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**Computational Physics and Engineering Division**

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

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## 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.

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ACKNOWLEDGMENTS

## 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 Schaerf[1] 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.

| | |
|---|---|
| ACTIVE-PC: | A Program to Process Gamma or X-ray spectra. |
| AMUSE: | Gamma-Ray Spectra Unfolding Code. |
| ANA: | Code System for Gamma-Ray Spectra Analyses. |
| BOB-7 SERIES: | Theory and Use of Gamma-Ray Spectrum Analysis Codes for Ge(Li) Detectors. |
| CERPI-CEREL: | Code Systems for Automatic Analysis of Gamma-Ray Spectra Obtained with Ge(Li) Detectors. |
| GAMAN: | Qualitative and Quantitative Evaluation of Ge(Li) Gamma-Ray Spectra. |
| GAMANAL. | RADIOACTIVE SPECIES MIX BY GAMMA SPECTRA |
| GAMX1: | A Computer Code System for Evaluating Spectra Peak Areas. |
| GASPAN-ZKD. | GE(LI) DETECTOR & MULTICHANNEL_ANALYSER |
| GAUSS: | A Code system for Analysis of Gamma-Ray Spectra from Ge(Li) Spectrometers. |
| GAUSS6 | EXPERIMENTAL GAMMA_SPECTRA ANAL, ISOTOPE_IDENTIFICATION, DECAY_RATES |
| GRETEL: | Analyzer and Processor of Ge(Li) Gamma-Ray Spectrometric Data. |
| GRPANL: | Code System for Analyzing Ge and Alpha-Particle Detector Spectra. |
| HYPERMET: | Gamma-Ray Spectra Analyzer Germanium Detector |
| JADSPE. | MULTI-CHANNEL GAMMA SPECTRA UNFOLDING |
| RICKI. | INTERACTIVE GAMMA SPECTRA UNFOLDING WITH ISOTOPE IDENTIFICATION |
| SAMPO-LRC: | Gamma-Ray Spectrum Analysis Code. |
| SAMPO80: | Gamma-Ray Spectrum Analysis Method for Minicomputers. |
| SKEWGAUS: | Skewed-Gaussian Line Peak Fitting Code -- Multichannel Analyzer (MCA) Spectra -- Ge(Li) and Semiconductor Detectors. |
| TPASS: | A Gamma-Ray Spectral Data-Reduction and Analysis Code System. |

## 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.

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|---|---|
| ALPHA-M: | Least-Squares Resolution of Gamma-Ray Spectra in Environmental Samples. |
| CONFOLD: | Least-Structure Unfolding Code System for Measured Neutron and Gamma-Ray Spectra. |
| CUPED: | Scintillation Spectrometer Polyenergetic Gamma Photon Experimental Distributions Unfolding Code. |
| DOMUS: | A Program for Decomposing A Two-Dimensional Spectrum |
| FERDO/FERD: | Multichannel Neutron and Gamma-Ray Spectrum Matrix Unfolding Code Systems. |
| FERD-PC: | Interactive Multichannel Neutron and Gamma-Ray Spectrum Matrix Unfolding Code System. |
| NAISAP: | Theory and Use of Gamma-Ray Spectrum Analysis Codes for NaI(Tl) Detectors. |
| RADAK. | MULTICHANNEL_ANALYSER N_SPECTRA & GAMMA_SPECTRA UNFOLDING |
| UNSPEC | X-RAY SPECTRUM UNFOLDING |
| UPEAK: | A Program for Decomposing A One-Dimensional Spectrum |

## 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 ORIGEN[1], 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:

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| 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

1. ORIGEN2.1, 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).

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|---|---|
| ALICE-91:<br><br>ALICE-87:<br><br>ALISO-PC: | Statistical Model Code System with Fission Competition.<br><br>Revised ALICE for Personal Computer.<br><br>Gives Isotopically Weighted Results. |
| CASTHY: | Statistical Model Calculation for Neutron Cross Sections and Capture Gamma-Ray Spectra. |
| EMPIRE: | A Pre-equilibrium Compound Nuclear Model Code For Personal Computers |
| ERINNI: | Optical Model Calculation of Multiple Cascading Particle Emissions. |
| EXIFON-GAMMA: | A Model For Statistical Multistep Direct and Multistep Compound Reactions |
| GNASH-FKK: | Pre-equilibrium, Statistical Nuclear-Model Code System for Calculation of Cross Sections and Emission Spectra. |
| PEGAS: | Pre-Equilibrium-Equilibrium Gamma-and-Spin Code System. |
| PEQAG-2: | A Pre-equilibrium Computer Code With Gamma Emission |
| TNG1: | A Multistep Statistical Model Based on the Hauser-Feshbach Theory For The Evaluation Of Neutron Data. |

## 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:

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| 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. |

## 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.

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| GAMDAT-78: | Library of Gamma-Ray Decay Data for 2055 Radionuclides. |
| GAMTAB: | Radioactive-Decay Gamma-Rays Ordered by Energy and Nuclide. |
| GAMTOT78: | Compilation of Radioactive Decay and Capture Gamma Rays. |
| NFCLIST: | Radionuclide Radiation Data from the Evaluated Nuclear Data File (ENDF/B) for Routine Releases from Nuclear Fuel Cycle Facilities. |
| NUCDECAY: | Nuclear Decay Data for Radiation Dosimetry Calculations for ICRP and MIRD. |
| RADDECAY 4.02: | Radioactive Decay Data for Radiological Assessments. |
| TPASGAM85: | Radioactive Decay Library of Gamma-Ray Energies, Branching Ratios, and Cross Sections. |
| XG-IAEA: | X-ray and Gamma-ray Standards For Detector Calibration |

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