package was extended to include GAUSS VII (PSR-45B) which runs on the CDC computer. The two have now been combined into this one package and called GAUSS.

2. CONTRIBUTORS

Aerojet Nuclear Company, Idaho Falls, Idaho (A).
EG&G Idaho, Inc., Idaho Falls, Idaho (B).

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 360/370 (A) AND CDC (B).

4. NATURE OF PROBLEM SOLVED

GAUSS determines gamma-ray energies and intensities from spectra obtained with a Ge(Li) detector and a multichannel pulse-height analysis system.

5. METHOD OF SOLUTION

The preliminary portions of the program can determine the energy and width calibration equations, locate individual peaks and define "peak regions" that are significantly above the local spectral background. The user may edit these lists of peaks and regions. Each peak region is fitted with one or more components in which the peaks are represented by a Gaussian function or a Gaussian with one or two additive exponential tails on the low-energy side and one on the high-energy side. A step-like background function can be used with each component. The program will automatically recycle to add one or more components to a region if needed to improve the fit. The gamma-ray energies and intensities are computed from the resulting Gaussian positions and peak areas. To allow the user to determine the best results, the results from the analyses for each region with different numbers of components can be printed and line-printer plots of the fits to the data can be made.

6. RESTRICTIONS OR LIMITATIONS

GAUSS will handle spectra of up to 4096 channels with up to 300 peaks and 50 energy calibration lines.

The quality of the results depends primarily on the ability of the program to define a good spectral region for each analysis and the ability to recycle to determine the proper number of components.

7. TYPICAL RUNNING TIME

Typical spectra can be analyzed at a rate of approximately 5 per minute.

8. COMPUTER HARDWARE REQUIREMENTS

GAUSS is operable on the IBM 360/370 computer (A) or the CDC computer (B). A printer and

punch are required.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran compiler is required.

10. REFERENCES

R. G. Helmer and M. H. Putnam, "GAUSS V, A Computer Program for the Analysis of Gamma-Ray Spectra from Ge(Li) Spectrometers," ANCR-1043 (January 1972).

C. M. McCullagh and R. G. Helmer, "GAUSS VII. A Computer Program for the Analysis of Gamma-Ray Spectra from Ge Semiconductor Spectrometers, Informal Report," EGG-PHYS-5890 (October 1982).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source codes and sample problem input written in EBCDIC card images, plus output from the sample problem written in list format; total records 4960 (A) or 13,591 (B).

12. DATE OF ABSTRACT

October 1983.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING

NEA CODE PACKAGE NESC0622/01

NESC0622 GAUSS -6, EXPERIMENTAL GAMMA SPECTRA
ANAL, ISOTOPE IDENTIFICATION, DECAY_RATES 801117

1. NAME OR DESIGNATION OF PROGRAM - GAUSS6

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
GAUSS-6	NESC0622/01	IBM 370 series	IBM 370 series	T

3. DESCRIPTION OF PROBLEM OR FUNCTION

GAUSS6 is used for the production analysis of gamma-ray spectra obtained with a Ge(Li) detector and a multichannel pulse-height analyzer system. In addition to determining gamma-ray energies and intensities, it provides isotopic identification, decay corrections and correlation of data from different peaks and different spectra to obtain isotopic decay rates.

4. METHOD OF SOLUTION

GAUSS6 carries out the following steps -

- Sorts master nuclide library to obtain a subset including only the nuclides of interest.
- Automatically locates peaks by means of an auto-correlation routine.
- Fits each peak with a Gaussian function plus a linear function representing the spectral background. Only the three Gaussian parameters (height, width, and position) are allowed to vary. The fit extends down to 1.5 times the width of the Gaussian (FWHM). Fits that fail to converge are repeated with a fixed width.
- Determines peak width and energy calibration functions from a Th228 spectrum. These functions as well as the energy calibration from any spectrum can be transferred to subsequent spectra.
- Attempts isotopic assignments for all peaks. Decay corrections are made.
- For spectra from the same sample, edits and averages the results to obtain the isotopic decay rates.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

GAUSS6 will handle any number of spectra of up to 4096 channels with up to 300 peaks and 20 energy calibration lines. The subset of the isotopic library is limited to 1000 gamma rays.

6. TYPICAL RUNNING TIME

Typical spectra can be analyzed at a rate of about 5 per minute.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

The program package includes the following auxiliary programs -

- (a) LCTAPE for putting nonlinearity correction and efficiency tables on disk.
- (b) UPDATE for updating the master nuclide library.
- (c) RASLIB for producing a subset of the master nuclide library (normally run as part of the analysis run).
- (d) MERGE for combining the output tapes from several GAUSS6 analyses.
- (e) CORLAT for carrying out the comparison and averaging of the several measurements for each sample.
- (f) LIBRER for generating a nuclide library data set from cards.
- (g) SECLIB for generating a secondary library subset for CORLAT.

GAUSS6 is based on GAUSS5 (NESC Abstract 605), but is written to analyze large groups of spectra efficiently and includes calculations beyond the gamma-ray energies and intensities and can compare results from different gamma-rays and different spectra to verify nuclide assignments for individual peaks.

9. STATUS

NESC0622/01: Arrived at NEADB
 : in preparation
 : Tested at NEADB

10. REFERENCES

J. E. Cline, M. H. Putnam, and R. G. Helmer, GAUSS VI, A Computer Program for the Automatic Batch Analysis of Gamma-ray Spectra from Ge(Li) Spectrometers, ANCR-1113, June 1973.

R. G. Helmer and M. H. Putnam, GAUSS V, A Computer Program for the Analysis of Gamma-ray Spectra from Ge(Li) Spectrometers, ANCR-1043, January 1972.

GAUSS6, ACC No. 622, Argonne Code Center Programming Note 74-29, March 29, 1974.
NESC0622/01:

11. MACHINE REQUIREMENTS

GAUSS6 requires storage devices for the spectral library, nuclide library subset, and the correlation data in addition to three scratch devices and the card reader and printer. CORLAT requires storage devices for the secondary library subset and the correlation data plus four scratch devices and the card reader and printer.

12. PROGRAMMING LANGUAGE USED

NESC0622/01: FORTRAN-IV

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

OS/360 MVT.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

The CORLAT program requires the IBM360 SORT package.

15. NAME AND ESTABLISHMENT OF AUTHORS

R. G. Helmer, J. E. Cline, and M. H. Putnam
EG&G Idaho, Inc.
P. O. Box 1625
Idaho Falls, Idaho 83401

16. MATERIAL AVAILABLE

NESC0622/01:

Report:

INFORMATION	1 records
LIBRER PROGRAM SOURCE (PL/1)	182 records
SAMPLE PROBLEM DATA	10 records
SAMPLE PROBLEM PRINTED OUTPUT	27 records
EXECUTION DD CARDS	4 records
LCTAPE PROGRAM SOURCE (F4)	170 records
SAMPLE PROBLEM DATA	60 records
SAMPLE PROBLEM PRINTED OUTPUT	140 records
EXECUTION DD CARDS	2 records
RASLIB PROGRAM SOURCE (PL/1)	461 records
SAMPLE PROBLEM DATA	5 records
SAMPLE PROBLEM PRINTED OUTPUT	28 records
EXECUTION DD CARDS	4 records
GAUSS-6 SOURCE MODULE (BAL)	2811 records
GAUSS-6 SOURCE MODULE (F4)	3825 records
SAMPLE PROBLEM DATA	2533 records
SAMPLE PROBLEM PRINTED OUTPUT	1043 records
EXECUTION DD CARDS	14 records
MERGE PROGRAM SOURCE MODULE (F4)	248 records
SAMPLE PROBLEM DATA	1 record
SAMPLE JCL	14 records
UPDATE PROGRAM SOURCE (PL/1)	518 records
SAMPLE JCL	9 records

17. CATEGORY = O ,

KEYWORDS Li-drifted Ge detectors
gamma spectra
isotopes

RSICC CODE PACKAGE PSR-100
NEA CODE PACKAGE NEA-0433

1. NAME AND TITLE

GRETEL: Analyzer and Processor of Ge(Li) Gamma-Ray Spectrometric Data.

2. CONTRIBUTOR

Joint Nuclear Research Centre, Ispra Establishment (EURATOM), Ispra, Italy.
OECD Nuclear Energy Agency Computer Program Library, Ispra, Italy.

3. CODING LANGUAGE AND COMPUTER

Fortran IV and Assembler language; IBM 370.

4. NATURE OF PROBLEM SOLVED

GRETEL performs the quantitative analysis of gamma-ray spectra obtained by Ge(Li) detectors using special "oriented libraries" which are prepared for each particular problem.

5. METHOD OF SOLUTION

The computer routines which detect and evaluate peak areas perform the following operations: 1) local smoothing of the spectrum, 2) first derivative of the smoothed spectrum, 3) peak location according to the change of sign of the first derivative, 4) computation of the net area of each peak found. GRETEL can also detect and compute double peaks from a study of the behavior of the first derivative.

An energy calibration source is counted by GRETEL as the first spectrum of the series; then the unknown neutron activated samples are successively counted. The analysis is carried out by the single @comparator method. Irradiation and decay times, weight of samples and neutron flux are manually assigned by the operator. Peaks in the gamma spectrum are searched, identified and measured by following the instructions of special "oriented" libraries which are prepared for each particular problem.

6. RESTRICTIONS OR LIMITATIONS

The maximum number of calibration peaks is 10. The maximum number of elements of the "oriented library" is 50. The maximum number of channels of the spectrometer which can be used is 4096. No limitation exists on the number of spectra to be treated. It is imperative that the calibration spectrum is always the first of the set.

CALCOMP plotting must be requested separately after the complete running of the program.

7. TYPICAL RUNNING TIME

For a typical analysis of 30 spectra of 2048 channels (calibration spectrum plus 29 unknown), with an "oriented library" of 30 elements, the running time is about 30 seconds (object program).

8. COMPUTER HARDWARE REQUIREMENTS

GRETEL is operable on the IBM 370 computers. The plotting routines are for a CALCOMP 900 off-line plotter.

9. COMPUTER SOFTWARE REQUIREMENTS

Fortran IV-G and Assembler language compilers are required.

10. REFERENCE

G. Guzzi and J. Cuypers, "GRETEL, A Computer Program for Gamma Ray Spectrometry with Ge(Li) Detectors," EUR 5117 e (1974).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, the plotting subroutines written in Fortran IV and Assembler Language, plus the output from the sample problem written in list format; total records 11,034.

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING

**RSICC CODE PACKAGE PSR-321
NEA CODE PACKAGE PSR-0321**

1. NAME AND TITLE

GRPANL: Code System for Analyzing Ge and Alpha-Particle Detector Spectra.

2. CONTRIBUTORS

Lawrence Livermore National Laboratory, Livermore, California through the Energy Science & Technology Software Center, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER/OPERATING SYSTEM

Fortran 77; VMS 4.7

4. NATURE OF PROBLEM SOLVED

GRPANL (GRouP ANaLysis) is a suite of programs which analyzes and interprets regions of germanium and alpha-particle detector pulse-height spectra. GRPANL is the main peak-fitting program; the other programs included are used in conjunction with GRPANL. GRPANL is particularly useful for accurately deconvoluting and interpreting complex clusters of peaks in a spectrum. GRPANL fits peaks in specified regions of a gamma-ray, x-ray, or alpha-particle spectrum, calculates their energies and intensities, and optionally calculates the photon emission rates for the sample from which they were emitted. It can also identify and measure isotopes in a sample. GRPANL output can be immediately analyzed for quantitative isotopic assays or stored in an intermediate data file. The other programs are EDIGRP, LIBRY, and GEVAL. EDISRP (EDIt GRouP) creates and edits an analysis control file that contains input parameters and analysis options for spectral regions analyzed by GRPANL; users can repeat or modify an analysis without retyping input. LIBRY (LIBRarY) assembles and cross references selected nuclear decay scheme data and stores it in decay scheme data files for use by GRPANL and GEVAL. GEVAL (Gamma ray EVALuation) uses these data files along with GRPANL intermediate results to identify isotopes, calculate their abundance in a sample, and print the corresponding disintegration rates and abundances at counting and zero times.

5. METHOD OF SOLUTION

The peaks in any x-ray or gamma-ray spectrum are always superimposed on a background distribution resulting from the Compton scattering process. GRPANL first removes the background continuum before starting the fitting process thus reducing the number of fitting parameters. GRPANL then estimates the initial peak heights and positions. The Gauss-Seidel, or Newton-Raphson, iterative least-squares technique is applied to fit the data because the equations describing the peak-shape are nonlinear in form. Convergence is determined by comparing the magnitude of the last change in each variable with a specified convergence criterion.

Once convergence is attained, final calculations are made for peak energies, intensities, and their respective uncertainties. The intensity uncertainties are based on counting statistics and on the goodness-of-fit.

6. RESTRICTIONS OR LIMITATIONS

Maxima of 1024 channels per peak, 40 degrees of freedom, and 40 peaks. GEVAL can evaluate a maximum of 200 peaks. The auxiliary programs CALDET, XDIST, LLFIT, and PKSHAP described in the reference reports are not included in the package. CALDET is used as an aid in

calibrating a new detector. LLFIT fits an nth order polynomial to the data and reports the coefficients of the fit. These coefficients may then be stored in the detector coefficients file for subsequent analysis using this newly calibrated detector.

7. TYPICAL RUNNING TIME

The programs are interactive.

8. COMPUTER HARDWARE REQUIREMENTS

The codes run on the VAX family of computers.

9. COMPUTER SOFTWARE REQUIREMENTS

GRPANL uses the LLNL DIGRAPH and DIGLIB codes to produce graphical output. These programs are supplied in object form only. The VMS Fortran compiler was used on the VMS operating system.

10. REFERENCES

a: included in document:

R. Gunnink, W. D. Ruhter, and J. B. Niday, "GRPANL: A Suite of Computer Programs for Analyzing Complex Ge and Alpha-Particle Detector Spectra, Volume 1," UCRL-53861, Vol. 1, (May 1988).

R. Gunnink, W. D. Ruhter, and J. B. Niday, "Operations Guide for GRPANL: A Suite of Computer Programs for Analyzing Complex Ge and Alpha-Particle Detector Spectra, Volume 2," UCRL-53861, Vol. 2 (May 1988).

GRPANL Sample Output (September 1988).

b: background information:

R. Gunnink and W. D. Ruhter, "GRPANL: A Program for Fitting Complex Peak Groupings for Gamma and X-ray Energies and Intensities," UCRL-52917 (January 1980).

11. CONTENTS OF CODE PACKAGE

Included in the package are the referenced documents and 1 DS/HD disk which includes the source files, test case input data and output.

12. DATE OF ABSTRACT

October 1992.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE;
PARAMETRIC MODELS; PLOTTING; UNFOLDING

**RSICC CODE PACKAGE PSR-101
NEA CODE PACKAGE PSR-0101**

1. NAME AND TITLE

HYPERMET: Gamma-Ray Spectra Analyzer Germanium Detector

2. CONTRIBUTOR

Naval Research Laboratory, Washington, D. C.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; CDC 3800 (A), T. I. ASC-7 IBM COMPATIBLE (B), FACOM M190 (C).

4. NATURE OF PROBLEM SOLVED

HYPERMET performs an automatic analysis of a multichannel gamma-ray pulse-height spectrum taken with a germanium detector. It has a number of options including an energy calibration, correction for radioactive decay, and a CALCOMP plot of each fit.

5. METHOD OF SOLUTION

A peak search is done by using a zero-area sliding transform on the data. A peak is indicated by a rise above a preset threshold. A fitting subregion is then defined about the peak and initial values are determined for the parameters of a semi-empirical peak-shape function plus background. Within this subregion, initial estimates are made for the parameters such as background level.

An iterative non-linear least-squares fit is done for the optimum values of the parameters. If programmed criteria for a good fit are not satisfied, the residuals (data minus fit) are searched for indication of an additional peak in the data. If found, the fit is repeated with the additional peak included.

6. RESTRICTIONS OR LIMITATIONS

HYPERMET is dimensioned for up to 8192 channel spectra with up to 100 peaks per spectrum.

7. TYPICAL RUNNING TIME

Running time varies linearly with peak width and quadratically with the number of multiplet peaks which must be fit simultaneously. Spectra with poor statistics are fit more rapidly than those with good statistics for which the statistical criteria for a good fit are more stringent.

For a typical spectrum with peak widths from 3 to 5 channels FWHM, moderate statistics, and mostly well separated peaks, running time on the CDC 3800 computer is on the order of one minute for every ten peaks in the spectrum.

8. COMPUTER HARDWARE REQUIREMENTS

HYPERMET is operable on the CDC 3800 (A), T. I. ASC-7 (B), or the FACOM M190 computers. Except for a few system input-output routines, it will fit into one 32 K word bank on a CDC 3800 computer.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

- G. W. Phillips, "Guide to Program HYPERMET Version 2.7," (August 1976).
G. W. Phillips and K. W. Marlow, "Program HYPERMET for Automatic Analysis of Gamma-Ray Spectra from Germanium Detectors," NRL-MR-3198 (January 1976).
G. W. Phillips, "Guide to Program HYPERMET Version A.1," (February 1977).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in BCD/EBCDIC/ASC card images, plus output from the sample problem; total records 4490 (A), 7145 (B), and 4001 (C).

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS;
GERMANIUM (Ge(Li)) DETECTOR; PLOTTING; UNFOLDING

NEA CODE PACKAGE IAEA0940

IAEA0940 JADSPE, MULTI-CHANNEL GAMMA SPECTRA UNFOLDING PROG 870706

1. NAME OR DESIGNATION OF PROGRAM - JADSPE.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
JADSPE	IAEA0940/01	ICL 4/72	ICL 4/72	A

3. DESCRIPTION OF PROGRAM OR FUNCTION

JADSPE is a package of eight programs to process multichannel gamma-ray spectra. The programs can be used to:

- locate automatically spectral peaks and calculate their positions, areas, and full widths at half maximum (FWHM);
- plot the spectra on a CALCOMP plotter, TEKTRONIX terminal or a line printer;
- add or subtract several spectra with the possibility of adjusting either their start and end channels or the maxima of the chosen corresponding peaks.

The JADSPE package comprises the following programs:

SPECTF: automatic location of peaks and calculation of their positions, areas and FWHMS. The standard deviations of peak parameters are also determined, and each evaluated region is plotted on the line printer.

SPECT1: The areas and FWHMs are calculated for peaks whose positions are known beforehand. The standard deviations of calculated parameters are also determined, and each evaluated region is plotted on the line printer.

PLOCHA: The peak net area is calculated by summing the channel contents in specified regions and by subtracting a linear background.

GRAPH: Spectrum plotting on the line printer.

PLTNEW: Spectrum plotting on CALCOMP plotter or on TEKTRONIX terminal.

SUMDIF: The channel contents of several gamma-ray spectra are added or subtracted.

SSPFP: The channel contents of several gamma-ray spectra are added with adjustment of the maxima of specified peaks.

SOU CET: The channel contents of several gamma-ray spectra are added with the adjustment of start and

end channels of the spectra.

4. METHOD OF SOLUTION

Non-linear least-square fit.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

The full energy peaks are approximated by a symmetrical Gaussian function and the underlying background is approximated by a first-order polynomial. A fixed spectrum length of 4096 channels is assumed.

Maxima of:

- number of peaks in one multiplet: 9
- number of peaks identified by the automatic search procedure: 300
- number of channels in one evaluated interval: 500
- dimensions of CALCOMP plots: 54 cm x 36 cm
- number of spectra, which may be added by SSPFP: 5
- number of peaks for spectra adjustment in SSPFP: 20
- number of spectra added by SOUCET: 10.

6. TYPICAL RUNNING TIME

SPECTF, SPECT1: running time depends on the spectrum complexity and the total number of peaks evaluated. The determination of peak positions, areas, and FWHM's requires from 10 to 60 ETU per spectrum (1 ETU = 3.6 seconds).

GRAPH: plotting on line printer requires about 25 ETU per spectrum.

PLTNEW: plotting on CALCOMP requires about 2 ETU per spectrum.

SUMDIF, SSPFP, SOUCET: running time depends on the number of spectra involved. To sum two spectra requires about 4 ETU.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

IAEA0940/01 : Requested by NEADB
 : Arrived at NEADB

10. REFERENCES

- J. R. Wolberg: "Prediction Analysis" Princeton, D. Van Nostrand Comp, Inc. 1967
- J. Pitha, R.N. Jones: Internal Report Division of Pure Chemistry, National Research Council, Ottawa Canada
- J. Rikovska, V. Zvoliska, V. Hnatowicz: Radioisotopy 13(5), 1007-1023 (1972)
- E. Stejskalova: Acta Polytechnica, 14 (IV,1) (1985)
- "Multijob Programming" TP4572, ICL

- "User's Guide to the MULTIJOB GRAFOR routine" University of Bath, Computer Unit
- J. Rikovska and E. Stejskalova: JADSPE - The Program Package for Analysis of the Gamma-Ray Energy Spectra (December 1987)

11. MACHINE REQUIREMENTS

Program execution requires from 41 to 106 bytes of mainm storage. CALCOMP plotter or TEKTRONIX 4010 terminal are required for spectrum plotting.

12. PROGRAMMING LANGUAGE USED

IAEA0940/01 : FORTRAN-IV

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

MULTIJOB (ICL/4-72)

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

J. RIKOVSKA and E. STEJSKALOVA
Technical Unigue
Faculty of Nuclear Science and Physical Engineering
Department of Mathematics
Brehova 7
115 19 PRAGUE 1 - Stare Mesto
CZECHOSLOVAKIA

16. MATERIAL AVAILABLE

SPECTF Source program
SPECTF JCL
SPECTF Sample Problem Input Data
SPECT1 Source program
SPECT1 JCL
SPECT1 Sample Problem Input Data
PLOCHA Source program
PLOCHA Macro (USERCODE)
PLOCHA JCL
PLOCHA Sample Problem Input Data
PLOCHA Sample Problem Input Data S0019
PLOCHA Sample Problem Printed Output
GRAPH Source program
GRAPH JCL
GRAPH Sample Problem Input Data

PLTNEW Source program
PLTNEW JCL
PLTNEW Sample Problem Input Data
SUMDIF Source program
SUMDIF JCL
SUMDIF Sample Problem Input Data
SUMDIF Sample Problem Printed Output
SSPFP Source program
SSPFP JCL
SSPFP Sample Problem Input Data
SSPFP Sample Problem Printed Output
SUCET Source program
SUCET JCL
SUCET Sample Problem Input Data
SUCET Sample Problem Printed Output
SPECTF Sample Problem Printed Output
SPECT1 Sample Problem Printed Output
GRAPH Sample Problem Printed Output
Report: JADSPE Report (December 1987)

17. CATEGORY = N , O ,

KEYWORDS data processing
gamma detectors
gamma spectra
least square fit
multi-channel analysers
spectra unfolding

NEA CODE PACKAGE NESC9580

NESC9580 RICKI, INTERACTIVE GAMMA SPECTRA UNFOLDING WITH ISOTOPE IDENTIFICATION 900918

1. NAME OR DESIGNATION OF PROGRAM - RICKI.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
RICKI	NESC9580/01	IBM PC	IBM PC	T

3. DESCRIPTION OF PROGRAM OR FUNCTION

RICKI is an interactive program for analysis of gamma spectra containing one or more peaks with possible multiplets. Algorithms are incorporated for peak fitting, analysis, and nuclide identification. Comprehensive output keeps the user informed of the analysis as it proceeds and presents the results. User-selectable options for plotting and neutron activation analysis are available to control this analysis. RICKI was developed to analyze spectra from examinations of severe fuel damage specimens. Two features included to streamline the analysis of Three Mile Island (TMI) core bore data are the edit of averaged activities and the output file created for generating a spreadsheet. Activity editing allows the user to select which gamma lines are used for a specific nuclide in average activity calculations. Contributions from peak areas which result from overlapping lines of two or more nuclides may be removed. For each averaged activity an edited activity file record is written containing the nuclide name, averaged activity, activity standard deviation, scan start position, and scan end position.

4. METHOD OF SOLUTION

The peak search algorithm utilizes an optimized second derivative filter for efficient and reliable determination of peak location. A linear Gaussian fitting technique, which is a modified version of Mukoyama's linear least squares fitting method in which the centroid, sigma, and peak height are free parameters, is used to calculate peak areas. An estimated background is computed for each peak using Gunnink's method. Nuclide activities are computed by matching centroids with nuclide library entries and averaging the activity calculated for each matching peak.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Maxima of - 500 gamma library entries 80 peaks/spectrum

6. TYPICAL RUNNING TIME

Running time varies from 20 seconds to 5 minutes.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

RICKI was developed from CINA, a simpler fitting and peak integration program. The CINA gamma line library and menu sections are retained in RICKI. Auxiliary programs GAMLIB, EFFCAL, and SPECMOD provide gamma library maintenance, detector efficiency table generation, and spectrum error correction, respectively. Auxiliary program CORESORT converts TMI core bore scan data to the format of a listing of activity versus scan position for each nuclide and produces a spreadsheet input file (nuclide activity listed by scan position) readable by LOTUS 1-2-3. RICKI is not intended to replace large-scale gamma analysis codes such as GAUSS8, GAMANAL (NESC 9654), or SAMPO, but provides rapid, accurate analysis for cases where detailed peak shapes and other parameters may not be known.

9. STATUS

NESC9580/01 : Offered to NEADB
 : Requested by NEADB
 : Arrived "as is"
 : in preparation
 : Tested at NEADB

10. REFERENCES

NESC9580/01 :
- A.E. Proctor: "An Implementation of the Pulse Injection Technique for Dead-Time and Pile-up Corrections in Gamma Spectroscopy Suitable for Automated Systems," EG&G Idaho (October 1986)
- M. Birgersson: "RICKI Flexible Disk Cartridge Description and Implementation Information," NESC Note 88-27 (December 31, 1987)
- A.E. Proctor: "RICKI: A Compact Gamma Analysis Code for the IBM Personal Computer," EGG-PHY-7545 (February 1987)
- A.E. Proctor: "RICKI: A Compact Gamma Analysis Code for the IBM Personal Computer," Addendum to EGG-PHY-7545

11. MACHINE REQUIREMENTS

An IBM PC, preferably equipped with math coprocessor and an enhanced graphics adapter, a minimum of two floppy disk drives, and an EPSON FX-286 or compatible printer for graphics printing. A hard disk is desirable to obtain reasonable nuclide sorting time.

NESC9580/01: Main storage requirements on an IBM PC/AT are as follows: RICKI and RICKI2: 175K; GAMLIB: 75K; EFFCAL: 95K; SPECMOD: 90K; CORESORT: 50K.

12. PROGRAMMING LANGUAGE USED

NESC9580/01 : BASIC

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

DOS 3.1.

NESC9580/01: The program ran under MSDOS version 3.30. The compiler Microsoft QuickBASIC version 4.00 and linker Microsoft Linker 3.63.08 were used.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

Because some DOS systems do not allow more than three open files, two RICKI source files are provided. RICKI2 edits the averaged activities and procedures output file (the fourth open file) for use by the CORESORT spreadsheet generation program. RICKI, which does not perform this editing, opens only three files.

15. NAME AND ESTABLISHMENT OF AUTHORS

A.E. Proctor
EG&G Idaho, Inc.

16. MATERIAL AVAILABLE

NESC9580/01 :
TMISPEC.PAR Menu file containing parameters
THORIUM.LIB Thorium library
TMIPEAKS.LIB TMI peak identification lib.
CALIB.LIB Calibration library
RICKI.BAS RICKI source
RICKI.MAP RICKI load map
RICKI.EXE RICKI executable file
TABLE.EFF Efficiency table
GAMLIB.BAS GAMLIB BASIC source
CORE.EFF Core efficiency table
GAMLIB.LST CAMLIB compilation listing
GAMLIB.MAP GAMLIB load map
GAMLIB.EXE GAMLIB executable file
TEST.EFF Demonstration efficiency table
EFFCAL.BAS EFFCAL BASIC source
EFFCAL.LST EFFCAL compilation listing
EFFCALL.MAP EFFCAL load map
EFFCAL.EXE EFFCAL executable file
CALIB.EFF Calibration efficiency table
TEST.PAR Test parameter
RODS.EFF Efficiency table for rods
PETE.EFF Test efficiency table for rods
SPECMOD.BAS SPECMOD BASIC source
SPECMOD.LST SPECMOD compilation listing
SPECMOD.MAP SPECMOD load map
SPECMOD.EXE SPECMOD executable file

RICKI2.BAS RICKI2 BASIC source	
CORESORT.BAS CORESORT BASIC source	
RICKI2.EXE RICKI2 executable file	
CORESORT.EXE CORESORT executable file	
GAMLIB.SC1 Gamma library spectrum file 1	
GAMLIB.SC2 Gamma library spectrum file 2	
86240001.GSR Spectral data file	
86240003.GSR Spectral data file	
Report: EG&G Idaho (October 1986)	
NESC Note 88-27 (December 31, 1987)	
Report: EGG-PHY-7545 (February 1987)	
Report: EGG-PHY-7545 ADDENDUM	
Information file	133 records
Spectral data file	848 records
Spectral data file	848 records
Calibration efficiency table	21 records
Calibration library	0 records
Core efficiency table	11 records
CORESORT BASIC source	401 records
CORESORT executable file	0 records
EFFCAL BASIC source	884 records
EFFCAL executable file	0 records
EFFCAL compilation listing	1038 records
EFFCAL load map	25 records
GAMLIB BASIC source	705 records
GAMLIB executable file	0 records
GAMLIB compilation listing	811 records
GAMLIB load map	25 records
Gamma library spectrum calculation file 1	0 records
Gamma library spectrum calculation file 2	9 records
Test efficiency table for rods	20 records
RICKI BASIC source	2297 records
RICKI executable file	0 records
RICKI load map	25 records
RICKI2 BASIC source	2364 records
RICKI2 executable module	0 records
Rod efficiency table with Ce/Eu strip stand.	20 records
SPECMOD BASIC source	918 records
SPECMOD executable file	0 records
SPECMOD compiling listing	1075 records
SPECMOD load map	25 records
Efficiency table	1 records
Demonstration efficiency table	7 records
Test parameter file	19 records
Thorium library	0 records
TMI peak identification library	0 records
File containing parameters for spect. analy.	19 records

DOS file-names

36 records

17. CATEGORY = 0 ,

KEYWORDS Gauss function

activation analysis

gamma spectra

spectra unfolding

RSICC CODE PACKAGE PSR-186

1. NAME AND TITLE

SAMPO-LRC: Gamma-Ray Spectrum Analysis Code.

SAMPO, originally called SISYPHUS, was developed on the CDC 6600 computer at the Lawrence Berkeley Laboratory at the University of California in 1969 in support of the author's doctoral dissertation. The IDENT subroutine included in this version carries out radioisotope identifications and elemental mass determinations after simple or cyclic thermal-neutron activation analysis. A minicomputer version of the code, PSR-204/SAMPO-80, was developed at the Helsinki University of Technology, Nuclear Engineering Laboratory, Finland.

2. CONTRIBUTOR

University of London Reactor Centre, Berkshire, England.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; CDC 6600.

4. NATURE OF PROBLEM SOLVED

SAMPO is a versatile gamma-ray spectrum analysis program used for the analysis of the complex spectra encountered in neutron-activation analysis. In particular, it is intended for photo-peak analysis of gamma-ray spectra obtained with semiconductor detectors. It includes routines for peak-finding, peak-fitting and peak intensity and energy determinations. It also makes complete statistical and calibration-error estimates. Different options are available to make the code applicable to accurate nuclear spectroscopic work as well as routine data reduction.

5. METHOD OF SOLUTION

SAMPO contains a mathematical formalism for the representation of photopeaks and the continua in their vicinity which is applicable to analysis of spectra measured under widely varying conditions. With this formalism, the line shape is defined for each peak in the spectrum. The region of data about a single peak is then fitted with the shape functions and a function representing the background continuum. The line-shape calculations and the fitting are performed by using a least-squares procedure with an iterative gradient minimization method with variable metric.

IDENT, a subroutine of SAMPO, carries out radioisotope identifications and elemental mass determinations after simple or cyclic thermal-neutron activation analysis by matching the peaks found with its nuclear data library.

6. RESTRICTIONS OR LIMITATIONS

IDENT is dimensioned to allow for a maximum of 15 peaks in any one interval and 50 unsuccessful identifications in each spectrum. These limits may be increased if necessary.

7. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for SAMPO.

8. COMPUTER HARDWARE REQUIREMENTS

SAMPO was designed to run on the CDC 6600 computer.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

a. Included in the documentation:

W. Carder, "A General Purpose Program for Semiconductor Spectral Analysis, User's Manual" (August 1977).

W. Carder, T. D. MacMahon, and A. Egan, "IDENT—A Radioisotope-Identification Subroutine for Use with the Gamma-Ray Spectrum Analysis Program SAMPO," *Talanta* 25, (1978) 21-40.

b. Background information:

J. T. Routti and S. G. Prussin, "Photopeak Method for the Analysis of Gamma-Ray Spectra from Semiconductor Detectors," *Nuclear Instruments and Methods* 72 (1969) 125-142.

Jorma T. Routti, "SAMPO, a Fortran IV Program for Computer Analysis of Gamma Spectra from Ge(Li) Detectors, and for Other Spectra with Peaks," UCRL-19452 (October 1969).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source codes, sample problem input, and JCL for the CDC 6600 written in EBCDIC card images, plus output from the sample problem; total records 7929.

12. DATE OF ABSTRACT

June 1982; revised October 1983; updated January 1984; revised April 1984; reviewed May 1984.

KEYWORDS: ACTIVATION SPECTRA ANALYSIS; GAMMA-RAY SPECTRUM ANALYSIS; GERMANIUM (Ge(Li)) DETECTOR

**RSICC CODE PACKAGE PSR-204
NEA CODE PACKAGE NEA-0691**

1. NAME AND TITLE

SAMPO80: Gamma-Ray Spectrum Analysis Method for Minicomputers.

AUXILIARY ROUTINES

SAMPOSHAPE: Performs peak shape calibration.

SAMPOFIT: Performs peak search and fitting.

SAMPOID: Performs nuclide identification.

SAMPO, originally called Sisyphus, was developed on the CDC 6600 computer at the Lawrence Berkeley Laboratory of the University of California in 1969 in support of the author's doctoral dissertation. The analysis methods employed in this minicomputer version are simplified from those in the original code. Another version of this code, PSR-186/SAMPO-LRC, was modified at the London Reactor Centre and runs on the CDC 6600 computer.

2. CONTRIBUTORS

Helsinki University of Technology, Nuclear Engineering Laboratory, Espoo, Finland.

OECD Nuclear Energy Agency Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 5; Data General Nova 2.

4. NATURE OF PROBLEM SOLVED

SAMPO80 is a rapid and accurate analysis program for gamma-ray spectra measured with Ge(Li) or HPGe detectors. SAMPO80 consists of three separate parts, the shape calibration part SAMPOSHAPE, the peak search and fitting part SAMPOFIT, and the nuclide identification part SAMPOID.

5. METHOD OF SOLUTION

The shape calibration procedure uses a non-linear least squares algorithm with a variable metric method. Some other features include: peak location with a smoothed second difference method, peak area calculation with a linear least squares fit to predefined peak shapes, and nuclide identification with a linear least squares fit based on associated lines.

6. RESTRICTIONS OR LIMITATIONS

Number of shape calibration points allowed:	20
Number of energy calibration points allowed:	20
Number of efficiency calibration points allowed:	20
Maximum number of found peaks:	100
Maximum number of fitted peaks:	100
Maximum number of peaks in a multiplet:	5
Maximum number of channels in a fitting interval:	50
Maximum number of peaks for nuclide identification:	80
Maximum number of identified nuclides:	30
Maximum number of lines per nuclide:	30

7. TYPICAL RUNNING TIME

On a Data General Eclipse S/140 with microcoded floating point instruction set, 25 seconds are required per shape calibration of one peak, 2 seconds per peak for peak search and fitting, and 3 seconds per identified nuclide for identification.

8. COMPUTER HARDWARE REQUIREMENTS

SAMPO80 is operable on the Data General Nova 2 minicomputer with a 32 kiloword central memory and a supporting disk unit.

9. COMPUTER SOFTWARE REQUIREMENTS

This version of SAMPO80 is run under the Data General Real Time Disk Operating System (RDOS) and requires a Fortran 5 compiler.

10. REFERENCES

P. A. Aarnio, J. T. Routti, J. V. Sandberg and M. J. Winberg, "Adapting Gamma-Spectrum Analysis Program SAMPO for Microcomputers," (May 1983).

J. T. Routti, "SAMPO, a Fortran IV Program for Computer Analysis of Gamma Spectra from Ge(Li) Detectors, and for Other Spectra with Peaks," UCRL-19452 (October 1969).

P. A. Aarnio, M. J. Koskela, "Computerized Gamma Spectrometry at the Helsinki University of Technology," *Nucl. Instrum. Meth.* 193 (1982) 129-134.

M. Koskela, P. Aarnio, and J. Routti, "SAMPO80: An Accurate Gamma Spectrum Analysis Method for Minicomputers," *Nucl. Instrum. Meth.* 190 (1981) 89-99.

M. J. Koskela, P. A. Aarnio, and J. T. Routti, "SAMPO80: Minicomputer Program for Gamma Spectrum Analysis with nuclide Identification," *Comput. Phys. Comm.* 24 (1981) 11-35.

J. T. Routti and S. G. Prussin, "Photopeak Method for the Analysis of Gamma-Ray Spectra from Semiconductor Detectors," *Nucl. Instrum. Meth.* 72 (1969) 125-142.

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source codes, sample problem input, and console dialogue written in EBCDIC card images, plus output from the sample problem; total records 4615.

12. DATE OF ABSTRACT

January 1984; revised April 1984, October 1991.

KEYWORDS: ACTIVATION SPECTRA ANALYSIS; GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE

RSICC CODE PACKAGE PSR-089

1. NAME AND TITLE

SKEWGAUS: Skewed-Gaussian Line Peak Fitting Code — Multichannel Analyzer (MCA) Spectra — Ge(Li) and Semiconductor Detectors.

2. CONTRIBUTOR

Ames Laboratory, USDOE, Iowa State University, Ames, Iowa.

3. CODING LANGUAGE AND COMPUTER

Fortran IV, PL/1; IBM 360/370.

4. NATURE OF PROBLEM SOLVED

SKEWGAUS fits a skewed-Gaussian line shape to peaks in multichannel analyzer (MCA) spectra obtained with Ge(Li) and Si(Li) semiconductor detectors.

5. METHOD OF SOLUTION

SKEWGAUS reads an entire multichannel analyzer (MCA) spectrum and retains this spectrum in core while all fits are being performed on it. Any number of fits may be performed on a spectrum and any number of spectra may be included in a single execution of the program. Each fit may include a superposition of up to nine peaks in addition to a linear or (optionally) quadratic background. Parameters of different peaks may be constrained to vary proportionately during the fit. Different convergence criteria are applied to different peak parameters. Several options are available for handling the background, permitting it to be fit either concurrently with the peaks or separately. A modified statistical weighting of the MCA data points takes into account the differential non-linearity of the analyzer. SKEWGAUS was designed to supply its own initial estimates for nearly all parameters so that the amount of input data which must be supplied is minimal.

6. RESTRICTIONS OR LIMITATIONS

The maximum number of channels included in the channel-by-channel output listing is 210; the maximum number of variable parameters in a fit is 40. It is possible to change these numbers following instructions in the documentation.

The maximum number of peaks in a fit is 9. This number cannot be changed easily.

7. TYPICAL RUNNING TIME

On an IBM 360/65 system, a sample problem involving 7 fits with an average of 36 data points and 10 variable parameters per fit and requiring an average of 11 iterations per fit took a total of 16 seconds of CPU time (exclusive of the plot step).

8. COMPUTER HARDWARE REQUIREMENTS

SKEWGAUS is operable on the IBM 360/370 computers. It was designed to fit into 128 K bytes (32 K words) of main core storage. Alternatively, the MCA data array may be placed in bulk (LCS) core storage to reduce the main core size to 96 K bytes.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCE

W. C. Schick, Jr., "SKEWGAUS: A Fortran Program for Fitting Peaks in Semiconductor Detector Spectra," IS-3460 (October 1974).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code input written in Fortran IV and PL/1; total records 1383.

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM
ANALYSIS; UNFOLDING

RSICC CODE PACKAGE PSR-164

1. NAME AND TITLE

TPASS: A Gamma-Ray Spectral Data-Reduction and Analysis Code System.

2. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; PDP-10.

4. NATURE OF PROBLEM SOLVED

TPASS is a collection of routines designed to assist data reduction of gamma-ray spectra obtained with a high-resolution detection system. It is intended to be used as a research tool to speed up data reduction and to present data in a manner which allows the researcher to determine the adequacy of the analysis.

5. METHOD OF SOLUTION

Using TPASS enables peaks in the spectrum to be identified, areas to be determined and corrected for detection efficiencies, and source identifications to be made, when possible, by comparisons with tabulated radionuclide decay data. Uncertainties assigned to peak area extractions are not derived from a "statistical" calculation but are determined from the estimated minimum continuum subtraction.

TPASS uses a direct comparison of E_{gamma} of the extracted data with tabulated values to indicate likely responsible radionuclides.

6. RESTRICTIONS OR LIMITATIONS

Up to 20 gamma-ray energies and branching ratios may be used for each identified radionuclide. The number of radionuclides is limited only by the contents of the data library which is used.

7. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for TPASS.

8. COMPUTER HARDWARE REQUIREMENTS

TPASS is operable on the PDP-10 computers.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

J. K. Dickens, "Radioactive Gamma-Ray Energy and Decay Branching Data," Informal note (June 1981).

J. K. Dickens, "TPASS, A Gamma-Ray Spectrum Analysis and Isotope Identification Computer Code," ORNL-5732 (March 1981).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source

code and sample problem input written in EBCDIC card images, plus output from the sample problem written in list format; total records 3811.

12. DATE OF ABSTRACT

April 1984.

KEYWORD: GAMMA-RAY SPECTRUM ANALYSIS

SECTION 3

UNFOLDING ANALYSIS CODES

These are programs designed to analyze gamma-ray pulse-height spectra obtained with a low-resolution detector, such as NaI or an organic scintillator. In most applications, the photon energy resolution is insufficient to resolve contributions to the measured spectra from photons having moderately different energies. These contributions would easily be identified in high-resolution Ge-detector data. This loss of resolution is usually compensated for by a substantial increase in efficiency.

Comments and assessments: as noted in the previous section, the computer codes usually evolve from some programmatic goal, involving a specific computer environment and/or a specific programming language. The compilers note that the quality of results is likely to be very dependent upon the adequacy of the user-supplied response matrix.

RSICC COMPUTER CODE PACKAGE PSR-169

1. NAME AND TITLE

ALPHA-M: Least-Squares Resolution of Gamma-Ray Spectra in Environmental Samples.

2. CONTRIBUTOR

Tennessee Valley Authority, Muscle Shoals, Alabama.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 360/370.

4. NATURE OF PROBLEM SOLVED

ALPHA-M is a standard least-squares computer program for analyzing gamma-ray spectral data obtained with NaI(Tl) scintillation detectors. This version of ALPHA-M has been prepared and tested to determine its capabilities and limitations for environmental monitoring. Either GEN4 or GENSTD is used to create standard libraries for ALPHA-M, and SIMSPEC is used to simulate spectra for ALPHA-M analysis.

5. METHOD OF SOLUTION

ALPHA-M determines the activities of radioisotopes by a weighted least-squares resolution of their gamma-ray spectra. The application of the least-squares method to gamma spectral data yields superior quantitative results as compared with any other commonly used technique:

1. Rapid data processing is possible.
2. Spectra with large statistical variations in counting can be handled.
3. The total spectrum, rather than just the photopeak regions, is used.
4. Spectra with superimposed peaks can be analyzed.
5. The standard error of the nuclide activity can be estimated.

6. RESTRICTIONS OR LIMITATIONS

Many gamma-ray emitting radionuclides can be quantified at activity levels of about 10 pico-Curies per liter or less, depending on counting time, at a confidence level of 95 percent.

7. TYPICAL RUNNING TIME

The sample problem input is a set of 3.5 liter water standards including 16 individual standard spectra for each of four 4" by 4" solid NaI crystals. The nuclide spectra are background stripped and the average background is an average of ten 4000-second backgrounds. The unit 5 input consists of a typical 3.5 liter water background spectrum and the spectrum from a 3.5 liter water cross-check from EPA. This problem took 7.73 cpu seconds on the IBM 370/3033.

8. COMPUTER HARDWARE REQUIREMENTS

On the IBM 370/3033 the sample problem required 196 K in the GO step.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler and an Assembler language compiler are required.

10. REFERENCE

L. G. Kanipe, S. K. Seale, and W. S. Ligget, "Least-Squares Resolution of Gamma-Ray Spectra

in Environmental Samples," TVA/EP-78/02, EPA-600/7-77-089, August 1977.

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 8154.

12. DATE OF ABSTRACT

January 1982.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS

RSICC CODE PACKAGE PSR-053

1. NAME AND TITLE

CONFOLD: Least-Structure Unfolding Code System for Measured Neutron and Gamma-Ray Spectra.

2. CONTRIBUTOR

Los Alamos National Laboratory, Los Alamos, New Mexico.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; CDC 6600 (A), IBM 360/370 (B).

4. NATURE OF PROBLEM SOLVED

CONFOLD solves integral equations of the first kind, subject to constraints on the structure of the solution.

5. METHOD OF SOLUTION

CONFOLD unfolds smooth, continuous spectra using a method called "least structure analysis."

6. RESTRICTIONS OR LIMITATIONS

It is necessary to use the correct uncertainties for the data and to use accurate response functions. Because no provision is made for including uncertainties in the response functions, it is important to determine how such uncertainties affect the unfolding and then to include them in the uncertainties assigned to the data.

7. TYPICAL RUNNING TIME

CONFOLD runs in a few seconds on the CDC 6600 computer.

8. COMPUTER HARDWARE REQUIREMENTS

CONFOLD is operable on the CDC 6600 computer. It requires about 13,000 words of storage for cases with 156 pulse-height channels and 21 response functions.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV and Assembler language compiler is required.

10. REFERENCE

A. A. Robba and L. R. Veaser, "A Least-Structure Unfolding Code," LA-5088 (November 1972).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in BCD/EBCDIC card images, plus output from the sample problem written in list format; total records 710 (A) and 918 (B).

12. DATE OF ABSTRACT

January 1984.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING

RSICC CODE PACKAGE PSR-032

1. NAME AND TITLE

CUPED: Scintillation Spectrometer Polyenergetic Gamma Photon Experimental Distributions Unfolding Code.

CUPED is a much modified version of CUBED.

2. CONTRIBUTOR

NUS Corporation, Rockville, Maryland.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 360/75/91.

4. NATURE OF PROBLEM SOLVED

CUPED unfolds sodium-iodide (thallium-activated) scintillation spectrometer polyenergetic gamma photon experimental distributions. It is designed to analyze the combination bremsstrahlung and monoenergetic gamma radiation field of cylindrical radioisotope power generators.

5. METHOD OF SOLUTION

CUPED generates the detector system response matrix function and applies it to the monoenergetic spectral components discretely and to the bremsstrahlung iteratively. It corrects for iodine K X-ray escape, detector non-linearity, system drift, source decay, background, and detection efficiency. Results are presented in digital form for differential and integrated photon number and energy distributions and exposure dose.

The standard spectra are normalized with respect to photopeak pulse-height and area and their photopeaks subtracted to obtain normalized Compton continua. The response matrix vectors are determined at each energy by interpolating the normalized continua and computing the associated Gaussian photopeaks. The thus interpolated vectors are redistributed in pulse-height to correspond to the detector system energy response and to satisfy the requirements of the spectra to be unfolded. Quadratic interpolation of the normalized continua is carried out either directly for gamma photon energies < 0.6616 MeV or by a method of parts, described in this report, for energies > 0.6616 MeV.

6. RESTRICTIONS OR LIMITATIONS

None noted.

7. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for CUPED.

8. COMPUTER HARDWARE REQUIREMENTS

CUPED is operable on the IBM 360/75/91 computers.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

J. J. Steyn, U. Born, J. T. Strahl, and R. Huang, "Code CUPED: A Code to Unfold Scintillation Spectrometer Polyenergetic Gamma Photon Experimental Distributions," NUS-557 (September 1969).

J. J. Steyn and D. G. Andrews, "A Comprehensive System for Computer Gain Changing of Scintillation Spectra," *J. Nucl. Sci. Eng.* Vol. 35, No. 3 (March 1968) 394-403.

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in BCD/EBCDIC card images, plus output from the sample problem written in list format; total records 5014.

12. DATE OF ABSTRACT

November 1983.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING

RSICC CODE PACKAGE PSR-301
NEA CODE PACKAGE IAEA0961

1. NAME AND TITLE

DOMUS: A Program for Decomposing A Two-Dimensional Spectrum

2. CONTRIBUTOR

Joint Institute of Nuclear Research, Dubna, USSR, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; IBM PC/XT; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED

DOMUS was written for the purpose of decomposing a two-dimensional spectrum into its components. DOMUS is a two-dimensional version of UPEAK (PSR-300).

5. METHOD OF SOLUTION

The spectrum of nuclear reactions may be formally considered as a linear combination: $s(x,y) = \sum_{i=1,n} (f_i(x,y) + b(x,y) + e(x,y))$; where $f_i(x,y)$ is the i -th component of interest, $b(x,y)$ is the background and $e(x,y)$ is the statistical error with zero-valued mean and variance $d(x,y)$; $s(x,y)$ is the spectrum in two dimensions. Each measured component is regarded as a result of a transformation of its model $m(x,y)$. The background is described by a second order surface. The method of least squares is used to determine the parameters in the equation.

6. RESTRICTIONS OR LIMITATIONS

A maximum of 12 peaks in the spectrum interval can be used.

7. TYPICAL RUNNING TIME

At the NEA Data Bank, the sample problem took about 5 minutes on an IBM PC/AT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS

IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77 and uses RM Fortran Version 2.42 or higher compiler. The PLINK86 overlay linker is also necessary.

10. REFERENCE

"The Long Write Up of the Program FIND2+DOMUS," informal notes by V. B. Zlokazov, JINR, Dubna, USSR.

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2 MB) 5.25 inch diskette.

12. DATE OF ABSTRACT

February 1991.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE;
MICROCOMPUTER

RSICC CODE PACKAGE PSR-102
NEA CODE PACKAGE PSR-0102

1. NAME AND TITLE

FERDO/FERD: Multichannel Neutron and Gamma-Ray Spectrum Matrix Unfolding Code Systems.

2. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 3033.

4. NATURE OF PROBLEM SOLVED

FERDO and FERD solve the integral equation which relates a measured pulse-height distribution and associated uncertainties to the true energy spectrum of the incident radiation.

5. METHOD OF SOLUTION

FERDO uses the method of constrained least-squares and biased estimation to solve a discretized representation of the integral unfolding problem and to compute a 2-sigma confidence interval for the true energy spectrum. FERD improves the FERDO solution by iteratively modifying the biased estimator.

6. RESTRICTIONS OR LIMITATIONS

FERDO/FERD require accurate estimations of the actual detector response and the idealized detector response (normally the detector energy resolution). In-core memory requirements are roughly three times the size of the response matrix (number of rows times the number of columns) for FERDO and four times the size of the response matrix for FERD. Additionally, a scratch storage device must be specified for both FERDO and FERD.

7. TYPICAL RUNNING TIME

Running time depends most strongly on the size of the response matrix. An 87 x 88 matrix problem required 4.5 s of IBM 3033 CPU time for FERDO and 15.2 s for FERD.

8. COMPUTER HARDWARE REQUIREMENTS

FERDO/FERD is operable on the IBM 3033 computer.

9. COMPUTER SOFTWARE REQUIREMENT

FERDO/FERD uses the proprietary DISSPLA graphics software package available from ISSCO, San Diego, California. It has been successfully run on the IBM 3033 computer under control of the MVS-JES2 Operating System. A Fortran IV compiler is required.

10. REFERENCE

B. W. Rust, D. T. Ingersoll, and W. R. Burrus, "A User's Manual for the FERDO and FERD Unfolding Codes," ORNL/TM-8720 (September 1983).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 5,332.

12. DATE OF ABSTRACT

October 1983.

KEYWORDS: UNFOLDING; GAMMA-RAY SPECTRUM ANALYSIS

RSICC CODE PACKAGE PSR-273
NEA CODE PACKAGE PSR-0273

1. NAME AND TITLE

FERD-PC: Interactive Multichannel Neutron and Gamma-Ray Spectrum Matrix Unfolding Code System.

AUXILIARY ROUTINE

PLOTFERD: Interactive Graphics Program for FERD-PC.

2. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

Fortran 77 and Basic; IBM PC and compatibles.

4. NATURE OF PROBLEM SOLVED

FERD-PC solves the integral equation which relates a measured pulse-height distribution and associated uncertainties to the true energy spectrum of the incident radiation. FERD-PC is a modified version of FERD, which is included in PSR-102. Several changes were made to include an interactive binning code, a flux integration code, and a plotting utility.

5. METHOD OF SOLUTION

The FERD method uses constrained least-squares and biased estimation to solve a discretized representation of the integral unfolding problem and to compute a 2-sigma confidence interval for the true energy spectrum. The mathematical method of FERD-PC differs from FERD only in that FERD-PC assumes no uncertainty in the response matrix, while FERD allows additional uncertainty by means of an upper and lower response matrix.

6. RESTRICTIONS OR LIMITATIONS

FERD requires an accurate estimation of the actual detector response and the idealized detector response (detector resolution). The limit on the size of the response is highly dependent on available computer memory. A 68 x 55 response matrix requires a minimum of 360 kilobytes of computer memory.

7. TYPICAL RUNNING TIME

Running time depends most strongly on the size of the response matrix and the number of output files it generates. The sample problem used 212 seconds on an IBM PC/XT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS

FERD is operable on IBM PC or compatibles running DOS version 2.1 or later. A minimum of 360 K of available user memory is required, and a math coprocessor must be installed. FERD-PC has been run on DEC VAX II and IBM PS/2 computers. PLOTFERD requires a HP 7475A or equivalent plotter.

9. COMPUTER SOFTWARE REQUIREMENT

FERD-PC uses the Microsoft Fortran (Version 4.01) compiler, and the Microsoft Quickbasic

compiler was used for PLOTFERD.

10. REFERENCE

B. D. Rooney, "User's Manual For FERD-PC," ORNL/TM-11028 (April 1989).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one double-sided, double density (360 K) diskette containing the source code and sample problem input, plus output from the sample problem.

12. DATE OF ABSTRACT

June 1989.

KEYWORDS UNFOLDING; GAMMA-RAY SPECTRUM ANALYSIS

RSICC CODE PACKAGE PSR-085

1. NAME AND TITLE

NAISAP: Theory and Use of Gamma-Ray Spectrum Analysis Codes for NaI(Tl) Detectors.

2. CONTRIBUTOR

Japan Atomic Energy Research Institute, Tokai Research Establishment, Ibaraki-Ken, Japan.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; FACOM 230-60.

4. NATURE OF PROBLEM SOLVED

NAISAP analyzes the NaI(Tl) gamma-ray spectrum and other types of spectra to determine the energies and intensities of the peaks detected. The spectrum is plotted in option.

5. METHOD OF SOLUTION

The analysis is carried out by the photopeak method on the basis of the NaI(Tl) response function represented in an analytical form. The peak search is based on the first derivative method accompanied with various peak shape tests. The usual least squares method is adopted for resolving the complex of peaks. Values of the parameters for constructing the NaI(Tl) response are stored as data for two detector sizes: 1-3/4" ϕ x 2" and 3" ϕ x 3."

6. RESTRICTIONS OR LIMITATIONS

NAISAP accepts a spectrum of a maximum of 1024 channels with up to 49 peaks. Response functions of detectors with dimensions different from those mentioned above must be given by the user in specifying the parameters as functions of the photon energy.

7. TYPICAL RUNNING TIME

NAISAP requires approximately one second for the analysis of each peak.

8. COMPUTER HARDWARE REQUIREMENTS

NAISAP is operable on the FACOM 230-60 computer. A 76 K word memory is required. A CALCOMP plotter is optional.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

Hiroshi Baba, Toshiaki Sekine, Sumiko Baba, and Hiroshi Okashita, "A Method of the Gamma-Ray Spectrum Analysis: Fortran IV Programs 'BOB 73' for Ge(Li) Detectors and 'NAISAP' for NaI(Tl) Detectors," JAERI 1227 (June 1973).

Toshiaki Sekine, Sumiko Baba, Hiroshi Baba, "Analytical Functions Representing Response Functions of NaI(Tl) Detector Systems to Gamma Rays," ORNL-tr-2941/JAERI-M 4590 (September 1971).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 3927.

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS;
UNFOLDING

NEA CODE PACKAGE NEA 0487

NEA 0487 RADAK, MULTICHANNEL_ANALYSER N_SPECTRA & GAMMA_SPECTRA UNFOLDING
810619

1. NAME OR DESIGNATION OF PROGRAM. RADAK.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
RADAK	NEA 0487/01	CDC 7600	CDC 7600	T
RADAK	NEA 0487/02	IBM 370 series	IBM 370 series	T

3. NATURE OF PHYSICAL PROBLEM SOLVED.

RADAK unfolds flux spectra from the output of multi-channel and single-channel neutron or gamma ray detectors. The errors, including correlations, of the flux solution are estimated.

4. METHOD OF SOLUTION.

The solution is determined which maximises the likelihood of the observed measurements subject to the fluxes remaining positive. The errors are estimated using Monte Carlo, by taking random samples about the measurements.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.

Maximum number of -
spectra unfolded simultaneously - 10
detector channels - 200
flux groups - 60

6. TYPICAL RUNNING TIME.

3 minutes CPU for unfolding (with error analysis) the output from 5 proportional counters and 3 threshold detectors at 3 positions. 60 flux groups were used, and a total of 76 channels.

7. UNUSUAL FEATURES OF THE PROGRAM.

The output from several multi-channel and single-channel detectors may be analysed simultaneously to produce a single-valued flux solution. Allowance may be made for the uncertainties in the detector response functions.

8. RELATED AND AUXILIARY PROGRAMS.

The program package also contains two auxiliary programs, PRC and NE213, which generate response matrices respectively for gas-filled spherical proportional counters and NE213 organic liquid scintillation spectrometers. The NE213 program may also be used for grouping or differentiating the counts from any type of spectrometer in preparation for input to RADAK. Several routines from the Harwell subroutine library are included.

9. STATUS

NEA 0487/01 : Arrived at NEADB
 : in preparation
 : Tested at NEADB
NEA 0487/02 : Arrived at NEADB
 : in preparation
 : Tested at NEADB

10. REFERENCES.

NEA 0487/01 :
- M.J. Grimstone: The RADAK Users Manual AEEW-M1455 (December 1976)
- M.J. Grimstone: Improved Facilities for Response Matrix Adjustment in RADAK AEEW-M1483 (July 1977)
- J. Patry: Three Programs for the Calculation of Flux Spectra from the Output of Neutron or Gamma-ray Detectors: PRC, NE213 and RADAKA TM-RZ-58/2 (December 7, 1978)
NEA 0487/02 :
- M.J. Grimstone: The RADAK Users Manual AEEW-M1455 (December 1976)
- M.J. Grimstone: Improved Facilities for Response Matrix Adjustment in RADAK AEEW-M1483 (July 1977)

11. MACHINE REQUIREMENTS.

The program requires 350 kbytes of code storage.

12. PROGRAMMING LANGUAGE USED

NEA 0487/01 : FORTRAN+ASSEMBLER
NEA 0487/02 : FORTRAN+ASSEMBLER

13. OPERATING SYSTEM OR MONITOR UNDER WHICH PROGRAM IS EXECUTED.

IBM 370 O.S. MVS.

14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.

15. NAME AND ESTABLISHMENT OF AUTHOR.

Mr. M.J. Grimstone
UKAEA
Atomic Energy Establishment
Winfrith
Dorchester, Dorset
United Kingdom.

16. MATERIAL AVAILABLE

NEA 0487/01 :
Report: AEEW-M1483 (July 1977)
Report: AEEW-M1455 (December 1976)
Report: TM-RZ-58/2 (December 7, 1978)
SOURCE (F4,ASSEMBLER) 2541 records
SAMPLE INPUT DATA 723 records
SAMPLE OUTPUT 2190 records
PRC (CAL. OF RESPONSE MATRIX FOR RADAK) 1232 records
SAMPLE INPUT FOR PRC 46 records
SAMPLE OUTPUT OF PRC 237 records
NE213 (PREPARATION OF RESPONSE MATRIX) 1042 records
SAMPLE INPUT FOR NE213 22 records
SAMPLE OUTPUT OF NE213 848 records
FEHLIM (COMPUTATION OF ERROR FUNCTION) 13 records

NEA 0487/02 :
Report: AEEW-M1483 (July 1977)
Report: AEEW-M1455 (December 1976)
INFORMATION 2 records
PRC ASSEMBLER ROUTINES 75 records
PRC F4 SOURCE EBCDIC 1782 records
PRC SAMPLE PROBLEM INPUT 14 records
PRC SAMPLE PROBLEM OUTPUT 764 records
NE213 ASSEMBLER ROUTINES 161 records
NE213 F4 SOURCE EBCDIC 1883 records
NE213 SAMPLE PROBLEM INPUT 41 records
NE213 SAMPLE PROBLEM OUTPUT 183 records
RADAK ASSEMBLER ROUTINES 267 records
RADAK F4 SOURCE EBCDIC 3239 records
RADAK SAMPLE PROBLEM INPUT 624 records
RADAK SAMPLE PROBLEM OUTPUT 6331 records
JCL AND INFORMATION 100 records

17. CATEGORY = O ,

KEYWORDS Monte Carlo method

gamma spectra
multi-channel analysers
neutron detectors
neutron flux
neutron spectra
spectra unfolding
spectrometers

NEA CODE PACKAGE ESTS0827

ESTS0827 UNSPEC,X-RAY SPECTRUM UNFOLDING 960430

1. NAME OR DESIGNATION OF PROGRAM - UNSPEC (Unfolding X-Ray Spectrums).

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
UNSPEC	ESTS0827/01	CRAY 1	CRAY 1	A

3. DESCRIPTION OF PROGRAM OR FUNCTION

UNSPEC is used to solve the problem of unfolding an observed X-ray spectrum given the response matrix of the measuring system and the measured signal valued.

4. METHOD OF SOLUTION

UNSPEC uses an iterative technique to solve the unfold problem. Qualitatively, the solution proceeds as follows: 1. Choose a trial spectrum consistent with the experiments criterion for smoothness, 2. Fold this spectrum with the known response matrix, 3. Compare the measured and calculated signal values, 4. Adjust the trial spectrum in order to improve the agreement between the measured and calculated signal values, 5. Repeat steps 1-4 until the final result is consistent with the measured signal values to some arbitrary criterion selected by the experimenter.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

6. TYPICAL RUNNING TIME

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

ESTS0827/01 : Known to NEADB
 : Requested by NEADB
 : Arrived at NEADB

10. REFERENCES

ESTS0827/01 :
- H.F. Finn:
 UNSPEC Reference Manual version 10/29/82
 UCID-19616 (December 1, 1982)

11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

ESTS0827/01 : LLNL-FORTRAN

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

Machine dependent.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

H.F. Finn

Lawrence Livermore National Lab., CA (United States)

16. MATERIAL AVAILABLE

ESTS0827/01 :

UNSPEC.SUB Source code

UNSPEC.CAR Sample problem (cards)

UNSPEC.SOC Sample problem (sock)

Report: UCID-19616 (December 1, 1982)

17. CATEGORY = O , W ,

KEYWORDS

gamma detectors

radiation detectors

spectra unfolding

x-rays

RSICC CODE PACKAGE PSR-300
NEA CODE PACKAGE IAEA0959

1. NAME AND TITLE

UPEAK: A Program for Decomposing A One-Dimensional Spectrum

2. CONTRIBUTOR

Joint Institute of Nuclear Research, Dubna, USSR, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; IBM PC/XT; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED

UPEAK was written for the purpose of decomposing a one-dimensional spectrum into its components.

5. METHOD OF SOLUTION

The spectrum of nuclear reactions may be formally considered as a linear combination: $s(x) = \sum_{i=1}^n (f_i(x) + b(x) + e(x))$; where $f_i(x)$ is the i -th component of interest, $b(x)$ is the background and $e(x)$ is the statistical error with zero-valued mean and variance $d(x)$; $s(x)$ is the spectrum. Each measured component is regarded as a result of a transformation of its model $m(x)$. Regression analysis is used to determine the least squares estimates of some of the parameters.

6. RESTRICTIONS OR LIMITATIONS

A maximum of 20 components in the spectrum interval can be used.

7. TYPICAL RUNNING TIME

At the NEA Data Bank, the sample problem took about 4 minutes on an IBM PC/AT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS

IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77 and uses RM Fortran Version 2.42 or higher compiler. The PLINK86 overlay linker is also necessary.

10. REFERENCES

"The Long Write Up of the Program UPEAK," informal notes by V. B. Zlokazov, JINR, Dubna, USSR.

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2 MG) 5.25 inch diskette.

12. DATE OF ABSTRACT

February 1991.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE;
MICROCOMPUTER

SECTION 4

MODEL PREDICTIONS OF PHOTON YIELDS

In this section are listed programs to predict photon yields. These computer codes are all based on compound-nucleus/statistical model formalisms; they also indicate that photon production is included in the calculations.

Programs of the inventory type, for example ORIGEN¹, are not listed in this compilation. However, in the next section is listed the program GABAS which can be used to interface with the output of an inventory code to calculate time-dependent photon spectra.

Also, we do not list Optical-Model analysis programs or other programs using direct-interaction calculations. The underlying theories for these programs are designed to predict angular distributions of outgoing nucleons or heavy ions and not for photon production.

It should be noted that the Information Centers have other programs of the statistical-model/compound-nucleus type but which do not indicate photon-production computations in the abstracts of the programs. Some of these other programs are:

CEM95	RSICC Code Package PSR-357; NEA Code Package IAEA1247;
COMNUC3B	RSICC Code Package PSR-302
HAUSER*5	RSICC Code Package PSR-152
NX1-NX2	RSICC Code Package PSR-310; NEA Code Packages IAEA0918 and IAEA0919;
PREANG	RSICC Code Package PSR-166
PREM	RSICC Code Package PSR-224; NEA Code Package NEA 0888;
SPECTER	RSICC Code Package PSR-023
STAPRE-H	RSICC Code Package PSR-325;

REFERENCE

¹ORIGEN2.1, RSICC Code Package CCC-371; A. G. Croff, "A User's Manual for the ORIGEN2 Computer Code," ORNL/TM-7175 (July 1980); A. G. Croff, "ORIGEN2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials," *Nucl. Technol.*, **62**, 335 (September 1983).

RSICC CODE PACKAGE PSR-146

1. NAME AND TITLE

ALICE-91: Statistical Model Code System with Fission Competition.
ALICE-87: Revised ALICE for Personal Computer.
ALISO-PC: Gives Isotopically Weighted Results.

2. CONTRIBUTORS

Lawrence Livermore National Laboratory, Livermore, California.
International Atomic Energy Agency, Vienna, Austria, through the Nuclear Energy Agency Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; Cray XMP (P00146CYOMP00), IBM PC (P00146PCAT00), SUN (P00146SUN0401).

4. NATURE OF PROBLEM SOLVED

Several types of calculations and combinations can be performed including a standard Weisskopf-Ewing evaporation with multiple particle emission, s-wave approximation to give an upper limit to the enhancement of gamma-ray deexcitation due to angular momentum effects, and an evaporation calculation that can include fission competition via the Bohr-Wheeler approach. ALICE91 calculates precompound decay via Hybrid and GDH models with multiple precompound decay algorithms, single and double differential spectra, and reaction product cross sections.

5. METHOD OF SOLUTION

ALICE/85/300 and later revisions of the ALICE/LIVERMORE 82 computer code do precompound, compound/statistical fission calculations in the general framework of the Weisskopf-Ewing evaporation model, the Bohr-Wheeler transition state model for fission, and the hybrid/geometry dependent models for precompound decay. ALICE/85/300 allows a variable energy mesh size, excitation energies up to 300 MeV, and incorporates several other improvements in calculational approaches.

ALICE91 includes options for shell dependent level densities, and an option to use systematics for angular distribution. The new version also includes gamma-ray competition with particle decay modes.

The IBM PC version (B) was converted from mainframe ALICE-87, which is a revision of ALICE/85/300. Input default options were included in this version. Refer to comments in the file ALICE1.FOR for information on modifications. ALISO differs only in that it will do calculations for natural isotopic targets, giving weighted results at the end.

The Sun version was converted from ALICE-91 that was released in April, 1991. This version differs from earlier releases in the following ways: 1) Level density options due to Katoria/Ramamurth may be selected.; 2) Level density options due to Ignatyuk may be selected.; 3) The systematics expressions for precompound angular distributions of C. Kalbach are an option. (These are faster than the option based on n-n scattering kinematics and agree more with experimental results).; 4) Gamma-ray spectra are given for the reactions, and gamma rays compete with nucleon emission (Mitigates problems with trapped protons for very proton rich nuclei.); 5) This version may be used to calculate for isotopically mixed targets (e.g. natural isotopic composition).

6. RESTRICTIONS OR LIMITATIONS

Users must refer to comments in the Fortran source files for input instructions and information. If running the PC version on 32-bit word-length machines, remove CXXXXX from double precision

statements for POW and GAM.

7. TYPICAL RUNNING TIME

The sample input took about 6 seconds of CPU time on the Cray XMP under UNICOS. The sample case for ALICE-87 took 23 minutes on an IBM PC/XT running at 4.7 megahertz with a math co-processor. The ALISO case took 4 minutes on the same computer.

8. COMPUTER HARDWARE REQUIREMENTS

Version A is operational on the Cray XMP, and Version B has run on both IBM PC/XT and /AT computers with math co-processors. Memory requirements for the executable modules on an IBM PC/AT are: 530 K (ALICE) and 525 K (ALISO). Version C is operational on Sun workstations.

9. COMPUTER SOFTWARE REQUIREMENTS

The Cray/CTSS version used the CIVIC compiler and the Cray/UNICOS version used the CFT77 compiler. For ALICE-87 IBM Professional Fortran Version 1.0 was used, and for ALISO, Microsoft's Fortran 4.01 was used. The Sun version was tested with the SC1.0 f77 compiler. The code was tested on a Sun SPARCstation SLC under SunOS 4.1.1 using SUN FORTRAN v1.4. The code was also tested on a Sun SPARCstation 2 under SOLARIS 2.3 (Sun 5.3) using SUN FORTRAN 2.0.

10. REFERENCES

a. Included in the documentation:

- M. Blann, "CODE ALICE/85/300," UCID-20169 (September 1984).
- M. Blann and J. Bisplinghoff, "CODE ALICE/LIVERMORE 82," UCID-19614 (November 1982).
- R. Roussin, Informal Input Instructions for ALICE/85/300 (February 1987).
- M. Blann and H. K. Vonach, "Global Test of Modified Precompound Decay Models," *Physical Review C*, 28(4), 1475-1492 (October 1983).
- D. E. Cullen and V. Goulo, "Precompound Nuclear Model Code Version for Personal Computer IBM/AT," Informal notes on PC implementation (May 1988).
- M. Blann, "Recent Progress and Current Status of Preequilibrium Reaction Theories and Computer Code ALICE," UCRL-JC-109052 (Preprint)(November 21, 1991).

b. Background information:

- M. Blann, "Recent Progress and Current Status of Pre-equilibrium Reaction Theories and Computer Code ALICE," in *SMR/284-1, ICTP Workshop on Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications* held in Trieste, Italy (February-March, 1988, and February-March, 1992).
- M. Blann, "Multiple Pre-equilibrium Decay Processes," UCRL-97778, from the NEANDC Specialists' Meeting on Pre-equilibrium Nuclear Reactions held in Semmerling, Austria (February 1988).
- Jens Bisplinghoff, "Configuration Mixing in Pre-equilibrium Reactions: A New Look at the Hybrid-Exciton Controversy," *Physical Review C*, 33(5), 1569-1580 (May 1986).
- M. Blann and J. Bisplinghoff, "Numerical Test of Approximations in the Hybrid Precompound Decay Model," *Atomic Nuclei*, 326, 429-434 (1987).
- M. Blann and T. T. Komoto, "Precompound Evaporation Analyses of Excitation Functions for (α ,xn) Reactions," *Physical Review C*, 29(5), 1678-1683 (May 1984).
- G. Reffo, M. Blann, B. A. Remington, "On the Origin of Medium Energy Gamma-Rays in Nuclear Reactions," UCRL-97866, Preprint submitted to *Physical Review C* (December 1987).
- M. Blann, W. Scobel, and E. Plechaty, "Precompound Nucleon Angular Distributions in the

Continuum," *Physical Review C*, 30(5), 1493-1508 (November 1984).

M. Blann, G. Reffo, F. Fabbri, "Calculation of Gamma-Ray Cascades in Code ALICE," UCRL-55374, Preprint submitted to *Nuclear Instruments and Methods* (September 1986).

F. Plasil, "ORNL ALICE: A Statistical Model Computer Code Including Fission Competition," ORNL/TM-6054, (November 1977).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents (a), the ALICE-91 source code, sample input and output for version A. Version B includes both the ALICE-87 and ALISO codes. Each package is available on one DS/HD (1.2MB) diskette in DOS format. The SUN version is alternately available on one DS/HD (1.44MB) diskette in UNIX tar format.

12. DATE OF ABSTRACT

February 1987, revised July 1989, June 1991, June 1994, October 1994.

KEYWORDS: NUCLEAR MODELS; WORKSTATION; MICROCOMPUTER

RSICC CODE PACKAGE PSR-316

1. NAME AND TITLE

CASTHY: Statistical Model Calculation for Neutron Cross Sections and Capture Gamma-Ray Spectra.

2. CONTRIBUTOR

Japan Atomic Energy Research Institute, Tokai-mura, Japan.

3. CODING LANGUAGE AND COMPUTER/OPERATING SYSTEM

Fortran 77, FACOM computers and IBM RISC 6000.

4. NATURE OF PROBLEM SOLVED

This code has been utilized as a tool for nuclear data evaluations. It is used to calculate neutron cross sections of total, shape elastic scattering and compound nucleus formation with the optical model, and compound elastic scattering, inelastic scattering and capture cross sections by the statistical model applying Hauser-Feshbach and/or Moldauer formula. The other cross sections such as the $(n,2n)$, (n,p) , (n,f) reactions are treated as cross sections of competing processes, and their sum is given through input data. This code calculates also capture gamma-ray spectra. Branching ratio for primary transition can be treated in a particular way, if necessary.

5. METHOD OF SOLUTION

The total transmission coefficient is modified so that the total reaction cross section obtained by using the optical model may be conserved. The transmission coefficients for neutrons and gamma-rays are rewritten by considering an effect of $(n,\text{gamma}-n')$ process.

6. RESTRICTIONS OR LIMITATIONS

For the normalization of cross section, the normalization energy point should be included in the incident energy points of input data. Some other limitations exist depending on options.

7. TYPICAL RUNNING TIME

On an IBM RISC system 550, sample problems 1, 2, and 3 took 14.6, 15.8 and 86.9 seconds respectively.

8. COMPUTER HARDWARE REQUIREMENTS

The code was developed on the FACOM computers and tested on the IBM RISC 6000.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77 and tested using the xlf Fortran compiler under the AIX 3.1 operating system on the IBM RISC 6000.

10. REFERENCE

S. Igarasi and T. Fukahori, "Program CASTHY - Statistical Model Calculation for Neutron Cross Sections and Gamma Ray Spectrum," JAERI-1321 (March 1991).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2MB) 5.25-in. diskette which includes the source files, sample input and output.

12. DATE OF ABSTRACT

September 1992.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; NEUTRON; NUCLEAR MODELS;
PARAMETRIC MODELS

RSICC CODE PACKAGE PSR-292

1. NAME AND TITLE

EMPIRE: A Pre-equilibrium Compound Nuclear Model Code For Personal Computers

2. CONTRIBUTOR

Institute of Nuclear Studies, Warsaw, Poland through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED

EMPIRE calculates spectra and cross sections for capture and/or multistep nuclear reactions in the frame of a combined pre-equilibrium and compound nucleus mechanism model.

5. METHOD OF SOLUTION

Angular momentum conservation is observed throughout the whole calculation. The decay of the compound nucleus is treated either in terms of the HRTW theory, to account for the width fluctuation effects, or in terms of standard Hauser-Feshbach theory if many open particle channels cause the fluctuations to cancel. The transmission coefficients of the nuclear potential are calculated with an optical model subroutine. The full gamma cascade is included in the calculations providing the gamma spectra and populations of the discrete levels in the residual nuclei.

6. RESTRICTIONS OR LIMITATIONS

The particles considered in the code are neutrons, protons and alphas. The energy discretization of the continuum is confined to 120 points. The maximum number of partial waves is 30.

7. TYPICAL RUNNING TIME

The sample input problems (test cases 1 and 2) were run at NEA Data Bank on an IBM PC/AT with a math coprocessor. With the PROFORT compiler, problem 1 took 15 minutes, 8 seconds; problem 2 took 32 minutes, 3 seconds. With the RM/Fortran compiler, problems 1 and 2 took 8 minutes, 48 seconds and 21 minutes, 55 seconds respectively.

8. COMPUTER HARDWARE REQUIREMENTS

EMPIRE runs on an IBM PC/AT with a math coprocessor.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77. The NEA Data Bank used IBM Professional Fortran version 1.0 and the RM/Fortran compiler, version 2.42 under the MS-DOS 3.20 operating system.

10. REFERENCE

A. Marcinkowski, "EMPIRE - Pre-equilibrium/Compound Nuclear Model For Personal Computer," IAEA-NDS-95, NEA Data Bank, France, June 2, 1988.

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2 MB) 5.25-inch diskette.

12. DATE OF ABSTRACT

November 1990.

KEYWORDS: MICROCOMPUTER; NUCLEAR MODELS; NEUTRON; PROTON

RSICC CODE PACKAGE PSR-219

1. NAME AND TITLE

ERINNI: Optical Model Calculation of Multiple Cascading Particle Emissions.

2. CONTRIBUTOR

Centro di Calcolo del CNEN, Bologna, Italy, through the NEA Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 360/370.

4. NATURE OF PROBLEM SOLVED

ERINNI offers an optical model calculation of multiple cascading particle emissions. It computes 42 cross sections for each incident energy representing all possible compound nucleus processes of types (x,a) , (x,ab) , and (x,abc) where x can be indifferently a neutron, proton, or alpha particle; a and b can be a neutron, a proton, an alpha or gamma particle; and c can be a neutron or a gamma particle. ERINNI is particularly useful for extensive cross section calculations such as those in the range of reactor calculation needs.

5. METHOD OF SOLUTION

The scattering amplitudes and the other optical model quantities are calculated in accordance with spherical local potentials by the usual methods.

Parameters are needed for 10 residual nuclei, hence particular care was devoted to reducing the input procedure. The table for pairing energies, the Mass excess table, the level density data systematics, and the optical model parameter sets most frequently used in literature are all incorporated in the program and can be used optionally as an alternative to more specific choices of data.

6. RESTRICTIONS OR LIMITATIONS

No width fluctuation is included because it is devised for high energy calculations.

7. TYPICAL RUNNING TIME

The OECD NEA Data Bank executed the test case included in the package on an IBM 3084Q computer in 375 seconds of CPU time. Computing time was reduced because the various optical model transmission coefficients and consequent decay probabilities at a given incident energy, when they are calculated within appropriately narrow energy intervals, lend themselves to interpolation.

8. COMPUTER HARDWARE REQUIREMENTS

ERINNI is operable on the IBM 360/370 computers. 240 kbytes of fast core memory is required if used together with the overlay structure.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCE

F. Fabbri and G. Reffo, "ERINNI: An Optical Model Fortran IV Code for the Calculation of Multiple Cascading Particle Emissions," RT/FI(77)4 (April 1977).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images; total records 2914.

12. DATE OF ABSTRACT

June 1986.

KEYWORD: NUCLEAR MODELS

RSICC CODE PACKAGE PSR-305

1. NAME AND TITLE

EXIFON-GAMMA: A Model For Statistical Multistep Direct and Multistep Compound Reactions

2. CONTRIBUTOR

Technische Universität Dresden, Germany, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; IBM PC/XT; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED

EXIFON-GAMMA predicts emission spectra for neutrons, protons, alphas, and photons including equilibrium, pre-equilibrium, direct as well as multiple particle emission processes.

5. METHOD OF SOLUTION

The model is based on random matrix physics with the use of the Green's function formalism. All calculations are performed without any free parameters. Results are presented for bombarding energies below 30 MeV.

6. RESTRICTIONS OR LIMITATIONS

None noted.

7. TYPICAL RUNNING TIME

The sample problem (as listed in RUN.BAT, using the FE56 data) took about 50 seconds on an IBM PC/AT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS

IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77 and uses RM Fortran Version 2.42 or Microsoft Fortran Version 4.01.

10. REFERENCE

H. Kalka, "EXIFON-GAMMA," INDC(GDR)-601L, Technische Universität Dresden, Germany, (August 1990).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2 MB) 5.25 inch diskette.

12. DATE OF ABSTRACT

March 1991.

KEYWORDS: MICROCOMPUTER; NEUTRON; NUCLEAR MODELS; PROTON

RSICC CODE PACKAGE PSR-125

1. NAME AND TITLE

GNASH-FKK: Pre-equilibrium, Statistical Nuclear-Model Code System for Calculation of Cross Sections and Emission Spectra.

AUXILIARY CODE

SEARCH3: Operates on the output of the FKK-GNASH code to produce ENDF/B-formatted cross section records.

DATA LIBRARY

STRUCTURE.DAT: Nuclear level energies, spins, parities, and gamma-ray branching ratios.

TRANS.COEF: Particle transmission coefficients from spherical or deformed optical model calculations.

MASS.DAT: Table of ground-state masses, spins, and parities.

2. CONTRIBUTOR

Los Alamos National Laboratory, Los Alamos, New Mexico.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; Cray (P00125/CY000/02).

4. NATURE OF PROBLEM SOLVED

GNASH provides a flexible method by which reaction and level cross sections, isomer ratios, and emission spectra (neutron, gamma-ray, and charged-particle) resulting from particle- and photon-induced reactions can be calculated. The September 1991 release of GNASH incorporated an additional option for calculating gamma-ray strength functions and transmission coefficients by including the Kopecky-Uhl model⁴. In addition, improvements were made to the output routines, particularly regarding gamma-ray strength function information. Major improvements in the 1995 FKK-GNASH release include added capabilities: to read in externally calculated preequilibrium spectrum from, e.g., Feshbach-Kermin-Koonin theory, to do multiple preequilibrium calculations, to calculate appropriate spin distributions for nuclear states formed in preequilibrium reactions, and to do incident-photon calculations. Additional improvements are noted in the READ.ME file.

5. METHOD OF SOLUTION

GNASH uses Hauser-Feshbach theory to calculate complicated sequences of reactions and includes a pre-equilibrium correction for binary tertiary channels. Gamma-ray competition is considered in detail for every decaying compound nucleus. A multi-humped fission barrier model is included for fission cross-section calculations. Three options for level densities are available.

6. RESTRICTIONS OR LIMITATIONS

In its present configuration, each calculation can handle decay sequences involving up to 38 compound nuclei and each decaying compound nucleus can emit a maximum of 5 types of radiation (neutrons, gamma rays, protons, alphas, etc.). Angular-momentum effects and conservation of parity are included explicitly. Each residual nucleus in a calculation can contain up to 78 discrete levels whereas its continuum region can be represented by up to 204 energy bins. The incident-particle types that are permitted are neutrons, protons, deuterons, tritons, ³He, and ⁴He. Angular distributions are not

calculated; i.e., isotropy is assumed in the center-of-mass (c.m.) system. Angular distribution effects can be added in postprocessing utility codes making use of, for example, Kalbach-Mann systematics.

7. TYPICAL RUNNING TIME

The running times typically range from a few seconds to a few minutes per incident energy depending upon incident particle energy, mass range of the target, number of compound nuclei included, and the energy bin width that is used.

8. COMPUTER HARDWARE REQUIREMENTS

GNASH was developed originally on the CDC 6600 and 7600 computers and is now maintained on Cray. It requires 3,500,000 words of storage in its present configuration. Storage requirements may be reduced by changing the value of 'nkdim' and other parameters in a PARAMETER statement. The current value for nkdim is 204 energy bins.

9. COMPUTER SOFTWARE REQUIREMENTS

The codes run on Cray computers under the UNICOS operating system. The gnash and search3 Fortran sources call routines which are Cray specific, but they can be ported to other Unix systems. Calls to filerep and qstart equate internal and external file names and may be removed. Substitutions need to be supplied for "date" and "second" which retrieve calendar data and time of day. Two "encode" statements in search3 may need to be changed.

10. REFERENCES

a. included in documentation:

P. G. Young, README (January 1996).

P. G. Young, M. B. Chadwick, "Code Input Description, Version T2/PGYC/93GNASH/GN7SRC (Update 12)" (January 6, 1996).

P. G. Young, E. D. Arthur, M. B. Chadwick, "Comprehensive Nuclear Model Calculations: Introduction to the Theory and Use of the GNASH Code," LA-12343-MS (July 1992).

b. background information:

J. Kopecky and M. Uhl, "Test of Gamma-Ray Strength Functions in Nuclear Model Calculations," *Phys. Rev. C* 41, 1941 (1990).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and one 3.5-in. DS/HD (1.44 MB) diskette containing the source code, data libraries, sample problem input and output in either compressed tar or DOS format.

12. DATE OF ABSTRACT

March 1984, revised June 1988, March 1989, September 1991, December 1992, January 1996.

KEYWORD: NUCLEAR MODELS

RSICC CODE PACKAGE PSR-336

1. NAME AND TITLE

PEGAS: Pre-Equilibrium-Equilibrium Gamma-and-Spin Code System.

2. CONTRIBUTORS

Institute of Physics, Slovak Academy of Sciences, Bratislava, Czechoslovakia through the NEA Data Bank, Issy-les-Moulineaux, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; IBM PC and compatibles.

4. NATURE OF PROBLEM SOLVED

PEGAS is a pre-equilibrium-equilibrium gamma-and-spin code, based on the unified model of nuclear reactions. Therein, the equilibrium (compound-nucleus) emission is treated as an organic part of the pre-equilibrium emission. The code has two important novel features: the angular-momentum couplings are correctly taken into account for all processes (equilibration, particle and gamma emission), and nucleon as well as gamma emissions are calculated with all possible cascades for all possible sequences of the ejectiles. PEGAS addresses the lack of possibilities, with currently existing codes, to trace a complete development of the reaction system including the consistent treatment of cascade emissions (e.g., the pre-equilibrium emission is often limited to the primary particle only). PEGAS also provides a full treatment of angular momentum conservation.

5. METHOD OF SOLUTION

Master equations of the exciton model are solved by the algorithm of Chatterjee and Gupta. Gamma emission is according to Oblozinsky. The general philosophy of the PEGAS code is derived from the nonspin version named PEQAG.

6. RESTRICTIONS OR LIMITATIONS

The present version of PEGAS is designed for reactions induced by nucleons, though other projectiles are allowed as well, leading to the composite system with the excitation energy not exceeding 30 MeV and with nuclear spins limited to $< 15\hbar$. The limitations in spin, energy, and number of successive nucleons may be shifted by adjusting the dimensions of the array.

7. TYPICAL RUNNING TIME

Sample problem execution time:
(on a Northgate 486/66) 9 minutes 43 seconds

8. COMPUTER HARDWARE REQUIREMENTS

PEGAS runs on an IBM PC or compatible with at least 578K of RAM (recommended) for compilation and linking and at least 520K for execution. Approximately 3.5 MB of free disk space is required for execution because the disk is used for temporary file swapping.

9. COMPUTER SOFTWARE REQUIREMENTS

PEGAS runs under DOS. The MS Fortran 5.0 compiler was used to create the executable included in the package.

10. REFERENCE

E. Betak and P. Oblozinsky, "PEGAS Pre-Equilibrium-Equilibrium Gamma-And-Spin Code (PC version)," Slovak Academy of Sciences unpublished report (October 1992).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and 1 DS/HD 5.25-in. (1.2 MB) diskette which contains the source code, executable, sample input/output, and a README.RSI file which describes the installation and operation of PEGAS.

12. DATE OF ABSTRACT

September 1993.

KEYWORDS: NUCLEAR MODELS; MICROCOMPUTER

RSICC CODE PACKAGE PSR-293

1. NAME AND TITLE

PEQAG-2: A Pre-equilibrium Computer Code With Gamma Emission

2. CONTRIBUTOR

Institute of Physics, Bratislava, Czechoslovakia, through IAEA, Vienna, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED

PEQAG-2 performs an exciton model calculation of angle-integrated nucleon and gamma energy spectra. All the emissions are treated consistently within the pre-equilibrium approach based on the master equations of the model. Multiple particle and/or multiple gamma emissions are included.

5. METHOD OF SOLUTION

Angle-integrated energy spectra of neutrons, protons and gammas, as well as the corresponding integrals are computed. No angle-dependent or spin-dependent calculations are included. The state density used is the equidistant-spacing model in the finite potential well. Inverse cross sections may be supplied by the program according to the approximation of Chatterjee et al, and the GDR shape is also built-in.

6. RESTRICTIONS OR LIMITATIONS

Up to four nucleons are emitted and interspersed and/or preceded by arbitrary number of gammas. The maximum energy is 100 times the energy step used.

7. TYPICAL RUNNING TIME

The sample input problem was run at NEA Data Bank on an IBM PC/AT with a math coprocessor. The problem took 8 minutes and 50 seconds.

8. COMPUTER HARDWARE REQUIREMENTS

PEQAG-2 runs on an IBM PC/AT with a math coprocessor.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77. The NEA Data Bank used Microsoft Fortran version 5.0 and the RM/Fortran compiler, version 2.42 under the MS-DOS 3.20 operating system.

10. REFERENCE

E. Betak, "PEQAG2: An Updated PC Version of Fully Pre-Equilibrium Computer Code With Gamma Emission," IAEA1185, NEA Data Bank, France, December 13, 1989.

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2 MB) 5.25-inch diskette.

12. DATE OF ABSTRACT

November 1990.

KEYWORDS: GAMMA RAY SOURCE ANALYSIS; MICROCOMPUTER; NUCLEAR
MODELS; NEUTRON; PROTON

RSICC CODE PACKAGE PSR-298

1. NAME AND TITLE

TNG1: A Multistep Statistical Model Based on the Hauser-Feshbach Theory For The Evaluation Of Neutron Data.

2. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; VAX 6000.

4. NATURE OF PROBLEM SOLVED

The TNG1 code is a multistep statistical model based on the Hauser-Feshbach theory including width-fluctuation corrections and pre-compound effects. Statistical model calculations are frequently performed for medium and heavy nuclei.

5. METHOD OF SOLUTION

The Hauser-Feshbach part of the TNG1 code is multi-step, but angular distribution can be calculated only for the binary step. The pre-compound portion is single step, in this case angular distribution is calculated on the basis of partial wave interference (partial relaxation of the random phase approximation in the H-F formalism). Quantities calculated include: elastic, total, inelastic, (n,g), (n,n'), (n,p), (n,a), (n,f), (n,2n), (n,np), (n,na), (n,nf),..., (n,4n),....., secondary particle and gamma ray production spectra, angular distributions of the first outgoing particles, and the production cross sections of isomeric states.

6. RESTRICTIONS OR LIMITATIONS

(n,gx) has not been included. Dimensions of the transmission coefficients are such that cross sections can be calculated up to 40 MeV for Ca-40 and 20 MeV for Pu-242. The maximum number of discrete levels is 40, the number of continuum bins is limited to 40 for each residual nuclide, and the number of outgoing particles is limited to 3.

7. TYPICAL RUNNING TIME

On an the VAX 6000, sample problem 1 took about 2 minutes of CPU time (wall clock time).

8. COMPUTER HARDWARE REQUIREMENTS

TNG1 runs on the VAX family of computers.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran 77 compiler is required. The code was compiled with VAX/Fortran on the VAX 6000 under the VAX/VMS operating system.

10. REFERENCE

K. Shibata and C. Y. Fu, "Recent Improvements of the TNG Statistical Model Code," ORNL/TM-10093 (August 1986).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and one DS/DD 5.25-inch diskette (360 K) which contains the source code and sample problem input and output.

12. DATE OF ABSTRACT

January 1991.

KEYWORDS: EXPERIMENTAL DATA ANALYSIS; NEUTRON; NUCLEAR MODELS

SECTION 5

MISCELLANEOUS PROGRAMS

This section contains computer codes of interest and application to photon data which are not in the previous categories. These programs and applications are as follows:

BOMJ	Using photon energies and uncertainties to develop level assignments.
COINC	To analyze coincident counting data.
CURVE	To determine the best fit to an arbitrary curve, useful, e.g., in determining Ge-detector efficiency curves.
DIMEN	To assist in assigning possible responsible nuclides for measured photon peaks.
GABAS	To generate time-dependent photon spectra from the output of an inventory-type program.
GASS	Compute self-shielding by an encapsulated photon source.
GRAP	Goal similar to that for BOMJ.
MARTHA	Compute NaI(Tl) scintillation-detector response functions.
MGA	Determines relative abundances of actinide isotopes from a spectrum obtained with a Ge-detection system.
PAPER.1	To compute solid angle and self-absorption factors for an inclined cylindrical source viewed by a cylindrical detector.
XRAY.AAC	To compute X-ray attenuation and absorption for any element.

NEA CODE PACKAGE IAEA1246

IAEA1246 BOMJ, LEVEL ASSIGNMENTS FROM GAMMA SPECTRA MEASUREMENTS 920317

1. NAME OR DESIGNATION OF PROGRAM - BOMJ.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
BOMJ	IAEA246/01	IBM PC	IBM PC	AN

3. DESCRIPTION OF PROGRAM OR FUNCTION

BOMJ uses measured gamma-ray energies with uncertainties and suggests level assignment to deduce a least-squares adjusted set of nuclear levels (similar to GTOL, see NESC-1149) and to find the places to dispose unassigned quanta among nuclear levels.

4. METHOD OF SOLUTION

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

204 nuclear levels,
1024 assigned quanta and 204 unassigned quanta.

6. TYPICAL RUNNING TIME

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

A non-standard string handling routine F77STR; and conversion routines NSDCNV for NSD applications.

9. STATUS

IAEA1246/01 : Requested by NEADB
 : Arrived, no report

10. REFERENCES

- B.J. Barton, J.K. Tuli:
 "Physics Analysis Programs for Nuclear Structure Evaluation"
 BNL-NCS-23375/R, October 1977
IAEA1246/01 :

11. MACHINE REQUIREMENTS

A 350KB virtual drive is recommended. To run BOMJ.EXE, the virtual drive must be named E: BOMJIC.EXE does not need a virtual drive, only hard disk space.

12. PROGRAMMING LANGUAGE USED

IAEA1246/01 : FORTRAN+ASSEMBLER

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

MS-DOS 4.1. The RM/FORTRAN compiler is required.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

F.E. Chukreev
C.A.J.A.D.
Kurchatov Institute
Moscow, Russia 123182

16. MATERIAL AVAILABLE

IAEA1246/01 :
ABSTRACT.TXT Abstract File
BOMJ.EXE Executable File
BOMJ.FOR Source File
BOMJ.LVL Test Case Data
BOMJIC.FOR Source File
README.DOC Information File
SHORT.RPT Short Report
TOTAL.RPT Total Report
PICTURE.LIB Symb. Data Lib.

17. CATEGORY = O ,

KEYWORDS ENSDF

data processing
evaluated data
gamma spectra
nuclear structure

NEA CODE PACKAGE NESC0248

NESC0248 COINC, PROCESSING OF EXPERIMENTAL COINCIDENCE COUNTING DATA 801118

1. NAME OR DESIGNATION OF PROGRAM. COINC.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
COINC	NESC0248/01	IBM 7090	IBM 7090	Z
COINC	NESC0248/02	CDC 3600	CDC 3600	T

3. NATURE OF PHYSICAL PROBLEM SOLVED.

Coincidence counting data are treated to obtain specific disintegration rates, channel efficiencies and count rates, weighted means, and all associated standard errors. Corrections are made for unequal deadtime loss in each channel, coincidence resolving time losses, decay during counting, decay from a reference time, and background in each of the three channels. Input variables include sample identification, start time for counting, sample reference time, counting interval, total number of counts in two single channels and one coincidence channel, and normalizing sample volume. Input parameters consist of deadtimes of each single channel, coincidence resolving time for all three channels, decay constant, background count rate for all three channels, and standard errors for each of the above parameters. Optional input allows date, group classification, and a 3-digit user code. Output contains corrected single channel, coincidence, and disintegration rates referred to start of count, specific disintegration rate (counts/second/unit volume or weight) referred to reference time, weighted mean and error of any number of problems in a group, efficiencies of the two independent detector channels, date, summary of background values used, identification number, count start time, and upper and lower limit (one standard deviation) of each of the computed quantities.

4. METHOD OF SOLUTION.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.

Decay constant greater than zero.
500 problems per set for CDC3600.

6. TYPICAL RUNNING TIME.

10 seconds are required for a 50 card problem on the CDC3600.

7. UNUSUAL FEATURES OF THE PROGRAM.

A very simple input format is available, allowing application to essentially any coincidence decay scheme.

Input data may be transcribed by hand and punched from standard format onto cards, or automatically punched card data may be utilized. Modifications for paper tape are complete. Complex adjustments of the accidental coincidence rates affected by deadtime are made. Both Poisson statistics for total accumulated counts and error propagation for correlated and uncorrelated quantities are compounded in determination of standard deviations. The program was designed for absolute beta-gamma coincidence counting, but it has also been used for gamma-gamma and neutron-fission coincidence work. Compensation for radioactive decay can be made to any reference time for any number of days.

8. RELATED AND AUXILIARY PROGRAMS.

9. STATUS

NESC0248/01 : Arrived at NEADB
 : Tested at NEADB
 : Obsolete
NESC0248/02 : Arrived at NEADB
 : Tested at NEADB

10. REFERENCES.

NESC0248/01 :
NESC0248/02 :

- A. De Volpi, K.G. Porges and G. Jensen:

Computer Code for Reduction of Coincidence Counting Data International Journal of Applied Radiation and Isotopes, vol. 17, (1966).

- G. Jensen:

COINC, For Reduction of Coincidence Counting Data ANL Program Library Report 1198/RP-258 (June 9, 1966).

11. MACHINE REQUIREMENTS.

12. PROGRAMMING LANGUAGE USED

NESC0248/01 : FORTRAN-II (IBM)
NESC0248/02 : FORTRAN-IV

13. OPERATING SYSTEM OR MONITOR UNDER WHICH PROGRAM IS EXECUTED. SCOPE

14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.

15. NAME AND ESTABLISHMENT OF AUTHOR.

A. De Volpi, K. G. Porges, and G. Jensen
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

16. MATERIAL AVAILABLE

NESC0248/01 :

Report:

SOURCE&DATA 0 records

OUTPUT 0 records

NESC0248/02 :

source program mag tape

test-case data mag tape

test-case output mag tape

Report: ANL 1198/RP-258 (June 9, 1966)

Reprint J. of App.Rad.&Isot. Vol.17 (1966)

SOURCE %CDC 3600< 0 records

DATA 0 records

OUTPUT 0 records

SOURCE %CDC 3600< 0 records

DATA 0 records

OUTPUT 0 records

17. CATEGORY = O ,

KEYWORDS Statistics

data processing

decay

NEA CODE PACKAGE NESC9533

NESC9533 CURVE LSFIT,GAMMA SPECTROMETER CALIBRATION BY INTERACTIVE FITTING
METH 900130

1. NAME OR DESIGNATION OF PROGRAM - CURVE,LSFIT.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
CURVE,LSFIT	NESC9533/01	DEC VAX 11/750	PC-80286	T

3. DESCRIPTION OF PROGRAM OR FUNCTION

CURVE and LSFIT are interactive programs designed to obtain the best data fit to an arbitrary curve.

CURVE finds the type of fitting routine which produces the best curve. The types of fitting routines available are linear regression, exponential, logarithmic, power, least squares polynomial, and spline.

LSFIT produces a reliable calibration curve for gamma ray spectrometry by using the uncertainty value associated with each data point. LSFIT is intended for use where an entire efficiency curve is to be made starting at 30 KeV and continuing to 1836 KeV. It creates calibration curves using up to three least squares polynomial fits to produce the best curve for photon energies above 120 KeV and a spline function to combine these fitted points with a best fit for points below 120 KeV.

4. METHOD OF SOLUTION

The quality of fit is tested by comparing the measured y-value to the y-value calculated from the fitted curve. The fractional difference between these two values is printed for the evaluation of the quality of the fit.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Maxima of -

2000 data points calibration curve output (LSFIT)

30 input data points

3 least squares polynomial fits (LSFIT)

The least squares polynomial fit requires that the number of data points used exceed the degree of fit by at least two.

6. TYPICAL RUNNING TIME

7. UNUSUAL FEATURES OF THE PROGRAM

CURVE and LSFIT can operate in the executive mode, which is faster than BASIC and requires less memory.

8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

NESC9533/01 : Requested by NEADB
: Arrived "as is"
: in preparation
: Tested at NEADB

10. REFERENCES

NESC9533/01 :
- Dale G. Olson:
Obtaining the Best Efficiency Curve by Curve Fitting Routines
- C. Yuelys-Miskis:
CURVE,LSFIT Tape Description and Implementation Information
NESC Note 88-101 (July 29, 1988).

11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

NESC9533/01 : BASIC

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

VMS 4.6.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

Compilation must be done with the GFloat qualifier.

15. NAME AND ESTABLISHMENT OF AUTHORS

D.G. Olson
Radiological & Environmental Sciences Laboratory
Idaho Operations Office

16. MATERIAL AVAILABLE

NESC9533/01 :
CURVE BASIC Source, curve fitting program
LSFIT BASIC Source, gamma-ray spectrometry
How to use by D.G. Olson
NESC Note 88-101 (july 29, 1988)
Information file 114 records
CURVE.BAS CURVE source (Turbo Basic) 627 records
CURVEVAX.BAS CURVE source (VAX Basic) 614 records

LSFIT.BAS	LSFIT source (Turbo Basic)	536 records
LSFITVAX.BAS	LSFIT source (VAX Basic)	522 records
CURVE.EXE	CURVE executable file	0 records
LSFIT.EXE	LSFIT executable file	0 records
XDATA.FIT	Sample input	29 records
YDATA.FIT	Sample input	29 records
ZDATA.FIT	Sample input	29 records
CURVE.OUT	CURVE sample output	75 records
LSFIT.OUT	LSFIT sample output	133 records
DOS	file-names	12 records

17. CATEGORY = 0,

KEYWORDS gamma spectra

least square fit

spectra unfolding

spectrometers

spline functions

RSICC CODE PACKAGE PSR-341

1. NAME AND TITLE

DIMEN: Code System for Isotope Identification by Gamma-Ray Analysis.

2. CONTRIBUTOR

Riga Radioisotope Research Institute, Riga, Latvia.

3. CODING LANGUAGE AND COMPUTER

Pascal; IBM PC (P00341/IBMPC/00).

4. NATURE OF PROBLEM SOLVED

For a set of a priori given nuclides taken from a work library, DIMEN uses median estimates of the peak areas and estimates of their errors to produce a list of possible nuclides matching a gamma-ray line and some measure of the reliability of this assignment.

5. METHOD OF SOLUTION

The identification of a given radionuclide is obtained by searching for a match with the energy information of a database. This procedure is performed in an interactive graphic mode by markers that superimpose, on the experimental data, the energy information provided by a previously elaborated data library. This library of experimental data includes approximately 16682 gamma-energy lines related to 749 known gamma emitter radioisotopes currently listed by the ICRP.

6. RESTRICTIONS OR LIMITATIONS

Number of channels: 4096.

7. TYPICAL RUNNING TIME

Interactive. No timing was attempted.

8. COMPUTER HARDWARE REQUIREMENTS

The code was tested on a PC 486 but should run on all IBM PC compatible computers.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Pascal. The original source code file was broken into several units by RSIC to test compilation using Microsoft QuickPascal.

10. REFERENCES

V. S. Kondrashov, Z. D. Moroz, A. A. Kolyshkin, and Remi Vaillancourt, "A Computer Program for the Identification of Nuclides by Using Median Estimates of Peak Areas in Gamma-Ray Spectra," Nucl. Inst. Meth. Phys. Res. A328, 542-546 (1993).

V. S. Kondrashov, I. Sajo-Bohus, and E. D. Greaves, "An Alternative Approach to Process Gamma-Ray Spectral Data," Spectrochimica Acta, 49B (9), 941-945 (1994).

Informal Notes: "Description of the MAKEBASE and DIMEN Programs" (1995).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and 2 3.5-in. DS/DD (1.44 MB) diskettes written in DOS format.

12. DATE OF ABSTRACT

January 1996.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; RADIONUCLIDES; INTERACTIVE,
ON-LINE; MICROCOMPUTER

RSICC CODE PACKAGE PSR-175

1. NAME AND TITLE

GABAS: A Code System for Generating Composite Time-Dependent Fission Produce Spectra.

AUXILIARY ROUTINES

ISPEC: Reads fission product spectral data and writes a binary file for input to GABAS.

2. CONTRIBUTORS

Instrumentation Research Technology, San Diego, California.

Sandia National Laboratories, Albuquerque, New Mexico.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; UNIVAC 1100/81.

4. NATURE OF PROBLEM SOLVED

GABAS calculates time-dependent beta- and/or gamma-ray spectra from decaying fission products.

5. METHOD OF SOLUTION

GABAS calculates composite fission-product beta and/or gamma-ray spectra based on the technique used by England, et al., in conjunction with the CINDER family of fission product codes. Multigroup beta and gamma-ray spectra for individual nuclides are folded with their corresponding time-dependent activities (usually generated by a fission product inventory code) to produce a composite time-dependent fission product spectrum. GABAS was intended to interface with the fission product inventory code RIBD-IRT; however, other codes like ORIGEN or CINDER could be utilized with appropriate modifications to their output format.

6. RESTRICTIONS OR LIMITATIONS

None noted.

7. TYPICAL RUNNING TIME

For 34 time steps and 180 fission products, the approximate CPU time was 10 seconds.

8. COMPUTER HARDWARE REQUIREMENTS

GABAS is operable on the UNIVAC 1100/81 computer. Two mass storage files, either tapes or discs, and a printer are needed.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

a. Included in documentation:

D. D. Thayer and N. A. Lurie, "A User's Manual for the GABAS Spectrum Computer Code," IRT 6406-004, January 1982.

b. Background information:

M. G. Stamatelatos and T. R. England, "FPDCYS and FPSPEC: Computer Programs for Calculating

Fission-Product Beta and Gamma Multigroup Spectra from ENDF/B-IV Data," LA-NUREG-6818-MS (May 1977).

D. D. Thayer and N. A. Lurie, "A User's Manual for Computer Code RIBD/IRT," IRT 6406-003, SAND 82-7013, NUREG/CR-2393 (January 1982).

T. R. England and M. G. Stamatelatos, "Multigroup Beta and Gamma Spectra of Individual ENDF/B-IV Fission Product Nuclides," LA-NUREG-6622-MS (December 1976).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document (a) and a reel of magnetic tape which contains the source program and sample problem input written in EBCDIC card images; total records 2565.

12. DATE OF ABSTRACT

February 1982; August 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS;
RADIATION SOURCE GENERATOR

RSICC CODE PACKAGE CCC-080

1. NAME AND TITLE

GASS: Monte Carlo Calculation of Self Shielding by Encapsulated Gamma-Ray Sources.

This code package originated in Office of Civil Defense programs in 1966; is retained by RSIC to preserve the technology.

2. CONTRIBUTORS

University of Illinois, Civil Engineering and Nuclear Engineering Program, Urbana, Illinois.

3. CODING LANGUAGE AND COMPUTER

FORTRAN IV; IBM 7090 and 7094.

4. NATURE OF PROBLEM SOLVED

GASS was designed to calculate the energy and angular distributions of photons emitted from a cylindrical or spherical encapsulated source.

5. METHOD OF SOLUTION

GASS represents an approximate solution by Monte Carlo methods to the steady state transport equation.

A time-saving procedure utilizing a "do-nothing" cross section allows ray tracing to proceed without many cross section look-ups and partial path length calculations. A choice is then made where the collision occurs between scattering, absorption, or the straight-ahead "do-nothing" reaction.

6. RESTRICTIONS OR LIMITATIONS

There are no known restrictions implied by storage allocation.

7. TYPICAL RUNNING TIME

Processing of 20,000 histories in the sample problem required 3 minutes on the IBM 7090 and 1.3 minutes on the 7094.

8. COMPUTER HARDWARE REQUIREMENTS

The code was designed for the 32 K IBM 7094 computer with 3 tape units.

9. COMPUTER SOFTWARE REQUIREMENTS

The code may be compiled and executed on the IBM FORTRAN IV IBJOB Monitor and other compatible systems. Standard I-O and systems tape assignments are made.

10. REFERENCE

K. Preiss, "Monte Carlo Calculation of Self Shielding by Encapsulated Gamma Ray Sources," UI-NRSS-3 (August 1966).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and a reel of magnetic tape which contains the source code and input for a sample problem written in BCD/EBCDIC card images and an output listing from running the problem; total records 734.

12. DATE OF ABSTRACT

January 1968; updated July 1981, February 1985.

KEYWORDS: MONTE CARLO; GAMMA-RAY; RAY-TRACING

NEA CODE PACKAGE IAEA1175

IAEA1175 GRAP,GAMMA-RAY LEVEL-SCHEME ASSIGNMENT 900219

1. NAME OR DESIGNATION OF PROGRAM - GRAP.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
GRAP	IAEA1175/01	IBM PC	IBM PC	A

3. DESCRIPTION OF PROGRAM OR FUNCTION

An interactive program for allocating gamma-rays to an energy level scheme.

Procedure allows for searching for new candidate levels of the form:

- 1) $L1 + G(A) + G(B) = L2$
- 2) $G(A) + G(B) = G(C)$
- 3) $G(A) + G(B) = C$ (C is a user defined number)
- 4) $L1 + G(A) + G(B) + G(C) = L2$

Procedure indicates intensity balance of feed and decay of each energy level. Provides for optimization of a level energy (and associated error). Overall procedure allows for pre-defining of certain gamma-rays as belonging to particular regions of the level scheme, for example, high energy transition levels, or due to beta-decay.

4. METHOD OF SOLUTION

Search for cases in which the energy difference between two energy levels is equal to a gamma-ray energy within user-defined limits.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Maximum number of gamma-rays	: 999
Maximum gamma ray energy	: 32000 units
Minimum gamma ray energy	: 10 units
Maximum gamma-ray intensity	: 32000 units
Minimum gamma-ray intensity	: 0.001 units
Maximum number of levels	: 255
Maximum level energy	: 32000 units
Minimum level energy	: 10 units
Maximum error on energy, intensity	: 32 units
Minimum error on energy, intensity	: 0.001 units
Maximum number of combinations	: 6400 (ca)
Maximum number of gamma-ray types	: 127

6. TYPICAL RUNNING TIME

Highly dependent on the number of transitions to be allocated and errors used. To generate the initial scheme (CRAG1) takes typically 10-15 minutes for 800 gamma-rays fitting to 120 levels.

7. UNUSUAL FEATURES OF THE PROGRAM

Intensity balance display of the feeding level and decaying level for particular transition gamma-ray energies.

Selective inclusion/removal of gamma-rays in multiple fit situation. Ability to force fit of gamma-ray even though errors dictate outside acceptance window.

8. RELATED AND AUXILIARY PROGRAMS

TRED - Raw data input, and edit, program.

GRAG1 - Preliminary assignment program.

9. STATUS

IAEA1175/01 : Requested by NEADB

: Arrived at NEADB

10. REFERENCES

- C. Hofmeyr et al:

74GE: Transitions and Levels Excited in Thermal-Neutron Capture
AIP Conference Proceedings No. 125 - Capture Gamma-Ray
Spectrometry and Related Topics - 1984.
Edited by S. Raman , pages 378-381.

IAEA1175/01 :

- C.B. Franklyn:

GRAP - Gamma Ray Allocations Program - A User's Guide
PEL-286 (May 1985)

11. MACHINE REQUIREMENTS

HP-version: HP-1000 series minicomputer, 192 Kbytes memory, disc drive, magnetic tape, terminal/monitor.

PC-version: IBM-PC XT or compatible, 512 Kbytes RAM, disc drive, printer, maths coprocessor (optional).

12. PROGRAMMING LANGUAGE USED

IAEA1175/01 : FORTRAN

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

HP version: Designed on RTE-IV B system, runs on RTE-VI.

PC version: MS-DOS 3.2 or higher.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

HP version: makes system calls to LOGLU, EXEC, OPEN, READF, WRITE, CLOSE, RMPAR, LURQ, IFBRK, FTIME. The printer for which the program was originally designed was a HP7310A.

15. NAME AND ESTABLISHMENT OF AUTHORS

Dr. C.B. Franklyn
Nuclear Energy Systems
Atomic Energy Corporation of South Africa
P.O. Box 582, Pretoria, South Africa

16. MATERIAL AVAILABLE

README File
GRAP Source Programs (HP Computer) (FTN4)
GRAG1 Source Programs (HP Computer) (FTN4)
TRED Source Programs (HP Computer) (FTN4)
GRAPEM Data File (HP Computer)
TREDED Data File (HP Computer)
1TRED Source Program (IBM PC/XT)
1CRAG1 Source Program (IBM PC/XT)
1GRAP Source Program (IBM PC/XT)
TREDED Data File (IBM PC/XT)
GRAPEM Data File (IBM PC/XT)
TREDTEST/CRAGTEST/GRAPTEST Data Files
README.TXT from DISC 1 & 2
Source Programs (4 files)
Data for TRED
Sample Output from GRAP
Sample Output from GRAG
Report: PEL-286 (May 1985)

17. CATEGORY = O ,

KEYWORDS gamma spectra
multilevel analysis
spectra unfolding

NEA CODE PACKAGE NEA 0983

NEA 0983 MARTHA,NAI(TL) GAMMA SCINTILLATION DETECTOR_RESPONSE BY M-C 860314

1. NAME OR DESIGNATION OF PROGRAM - MARTHA.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
MARTHA	NEA 0983/01	FACOM M-380	IBM 3084Q	T

3. DESCRIPTION OF PROGRAM OR FUNCTION

The program MARTHA calculates NaI(Tl) scintillation detector response functions to gamma rays. There are four versions of the program according to the detector shape and gamma-ray energy.

4. METHOD OF SOLUTION

Using a Monte Carlo method, every photon and electron produced by one incident photon are traced in a detector assembly, and the total energy deposited in the crystal is recorded as a pulse height. Repeating this procedure several times, a response function is obtained.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Response functions can be calculated for cylindrical or spherical detectors. The program was originally designed to calculate response functions for gamma energies from 0.01 MeV to 10 MeV. But the program should work up to 20 MeV. Available source conditions are a point source on the detector axis and a parallel beam. The maximum channel number of a spectrum is 300.

6. TYPICAL RUNNING TIME

Running time depends among other factors on the incident gamma energy. For 10,000 gamma quanta of 1.0 MeV incident on a 3 in. x 3 in. cylindrical crystal, execution time is approximately 11 seconds on an FACOM 380.

NEA 0983/01: NEA-DB executed the test cases included in this package on an IBM 3084Q computer. The following CPU times were required: 22 seconds (version 1); 15 seconds (version 2); 53 seconds (version 3); 21 seconds (version 4).

7. UNUSUAL FEATURES OF THE PROGRAM

The program takes the following two effects into account: (1) The housing material of the NaI(Tl) crystal; (2) the non-linear response of a NaI(Tl) detector to electron energy.

8. RELATED AND AUXILIARY PROGRAMS

Five programs to prepare the input data for MARTHA. These data are already given in the sample input.

9. STATUS

NEA 0983/01 : Arrived at NEADB
 : in preparation
 : Tested at NEADB

10. REFERENCES

- K. Saito and S. Moriuchi:
Monte Carlo Calculation of Accurate Response Functions for a NaI(Tl) Detector for Gamma Rays.
Reprinted from: Nuclear Instruments & Methods, 185(1981)299-308
- K. Saito and S. Moriuchi:
Monte Carlo Calculation of Accurate Response Functions for a NaI(Tl) Detector for Gamma Rays and
Analysis of Pulse Height Spectrum Formation Mechanism.
JAERI-M 9741 (In Japanese) (September 1981)

11. MACHINE REQUIREMENTS

NEA 0983/01: The test cases were run in 550K bytes of IBM 3084Q main storage.

12. PROGRAMMING LANGUAGE USED

NEA 0983/01 : FORTRAN-IV

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

FACOM OS 4-F4-MSP.
NEA 0983/01: MVS-SP (IBM 3084Q).

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

K. Saito
Department of Environmental Safety Research
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken
Japan

16. MATERIAL AVAILABLE

Source Program (Fortran-IV)	(Version 1)
Subroutine Source (fortran-IV)	(Version 1)
Sample Input	(Version 1)
Input Library (FT31)	(Version 1)

Input Library (FT32)	(Version 1)
Input Library (FT33)	(Version 1)
JCL	(Version 1)
Sample Output	(Version 1)
Source Program (Fortran-IV)	(Version 2)
Subroutine Source (fortran-IV)	(Version 2)
Sample Input	(Version 2)
JCL	(Version 2)
Sample Output	(Version 2)
Source Program (Fortran-IV)	(Version 3)
Subroutine Source (fortran-IV)	(Version 3)
Sample Input	(Version 3)
Input Library (FT33)	(Version 3)
Input Library (FT32)	(Version 3)
Input Library (FT33)	(Version 3)
JCL	(Version 3)

NEA 0983/01 :

Sample Output	(Version 3)
Source Program (Fortran-IV)	(Version 4)
Subroutine Source (fortran-IV)	(Version 4)
Sample Input	(Version 4)
JCL	(Version 4)
Sample Output	(Version 4)

Nucl. Instr. & Methods 185(1981)299-308

Input Description

Report: JAERI-M 9741 (In Japanese) (September 1981)

This information file	119 records
Program to convert EBCDIC to binary	26 records
Routine RANDOM from SLATEC library	117 records
Program MARTHA source, Version 1	2496 records
JCL to run MARTHA version 1	101 records
Input for version 1	57 records
Library for version 1 (file code 31)	216 records
Library for version 1 (file code 32)	594 records
Library for version 1 (file code 33)	540 records
Test case output, version 1	768 records
Program MARTHA source, version 2	1972 records
JCL to run version 2	74 records
Input for version 2	20 records
Test case output, version 2	425 records
Program MARTHA source, version 3	1968 records
JCL to run version 3	101 records
Input for version 3	48 records
Library for version 3 (file code 31)	216 records
Library for version 3 (file code 32)	594 records
Library for version 3 (file code 33)	540 records

Test case output, version 3	1076 records
Program MARTHA source, version 4	1557 records
JCL to run version 4	74 records
Input for version 4	15 records
Test case output, version 4	663 records

17. CATEGORY = O ,

KEYWORDS gamma detectors
response functions
scintillation detectors

NEA CODE PACKAGE NESC9479

NESC9479 MGA,PU ISOTOPE ABUNDANCE FROM MULTICHANNEL ANALYZER GAMMA SPECTRA
930309

1. NAME OR DESIGNATION OF PROGRAM - MGA.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name	Package-ID	Orig. Computer	Test Computer	Status
MGA	NESC9479/01	DEC VAX series	DEC VAX 8810	T
MGA	NESC9479/02	IBM PC	IBM PC	K

3. DESCRIPTION OF PROGRAM OR FUNCTION

The MGA (Multiple Group Analysis) program determines the relative abundances of plutonium and other actinide isotopes in different materials. The program analyzes spectra taken of such samples using a 4096-channel germanium (Ge) gamma-ray spectrometer. The code can be run in a one or two detector mode. The first spectrum which is required and must be taken at a gain of .075 Kev/channel with a high resolution planar detector, contains the 0-300Kev energy region. The second spectrum, which is optional, must be taken at a gain of 0.25 Kev/channel; it becomes important when analyzing high burnup samples (concentration of Pu(241) greater than one percent). Isotopic analysis precisions of one percent or better can be obtained, and no calibrations are required. The system also measures the abundances of U(235,238), Np237, and Am241. A special calibration option is available to perform a one-time peak-shape characterization when first using a new detector system.

4. METHOD OF SOLUTION

The basic method for determining the relative abundance of the isotopes of plutonium is to measure the intensity of two or more peaks from gamma rays of similar energy, but arising from different isotopes. Since the gamma-ray emission probabilities and half-lives are known, the atom ratios can be calculated provided relative detection efficiencies for the peaks can be estimated.

NESC9479:

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

6. TYPICAL RUNNING TIME

Analysis time is less than one minute.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

NESC9479/01 : Offered to NEADB
: Requested by NEADB
: Arrived "as is"
: in preparation
: Tested at NEADB

NESC9479/02 : Requested by NEADB
: Known to NEADB

10. REFERENCES

- R. Gunnink:
MGA2 - A One-Detector Code for Rapid High-Precision Plutonium Measurements
UCRL-96016 Rev. 1, Preprint (July 1987).
- NESC9479/01 :
- R. Gunnink:
MGA - A Gamma-Ray Spectrum Analysis Code for Determining Plutonium Isotopic Abundances Volume
1, Methods and Algorithms UCRL-LR-103220, Vol.1 (April 3, 1990).
- R. Gunnink:
A New One-Detector Analysis Method for Rapid High-Precision Plutonium Isotopic Measurements
Reprinted from the Proceedings of the 9th ESARDA Symposium on Safeguards and Nuclear Material
Management, London, UK., pp. 167-171 (May 12-14, 1987).

11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

NESC9479/01 : FORTRAN-77
NESC9479/02 : FORTRAN-77

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

VMS.

NESC9479/01: The program was compiled by NEA-DB on a DEC VAX 8810 computer under VMS
V5.4-2 using the DEC/VAX FORTRAN-77 compiler. The test case was run interactively.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

R. Gunnink
Lawrence Livermore National Laboratory

16. MATERIAL AVAILABLE

NESC9479/01 :

MGA Source File
 Executable Image
 Object Modules
 Object Library
 Sample Problem Data (BINARY)
 Auxiliary Information
 Control Information
 Sample Output
 Report: UCRL-LR-103229, Vol.1 (April 3, 1990)
 ESARDA Reprint
 Information file 102 records
 000004.Z17 0 records
 000575.H27 0 records
 AVE FOR 0 records
 BKGD.FOR 103 records
 BKGRD.FOR 131 records
 BWF.FOR 71 records
 C2JDAT.FOR 24 records
 CALERR.FOR 20 records
 FOR007.DAT Sample problem output 103 records

NESC9479:
 GFIT.FOR 102 records
 GRP100.DAT 31 records
 GRP340.DAT 22 records
 GRP660.DAT 18 records
 J2CDAT.FOR 30 records
 MATINV.FOR 80 records
 MAXVAL.FOR 48 records
 MGA.COM 16 records
 MGA.FOR 129 records
 MGA.RUN 5 records
 MGA100.FOR 353 records
 MGA235.FOR 174 records
 MGA300.CMN 31 records
 MGA300.FOR 253 records
 MGA45.FOR 178 records
 MGA600.FOR 250 records
 MGA94.FOR 636 records
 MGAABS.FOR 548 records
 MGACAL.CMN 5 records
 MGACAL.FOR 545 records
 MGACOM.CMN 104 records
 MGADAT.CMN 8 records
 MGAEQS.FOR 273 records
 MGAGAN.FOR 250 records
 MGAHIE.FOR 528 records

MGAOUT.FOR	307 records
MGAPKS.FOR	437 records
MGASPC.FOR	461 records
NCNTS.FOR	61 records
PKFIT.CMN	4 records
PKFIT.FOR	691 records
RDCHN.FOR	9 records
RDCHN2.FOR	54 records
RDCHN3.FOR	58 records
SHAPC.Z1	15 records
SHAPC2.H2	10 records
SPRAM.FOR	85 records
STRIP1.FOR	85 records
UTFSBS.FOR	397 records
UTLIB.OLB	0 records

17. CATEGORY = D , O ,

KEYWORDS plutonium
spectra

RSICC COMPUTER CODE PSR-097

1. NAME AND TITLE

PAPER 1: Monte Carlo Calculation of Solid Angle and Self-Absorption Factors for an Inclined Cylindrical Source Viewed by a Cylindrical Detector.

2. CONTRIBUTOR

Department of Physics, Ben Gurion University of the Negev, Beersheva, Israel.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; CDC 6600.

4. NATURE OF PROBLEM SOLVED

PAPER 1 calculates the self absorption of gamma radiation in an inclined cylindrical source and, also, the solid angle of the source subtended by a cylindrical detector. It can be used in any situation in which a transformation composed of a translation and a rotation between the source and detector coordinate systems is required.

5. METHOD OF SOLUTION

PAPER 1 uses the Monte Carlo method for determining self-absorption and solid-angle correction factors in the inclined cylindrical geometry. The Monte Carlo method used in PAPER 1 is extremely flexible and many geometric configurations can be treated with only trivial modifications of the computer program.

6. RESTRICTIONS OR LIMITATIONS

No weighting factor was assigned to the gamma ray as a function of its angle of incidence on the detector.

7. TYPICAL RUNNING TIME

The Monte Carlo method for determining self-absorption and solid-angle correction factors in the inclined cylindrical geometry requires fairly large amounts of computer time to acquire statistical accuracy of the order of 1%. A total of 1000 s of computer time was used to run 40,000 case histories per point on the CDC-6000 computer.

8. COMPUTER HARDWARE REQUIREMENTS

PAPER 1 is operable on the CDC 6600 computer.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES

"User's Instructions," Informal Note.

Y. S. Horowitz, S. Mordechai and A. Dubi, "Solid-Angle and Self-Absorption Factors for an Inclined Cylindrical Source Viewed by a Cylindrical Detector," *Nucl. Instr. and Meth.* 123 (1975) 551-555.

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code input written in EBCDIC card images; total records 76.

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: GAMMA-RAY SOURCE ANALYSIS; SELF ABSORPTION

RSICC CODE PACKAGE CCC-525

1. NAME AND TITLE

XRAY_AAC: X-ray Attenuation and Absorption Calculations.

AUXILIARY ROUTINES

UPDATE_COEFF: Convert data library to binary indexed file.

AAC_1: Application program to demonstrate calling XRAY_AAC.

AAC_2: Interactive application program to call XRAY_AAC.

AAC_3: Interactive application program to provide easy access to Function XRAY_AAC.

DATA LIBRARY

ELEMENTS.DAT: Subset of DLC-99/HUGO including attenuation and absorption coefficients.

2. CONTRIBUTOR

Boeing Aerospace Company, Seattle, Washington.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; VAX.

4. NATURE OF PROBLEM SOLVED

This point-source, polychromatic, discrete energy X-ray transport and energy deposition code system calculates first-order spectral estimates of X-ray energy transmission through slab materials and the associated spectrum of energy absorbed by the material.

5. METHOD OF SOLUTION

X-ray source spectra may be internally generated and normalized (Kramer or Planck spectrum), read from data files, or read from an electronic library. Virtually any material consisting of the first 100 atomic elements may be specified as a shield or absorber using a common symbolic format. The calculated spectra may be selectively written to data files which in turn may be used as input to further calculations. One aspect of this software that is believed unique is its ability to parse chemical compounds and alloys that are entered in a conventional symbolic format and calculate the relative mass of the constituent elements.

6. RESTRICTIONS OR LIMITATIONS

Because this software is written in Vax Fortran, which is a superset of ANSI Fortran 77, and takes appropriate advantage of VMS system routines and run-time library functions, its transportability is limited.

7. TYPICAL RUNNING TIME

The programs take only a few seconds to execute interactively.

8. COMPUTER HARDWARE REQUIREMENTS

The codes run on VAX 11/750 or VAX 8600 computers.

9. COMPUTER SOFTWARE REQUIREMENTS

The codes were developed using Vax/VMS Version 4.5 and Vax Fortran Version 4.6.

10. REFERENCE

Alan MacArthur, "XRAY_AAC: X-ray Attenuation and Absorption Calculations," Boeing Aerospace Company, Seattle, Washington (Unpublished document 1987).

11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD 5.25 (1.2MB) diskette in compressed DOS files.

12. DATE OF ABSTRACT

February 1988.

KEYWORDS: BEAM TRANSPORT; ENERGY DEPOSITION; GAMMA-RAY SOURCE;
GAMMA-RAY; INTERACTIVE; X-RAY

SECTION 6

DATA LIBRARIES

These libraries contain photon energies and branching ratios of decay gamma rays. These data are used in identification of isotopes responsible for data observed in measured photon spectra.

As in the case of computer codes discussed in previous sections, these compilations reflect scientific evaluations usually related to an ongoing experimental program (or programs), and may be written for specific computer environments. Although there is a substantial overlap in the information presented, the individual data libraries are unique. The compilers do not make a recommendation for the choice of library to use.

RSICC DATA LIBRARY DLC-083

1. NAME AND TITLE OF DATA LIBRARY

GAMDAT-78: Library of Gamma-Ray Decay Data for 2055 Radionuclides.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

No retrieval program is included in the package.

3. CONTRIBUTOR

Central Division of Chemical Analysis, Nuclear Research Establishment, Jülich, Federal Republic of Germany.

4. HISTORICAL BACKGROUND AND INFORMATION

Gamma-ray spectrometry, which in every case includes the step of gamma-ray spectra evaluation, is an indispensable tool in nearly all fields where radioactive materials and substances are handled or investigated.

5. APPLICATION OF THE DATA

However, not only in connection with the production of energy by nuclear fission is gamma-ray spectrometry required. Fusion reactors also will produce radioactive materials and must use this method.

Gamma-ray spectrometry is also vital to nuclear medicine and gamma-ray spectrometry is the most important measuring technique used in radioanalytical chemistry, as well as planning for the shielding required for radioactive materials.

6. SOURCE AND SCOPE OF DATA

Starting from a collection of gamma-ray data used for gamma-ray spectra evaluation in the authors' laboratory, this data set was completed by systematic compilation of all gamma-ray data available. The first edition of the data collections was available in 1973; in 1978 an updated, completed and corrected version was finished.

The latest version contains 1) all radionuclides known until 1977; 2) their half-lives; 3) their daughter-nuclides; 4) their long-lived precursor-nuclides (parents); 5) their genesis or mode of artificial production; 6) hints to the references where the gamma-ray data have been found; 7) the energies of the gamma-ray and X-ray lines; 8) the abundances (intensities) of the gamma rays and X-rays.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

Not applicable.

8. DATA FORMAT AND COMPUTER

EBCDIC card images; IBM 370/3033.

9. TYPICAL RUNNING TIME

Not applicable.

10. REFERENCE

G. Erdtmann and W. Soyka, "The Radionuclide Gamma Ray Data File GAMDAT-78," Jul-Spez-34 (April 1979).

11. CONTENTS OF LIBRARY

Included are the referenced document and a reel of magnetic tape which contains the radionuclide gamma-ray data file GAMDAT 78; total records 52,015.

12. DATE OF ABSTRACT

April 1985.

KEYWORDS: RADIOACTIVE DECAY SPECTRA

RSICC DATA LIBRARY DLC-032

1. NAME AND TITLE OF DATA LIBRARY

GAMTAB: Radioactive-Decay Gamma-Rays Ordered by Energy and Nuclide.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAM

No retrieval program is included in the package.

3. CONTRIBUTOR

Savannah River Laboratory, Aiken, South Carolina, through the Argonne Code Center, Argonne, Illinois.

4. HISTORICAL BACKGROUND AND INFORMATION

Since the first Catalogue of Gamma-Rays Emitted by Radionuclides was published by M. A. Wakat in 1971, the continued use of Ge(Li) detectors of high resolution has resulted in a general upgrading of nuclear decay data. The present work consists of data from the original catalogue card files with additions and corrections where newer, superior data were at hand.

5. APPLICATION OF THE DATA

Because of the increased precision of the revised data, several minor policy changes were made to allow for: 1) Energy listings to 0.01 keV, where available; 2) Uncertainty listings for the energy, where available; 3) Use of exponential notation for half-lives and gamma-ray abundances; 4) Revision of the production mode code; 5) Listing the two most-abundant associated gamma rays to the nearest keV.

6. SOURCE AND SCOPE OF DATA

GAMTAB has a separate table of the data listed by nuclide. By means of the original Catalogue, the source of a gamma ray could be narrowed initially via two associated gamma rays to several possibilities. However, to reduce these possibilities to one, much further searching through the Catalogue and spectrum was required. In this work, TABLE II, the listing by nuclide of up to 50 associated gammas, will allow a more rapid and thorough search of the data for each of the possible nuclides and eliminate the less abundant gamma rays from further scrutiny.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

Not applicable.

8. DATA FORMAT AND COMPUTER

EBCDIC card images; IBM 360/370.

9. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for GAMTAB.

10. REFERENCE

W. W. Bowman and K. W. MacMurdo, "Radioactive-Decay Gammas Ordered by Energy and Nuclide," *Atomic Data and Nuclear Data Tables* 13 (1974) 89-92.

11. CONTENTS OF LIBRARY

Included are the referenced document and a reel of magnetic tape which contains the gamma-ray data

listed in ascending energy, data listed by nuclide, and references written in EBCDIC card images; total records 26,871.

12. DATE OF ABSTRACT

June 1984.

KEYWORD: RADIOACTIVE DECAY SPECTRA

RSICC DATA LIBRARY DLC-109

1. NAME AND TITLE OF DATA LIBRARY

GAMTOT78: Compilation of Radioactive Decay and Capture Gamma Rays.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAM

GAMIDEN: An Aid to the Identification of Unknown Materials through Gamma-Ray Spectroscopy.

3. CONTRIBUTOR

Lawrence Livermore Laboratory, Livermore, California.

4. HISTORICAL BACKGROUND AND INFORMATION

The intent of GAMIDEN is to help identify isotopes by their gamma-ray emissions and, thus, to assist in the nondestructive assay of unknown materials from both radioactive decay and neutron captures.

5. APPLICATION OF THE DATA

GAMIDEN searches GAMTOT78, a file of gamma-ray spectra, for matches with observed photon energies. The gamma-rays emitted by an isotope undergoing radioactive decay or neutron capture have energies and intensities that are characteristic of that isotope. A useful method for the nondestructive assay of unknown materials is based on identifying the signature of the isotope.

Since there are thousands of known gamma-rays, the automated search procedure searches for isotopes that satisfy the input criteria. Each such isotope is printed out, accompanied by a list of other gamma emissions from the isotope that one might expect to see.

The data file is taken from two compilations of gamma-ray spectra. The compilation of radioactive-decay gammas includes the half-life for each isotope and the energy and probability of emission per decay for each gamma emitted by that isotope.

6. SOURCE AND SCOPE OF DATA

Included are photon energies greater than 1 MeV and probabilities greater than 0.01. A total of 43,940 entries are provided.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

GAMIDEN lists the matching isotopes, eliminates isotopes that are likely to be the source of the observed protons, and then lists the isotopes that are left. It is designed for the Cray 1. It is written in standard Fortran (ANSI), but contains some LRLTRAN instructions to make use of the Livermore time-sharing system.

8. DATA FORMAT AND COMPUTER

Character type EBCDIC; GAMTOT78 data 120 character records, Cray 1, IBM 3033.

9. TYPICAL RUNNING TIME

For GAMIDEN, the typical problem requires less than 0.75 min. Please note that disk file GAMTOT78 must be present. No input data required.

10. REFERENCES

a. Included in the documentation:

R. J. Howerton, "GAMIDEN: A Program to Aid in the Identification of Unknown Materials by Gamma-Ray Spectroscopy," UCRL-50400, Vol. 22 Rev. 1 (June 1982).

b. Background information:

G. Erdtmann and W. Soyka, "The Gamma Rays of the Radionuclides," in *Verlag Chemie* (Weinheim, New York, 1979).

V. J. Orphan et al, "Line and Continuum Gamma-Ray Yields from Thermal-Neutron Capture in 75 Elements," DASA 2570 GA-10248 (1970).

11. CONTENTS OF LIBRARY

Included are the referenced document (a) and a reel of magnetic tape which contains the program to search the data file and the data file written in BCD/EBCDIC card images; total records 44,390.

12. DATE OF ABSTRACT

March 1984.

KEYWORD: RADIOACTIVE DECAY SPECTRA

RSICC DATA LIBRARY DLC-062

1. NAME AND TITLE OF DATA LIBRARY

NFCLIST: Radionuclide Radiation Data from the Evaluated Nuclear Data File (ENDF/B) for Routine Releases from Nuclear Fuel Cycle Facilities.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

No retrieval program is in the package.

3. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

4. HISTORICAL BACKGROUND AND INFORMATION

The calculation of radiation doses from exposure to radionuclides requires a knowledge of the energies and intensities of the atomic and nuclear radiations emitted during the decay process. NFCLIST provides tabulations of decay data for radionuclides expected to occur in routine releases of effluents from nuclear fuel cycle facilities.

5. APPLICATION OF THE DATA

NFCLIST gives tabulations of the atomic and nuclear radiations emitted by 240 radionuclides. Most of these are the ones expected to occur in routine releases of effluents from nuclear fuel cycle facilities. The half-life and recommended values for the energies, intensities, and equilibrium absorbed-dose constants for each of the atomic and nuclear radiations are given for each radionuclide. Also given are the daughter radionuclides produced and recommended values for decay branching ratios, where applicable. The radioactivity decay chains and branching ratios are displayed in diagram form.

6. SOURCE AND SCOPE OF DATA

Most of the decay data are for the radionuclides given in Table A-3 of Regulatory Guide 1.109, USNRC, and their radioactive daughter products.

Nuclear fuel cycle data was contributed by ORNL Nuclear Data Project. The data are taken from atomic and nuclear radiations emitted by 240 radionuclides which are expected to occur in routine releases of effluents for nuclear fuel cycle facilities. They were derived from a computer file used to prepare NUCLEAR DATA SHEETS (the Evaluated Nuclear Structure Data File).

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

Not applicable.

8. DATA FORMAT AND COMPUTER

EBCDIC card images; IBM 360.

9. TYPICAL RUNNING TIME

Not applicable.

10. REFERENCE

D. C. Kocher, "Nuclear Decay Data for Radionuclides Occurring in Routine Releases from Nuclear Fuel Cycle Facilities," ORNL/NUREG/TM-102 (August 1977).

11. CONTENTS OF LIBRARY

Included are the referenced document and a reel of magnetic tape which contains the decay data and the MEDPRINT source file written in EBCDIC card images, plus output from the sample problem; total records 38,175.

12. DATE OF ABSTRACT

March 1985.

KEYWORDS: RADIOACTIVE DECAY SPECTRA

RSICC DATA LIBRARY DLC-172

1. NAME AND TITLE OF DATA LIBRARY

NUCDECAY: Nuclear Decay Data for Radiation Dosimetry Calculations for ICRP and MIRD.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

DEXRAX: Extracts decay data from the library for radionuclide(s) specified by the user.

3. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

4. HISTORICAL BACKGROUND AND INFORMATION

The Dosimetry Research Group (DRG) of the Health Sciences Research Division at ORNL has for several years maintained data bases of nuclear decay data for use in dosimetric calculations. The data on mean and unique energy plus intensity have been previously published, in abridged form, in Publication 38 of the International Commission on Radiological Protection (ICRP 1983) and a monograph¹ for the Medical Internal Radiation Dose (MIRD) Committee of the Society of Nuclear Medicine; but the unabridged data included here and the beta spectra have not been previously published.

5. APPLICATION OF THE DATA

This data base has been designed to address the needs in medical, environmental, and occupational radiation protection. Calculations of the spatial distribution of absorbed dose (depth-dose) requires information on the beta spectra, and these are compiled in a separate data file also included here. NUCDECAY is required by the CCC-620/SEECAL program to calculate age-dependent specific effective energies.

6. SOURCE AND SCOPE OF DATA

The unabridged data used in preparing ICRP Publication 38 and a monograph of the MIRD Committee are distributed in electronic form in this package. The data are assembled in two collections. The collection referred to as ICRP38 consists of data on the energies and intensities of radiations emitted by the 825 radionuclides reported, although abridged, in ICRP Publication 38 plus an additional 13 radionuclides evaluated during preparation of a monograph for the MIRD Committee. The second collection, denoted as MIRD, contains data for the 242 radionuclides in the MIRD monograph noted above. Each collection consists of three ASCII files:

- (1) the index file (ICRP38.IDX or MIRD.IDX) is a sorted list of the radionuclides with pointers into the data files.
- (2) the radiation file (ICRP38.RAD or MIRD.RAD) contains data on the energies and intensities of the emitted radiations.
- (3) the beta spectra file (ICRP38.BET or MIRD.BET) contains the spectra for all beta emitters in the collection.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

Four utility codes are provided. The code DEXRAX is used to extract the decay data from the library for radionuclide(s) specified for the user. The utility CHAIN lists the decay chain headed by a user-specified radionuclide. The RADLINE code identifies radionuclides which emit alpha or photon radiations of a user-specified energy. The executables and most of the source codes are provided. The Microsoft Fortran 5 compiler was used to compile the CHAINS code and the READDEC portion of the

DEXRAX code. The full source for DEXRAX is not provided as that implementation must be linked with two special libraries. The source code is provided for a QBASIC version of the utility RADSUM. This version of RADSUM does include plotting of the beta spectra or computations of the gamma constant. Other utilities were written in Microsoft BASIC Professional Development System.

8. DATA FORMAT AND COMPUTER

ASCII; PC 386. (D00172/PC386/01)

9. TYPICAL RUNNING TIME

The codes are interactive.

10. REFERENCES

a. Documentation available with library

K. F. Eckerman, R. J. Westfall, J. C. Ryman, M. Cristy, "Nuclear Decay Data files of the Dosimetry Research Group," ORNL/TM-12350 (December 1993).

K. F. Eckerman, R. J. Westfall, J. C. Ryman, and M. Cristy, "Availability of Nuclear Decay Data in Electronic Form, Including Beta Spectra not Previously Published," Health Phys. 67(4):338-345 (1994).

b. Other useful documentation

D. Weber, K. F. Eckerman, L. T. Dillman, and J. C. Ryman, "MIRD: Radionuclide Data and Decay Schemes," Society of Nuclear Medicine, New York (1989).

11. CONTENTS OF LIBRARY

Included are the referenced documents and two DS/HD 3.5-in. (1.44 MB) diskette written in compressed DOS files which include the data library, the installation code, and the utility codes.

12. DATE OF ABSTRACT

November 1994; revised May 1995.

KEYWORDS: BETA-RAY SPECTRA; MICROCOMPUTER; RADIOACTIVE DECAY SPECTRA; ELECTRON SPECTRA; EXTERNAL DOSE; INTERNAL DOSE; RADIONUCLIDES

RSICC DATA PACKAGE DLC-134

1. NAME AND TITLE OF DATA LIBRARY

RADDECAY 4.02: Radioactive Decay Data for Radiological Assessments.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

RADDECAY 4.02 (DK4.EXE) - Display Decay Information of Radioactive Nuclides.
MEV 1.03 Nuclide Search and Analysis Utility.

3. CONTRIBUTORS

Original Contributor:

Grove Engineering, Inc., Rockville, Maryland.

Other Contributor:

University of Connecticut, Storrs, Connecticut.

4. HISTORICAL BACKGROUND AND INFORMATION

The data are derived from DLC-80/DRALIST, a data set giving radioactive decay energies, spectra, half lives, and other information. RADDECAY 4.02 is an interactive program for the IBM PC, or compatible, for retrieving and displaying decay information for 497 radionuclides. Data provided include the half life, radioactive daughter nuclides, probabilities per decay, and decay product energies for alpha particles, beta rays, positrons, electrons, x-rays, and gamma rays.

5. APPLICATION OF THE DATA

The estimation of radiation dose to man from either external or internal exposure to radionuclides requires a knowledge of the energies and intensities of the atomic and nuclear radiations emitted during the radioactive decay process. The availability of evaluated decay data for the large number of radionuclides of interest is of fundamental importance for radiation dosimetry.

The library includes radionuclides occurring naturally in the environment, those of potential importance in routine or accidental releases from the nuclear fuel cycle, those of current interest in nuclear medicine and fusion reactor technology, and some of those of interest in the estimation of annual limits on intake via inhalation and ingestion for occupationally exposed individuals.

6. SOURCE AND SCOPE OF DATA

The radioactive decay data in the library were published in DOE/TIC-11026 (see reference below) and made available as DLC-80/DRALIST in the MEDLIST format.

In addition to the radionuclides of interest in the nuclear fuel cycle, the data base comprises most of the nuclides occurring naturally in the environment, those of current interest in nuclear medicine and fusion reactor technology, and some additional radionuclides of use in the estimation of annual limits of intake and derived air concentrations for occupationally exposed individuals. The current data base contains approximately 500 radionuclides. It is believed that, with few exceptions, the decay data contained in this report are not likely to change significantly over the next few years as the result of new measurements.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAMS

RADDECAY (DK4.EXE) is a program for the IBM PC and compatibles for the retrieval and display of the decay information of radioactive nuclides. It is written in TrueBasic and compiled. The

executable program is on the distribution diskette. The data are in a special format for retrieval by RADDECAY which is defined in the documentation. A math co-processor is desirable but not necessary. The data files can be "exported" to an ASCII format. A search routine allows finding the radionuclides that have photon decay in a user specified energy range.

At the University of Connecticut the MEV Search and Analysis program was developed to assist in the identification of nuclides producing a spectrum on their Multi Channel Analyzer. MEV will search through either Alpha, Beta, or Gamma libraries for single energy line or for a group of energy lines. Each energy line is described by a specific energy in Mev, an uncertainty above and below this value to extend the search through, and a probability lower limit of yield to discriminate out low probability energy lines. Single energy line searches will result in a list of possible nuclides. Multiple energy line searches of up to six lines provide a list of possible nuclides and how many energy lines each nuclide matched. Also available is an option to display all the energy lines of any nuclide.

8. DATA FORMAT AND COMPUTER

Executable and coded data files on one DS/HD 3.5-inch diskette (1.44 MB); IBM PC.

9. TYPICAL RUNNING TIME

Interactive.

10. REFERENCES

a. Included in package:

C. A. Negin and G. Worku, "RadDecay - Radioactive Nuclide Library and Decay Software," Version 4 (September 1993).

M. W. Rota and E. L. Wilds, "READ.ME File of MEV Search and Analysis, Version 1.3" (1993).

b. Background information:

D. C. Kocher, "Radioactive Decay Tables--A Handbook of Decay Data for Application to Radiation Dosimetry and Radiological Assessment," DOE/TIC-11026 (1981).

11. CONTENTS OF LIBRARY

Included are the documents in 10.a. and one 3.5-in. (1.44 MB) DS/HD diskette written in DOS format which contains the data files and executable file and MEV program.

12. DATE OF ABSTRACT

December 1987; revised November 1990, October 1992, March 1994.

KEYWORDS: RADIOACTIVE DECAY SPECTRA; MICROCOMPUTER

RSICC DATA PACKAGE DLC-088

1. NAME AND TITLE

TPASGAM85: Radioactive Decay Library of Gamma-Ray Energies, Branching Ratios, and Cross Sections.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

FIXISO: To update the gamma-ray data file ordered by nuclide number.

DECAYDAT: To read and list the gamma-ray data file ordered by nuclide number.

NUCLIDE ID: To display data for a particular nuclide or list nuclides which emit gamma rays in a narrow energy range (IBM PC).

TPASLIST: To read and list data file ordered by energy.

3. CONTRIBUTORS

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

EG&G Energy Measurements, Inc., Goleta, California.

4. HISTORICAL BACKGROUND INFORMATION

The data reported in DLC-19/DECAYGAM were the parent data for this library. Additions and changes have been primarily for fission product radionuclides and for heavy actinides. Other changes include determining the absolute normalization for most of the relative branching ratios given in the parent file.

The original data library was made available April 1982. A major revision was made August 1983, another in September 1984, and another in October 1985.

5. APPLICATIONS OF THE DATA

This compilation of radionuclide decay data contains, for those radionuclides tabulated, all necessary data for qualitatively and quantitatively measuring the concentration of photon emitting radionuclides as well as conducting activation analyses using gamma-ray spectrometry. It was developed specifically for use with RSICC code package PSR-164/TPASS.

6. SOURCE AND SCOPE OF DATA

The TPASGAM data library contains gamma-ray decay information for 1438 radionuclides. The data consist of gamma-ray energies and intensities as well as cross-section information useful in activation analysis.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAMS

D00088ALLCP04

FIXISO, the program for editing the data library ordered by nuclide number, is an interactive PDP-10 Fortran IV program. The user is prompted to name the data file, to identify the nuclide to be edited and then for the datum to be replaced and its new value. More than one element may be changed while executing the program; however, the changes must be ordered by nuclide number since the input file is not rewound.

DECAYDAT runs on the IBM 3033 and reads the data library ordered by nuclide number from unit 5 and prints it on unit 6 with comments.

TPASLIST runs interactively on Vax computers. It reads the file ordered by energy and lists data for selected nuclides.

SEARCH.FOR is a Fortran program to perform searches for records on the data library ordered by nuclide number. It can be linked with additional subprograms to perform calculations required for user's applications.

D00088IBMPC03

NUCLIDE ID is a compiled IBM PC program which displays data for a particular nuclide or lists nuclides which emit gamma rays in a specified energy range. The program is interactive. The data are stored in dBase III DBF format.

8. DATA FORMAT AND COMPUTERS

EBCDIC card images; FIXISO, PDP-10; DECAYDAT, IBM 3033; TPASLIST, VAX.

ASCII files of the nuclide ordered table; dBase III DBF files for NUCLIDE ID, IBM PC.

9. TYPICAL RUNNING TIME

Several changes to the data file can be made running FIXISO in less than 15 CPU seconds. DECAYDAT runs in less than 3 CPU seconds.

NUCLIDE ID is interactive.

10. REFERENCES

a Included in package:

J. K. Dickens, Informal Notes (October 1985).

b. Background information:

RSICC Data Package DLC-19/DECAYGAM.

11. CONTENTS OF LIBRARY

Included are the referenced document (a) and a reel of magnetic tape which contains three Fortran programs and the three data libraries ordered by nuclide number, energy and half life written in EBCDIC card images; total records 20,479.

ASCII files (PC-DOS) for IBM PC (1 5.25-in. diskette). DBF files for IBM PC (3 5.25-in. diskettes).

12. DATE OF ABSTRACT

August 1983; updated October 1984, January 1986, April 1986, June 1988, November 1993.

KEYWORD: RADIOACTIVE DECAY SPECTRA

RSICC DATA PACKAGE DLC-163

1. NAME AND TITLE OF DATA LIBRARY

XG-IAEA: X-ray and Gamma-ray Standards For Detector Calibration

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

XG: Executable X-Ray and Gamma-Ray DBASE program.

3. CONTRIBUTOR

International Atomic Energy Agency, Vienna, Austria.

4. HISTORICAL BACKGROUND AND INFORMATION

IAEA established a Coordinated Research Program (CRP) on the Measurements and Evaluation of X- and Gamma-ray Standards for Detector Efficiency Calibration in 1986 with the aim of alleviating the generation of data discrepancies. Representatives of nine research groups and one international organization performed precise measurements and systematic in-depth evaluations of the required decay data. They have also contributed to the development of evaluation methodology and measurement techniques and stimulated a number of such studies. Results of the work finished in 1990 are incorporated in XG-IAEA data base.

5. APPLICATION OF THE DATA

Values of half-lives and photon emission probabilities are given for a selected set of radionuclides that are suitable for detector efficiency calibration.

6. SOURCE AND SCOPE OF DATA

Data were evaluated from the open literature and laboratory reports published over a considerable period of time. The eventual omission of individual values had to be justified on the basis of their quality or other specific grounds. An evaluation procedure was developed for the half-life data. This procedure was also applied to the gamma-ray emission probabilities whenever appropriate. Included for 36 selected radionuclides are three tables of recommended evaluated values and uncertainties of their half-lives; energies and emission probabilities of X-rays, energy range 5-90 keV; energies and emission probabilities of gamma-rays, energy range 14-3600 keV.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAMS

The file XG.EXE is a DBASE program. At the PC prompt, one need only type XG. The data are shown in either nuclide sort or energy sort.

8. DATA FORMAT AND COMPUTER

The data files are in DBASE format; IBM PC.

9. TYPICAL RUNNING TIME

None noted.

10. REFERENCES

H. D. Lemmel, "XG Standards," Informal Notes (1 page) (December 6, 1991).

H. D. Lemmel, "X-ray and Gamma-ray Standards for Detector Calibration," IAEA-TECDOC-619 (September 1991).

11. CONTENTS OF PACKAGE

The package contains the documents referenced, and an executable DBASE program and binary DBASE data files are transmitted on one DS/HD 5.25-inch diskette (1.2MB).

12. DATE OF ABSTRACT

September 1992.

KEYWORDS: MICROCOMPUTER; RADIOACTIVE DECAY SPECTRA

ACKNOWLEDGMENTS

This work was partially supported by the U.S. Department of Energy Office of Energy Research/Basic Energy Sciences and by the Joint Institute for Heavy Ion Research through contract number DE-FG05-87ER40361 with the University of Tennessee, Vanderbilt University and Oak Ridge National Laboratory. Valuable help with the electronic document preparation was provided by A. F. Rice.

INTERNAL DISTRIBUTION

1-2.	Laboratory Records Dept.	7.	J. B. Mannes Schmidt
3.	Laboratory Records, ORNL-RC	8.	R. W. Roussin
4.	Central Research Library	9.	J. E. White
5.	S. Y. Finch	10.	RSICC
6.	M. A. Kuliasha		

EXTERNAL DISTRIBUTION

11. John E. Baublitz, EM-40, Office of Environmental Restoration and Waste Management, U. S. Department of Energy, Washington, DC 20585
12. Mr. Sam E. Berk, Bldg. ER-533 MS G-234/GTN, Div. of Devel. & Tech., Office of Fusion Energy, U.S. Dept. of Energy, Washington, DC 20545
13. Alois J. Burda, End User Support Services Branch, Office of Information Resources Management, Nuclear Regulatory Commission, Washington, DC 20555-0001
14. Dr. Frank Dietrich, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551-0808
15. Kirk Dickens, 367 Jefferson Ave, Oak Ridge, TN 37830-3647
16. Albert Evans, ER-13, J-311, Materials Sciences Division, U.S. Department of Energy, Washington, DC 20585
17. Dr. Sheldon L. Kahala, Acting Tech. Dir. Off. of Research & Testing, Office of Research and Development, DP-20, A-359 GTN, U.S. Department of Energy, Washington, DC 20545
18. R. Kehlet, Director, Defense Special Weapons Agency, ATTN: WEP, 6801 Telegraph Rd., Alexandria, VA 22310-3398
19. Terry R. Lash, Director, Office of Nuclear Energy, U.S. Department of Energy, Washington, DC 20545
20. Robert M. Loesch, GTN270CC, EH-52, U. S. Department of Energy, Germantown, MD 20874-1290
21. Ronald A. Milner, RW-30, 7F-059/GTN, U. S. Department of Energy, OCRWM, Washington, DC 20545
22. Doug Minnema, Mail Stop DP-311, U.S. Department of Energy, 19901 Germantown Road, Washington, DC 20874-1290
- 23-27. Dr. Pavel Oblozinsky, IAEA, P.O. Box 100, A-1400 Vienna
28. E. Tourigny, Chief, Technical Support Branch, NE-443, F-414/GTN, U.S. Department of Energy, Washington, DC 20585