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ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data File
ENDF/B-VI and ENDF/B-VII

Written by the Members of the Cross Sections Evaluation Working Group

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PREFACE

In December 2006, the Cross Section Evaluation Working Group (CSEWG) of the United States released the new ENDF/B-VII.0 library. This represented considerable achievement as it was the 1st major release since 1990 when ENDF/B-VI has been made publicly available. The two libraries have been released in the same format, ENDF-6, which has been originally developed for the ENDF/B-VI library. In the early stage of work on the VII-th generation of the library CSEWG made important decision to use the same formats. This decision was adopted even though it was argued that it would be timely to modernize the formats and several interesting ideas were proposed. After careful deliberation CSEWG concluded that actual implementation would require considerable resources needed to modify processing codes and to guarantee high quality of the files processed by these codes. In view of this the idea of format modernization has been postponed and ENDF-6 format was adopted for the new ENDF/B-VII library.

In several other areas related to ENDF we made our best to move beyond established tradition and achieve maximum modernization. Thus, the "Big Paper" on ENDF/B-VII.0 has been published, also in December 2006, as the Special Issue of Nuclear Data Sheets **107** (1996) 2931-3060. The new web retrieval and plotting system for ENDF-6 formatted data, Sigma, was developed by the NNDC and released in 2007. Extensive paper has been published on the advanced tool for nuclear reaction data evaluation, EMPIRE, in 2007. This effort was complemented with release of updated set of ENDF checking codes in 2009. As the final item on this list, major revision of ENDF-6 Formats Manual was made. This work started in 2006 and came to fruition in 2009 as documented in the present report.

I would like to thank Mike Herman, the ENDF library data manager at the NNDC, as well as Andrej Trkov, IJS Ljubljana, for their dedicated effort on the revised manual. They converted it into LaTeX, carefully checked and implemented updates since the latest 2005 release and consolidated Manual into fully updated and revised version. Many thanks are due to numerous CSEWG members and international colleagues for their useful comments and observations on several draft versions. It should be stressed that even though the Manual is maintained by the United States, active contribution from the international data community is essential for achieving its high quality.

It is my expectation that this major revision will be embraced by the data evaluators as well as members of numerous user communities worldwide.

Upton, June 2009

Pavel Obložinský
CSEWG chair until January 2009

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Chapter 0

INTRODUCTION

This revision of "ENDF-6 Formats Manual" pertains to version 6 of the ENDF formats. The seventh version of the ENDF/B library, namely ENDF/B-VII, uses ENDF-6 formats.

The manual is based on the previous version of the document, revised in June 2005, In some cases the older version from October 1991 was consulted in order to resolve some ambiguities and errors that were introduced when the reference document was translated from WordPerfect in Word format.

Below is a list of changes to the formats and procedures that appear in this edition. In addition, many typographical error corrections and improvements to the text for clarity are included. Users of this manual who note deficiencies or have suggestions are encouraged to contact the National Nuclear Data Center.

Major updates to Manual for Revision June 2009

- Detailed review of the entire manual.
- Conversion to LaTeX.
- Inclusion of recommendations from previous CSEWG Meetings that were not incorporated into the text.
- Inclusion of recommendations from the November 2008 CSEWG Meeting.

0.1 Introduction to the ENDF-6 Format

The ENDF formats and libraries are decided by the Cross Section Evaluation Working Group (CSEWG), a cooperative effort of national laboratories, industry, and universities in the U.S. and Canada, and are maintained by the National Nuclear Data Center (NNDC).

Earlier versions of the ENDF format provided representations for neutron cross sections and distributions, photon production from neutron reactions, a limited amount of charged-particle production from neutron reactions, photo-atomic interaction data, thermal neutron scattering data, and radionuclide production and decay data (including fission products). Version 6 of the formats (ENDF-6) allows higher incident energies, adds more complete descriptions of the distributions of emitted particles, and provides for incident charged particles and photonuclear data by partitioning the ENDF library into sub-libraries. Decay data, fission product yield data, thermal scattering data, and photo-atomic data have also been formally placed in sub-libraries.

0.2 Philosophy of the ENDF System

The ENDF system was developed for the storage and retrieval of evaluated nuclear data to be used for applications of nuclear technology. These applications control many features of the system including the choice of materials to be included, the data used, the formats used, and the testing required before a library is released. An important consequence of this is that each evaluation must be ***complete*** for its intended application. If the required data are not available for some particular reactions, the evaluator should supply them by using systematics or nuclear models.

The ENDF system is logically divided into formats and procedures. ***Formats*** describe how the data are arranged in the libraries and give the formulas needed to reconstruct physical quantities such as cross sections and angular distributions from the parameters in the library. ***Procedures*** are the more restrictive rules that specify what data types must be included, which format can be used in particular circumstances, and so on. Procedures are, generally, imposed by a particular organization, and the library sanctioned by the Cross Section Evaluation Working Group (CSEWG) is referred to as ENDF/B. Other organizations may use somewhat different procedures, if necessary, but they face the risk that their libraries will not work with processing codes sanctioned by CSEWG.

0.2.1 Evaluated Data

An ***evaluation*** is the process of analyzing experimentally measured physical parameters (such as cross sections), combining them with the predictions of nuclear model calculations, and attempting to extract the true values of such parameters. Parameterization and reduction of the data to tabular form produces an ***evaluated data set***. If a written description of the preparation of a unique data set from the data sources is available, the data set is referred to as a ***documented evaluation***.

0.2.2 ENDF/B Library

The ENDF/B library maintained at the National Nuclear Data Center (NNDC) contains the recommended evaluation for each material. Each material is as complete as possible; however, completeness depends on the intended application. For example, when a user is interested in performing a reactor physics calculation or in doing a shielding analysis, he needs evaluated data for all neutron-induced reactions, covering the full range of incident neutron energies, for each material in the system that he is analyzing. Also, the user expects that the file will contain information such as the angular and energy distributions for secondary neutrons. For another calculation, the user might only be interested in some minor isotope activation, and would then be satisfied by an evaluation that contains only reaction cross sections.

ENDF/B data sets are revised or replaced only after extensive review and testing. This allows them to be used as ***standard reference data*** during the lifetime of the particular ENDF/B library version.

There may be other libraries not endorsed by CSEWG that adopt the ENDF-6 format. In the text that follows, any library in ENDF-6 format will be referred to as an ENDF library.

0.2.3 Choices of Data

The data sets contained in the ENDF/B library are those chosen by CSEWG from evaluations submitted for review. The choice is made on the basis of requirements for applications, conformance of the evaluation to the formats and procedures, and performance in testing. The data set that represents a particular material may change when:

- new significant experimental results become available,
- integral tests show that the data give erroneous results, or
- users' requirements indicate a need for more accurate data and/or better representations of the data for a particular material.

New or revised data sets are included in new releases of the ENDF/B library.

0.2.4 Experimental Data Libraries

The CSISRS/EXFOR library of experimentally measured nuclear reaction data is maintained internationally by the Nuclear Reaction Data Centers Network (NRDC)[1]. In addition to numerical data, the CSISRS/EXFOR library contains bibliographic information, as well as details about the experiment (standards, renormalization, corrections, *etc.*).

At the beginning of the evaluation process the evaluator may retrieve the available experimental data for a particular material by direct access to the CSISRS/EXFOR database via the World Wide Web[2]

[1] "http://www-nds.iaea.org/nrdc.html"

[2] "http://www.nndc.bnl.gov/exfor/" or "http://www-nds.iaea.org/exfor/".

0.2.5 Processing Codes

Once the evaluated data sets have been prepared in ENDF format, they can be converted into forms appropriate for testing and actual applications using processing codes. Processing codes that generate pointwise and group-averaged cross sections for use in neutronics calculations from an ENDF library are available. These codes[3] [4] include functions such as resonance reconstruction, Doppler broadening, multigroup averaging, and/or rearrangement into specified interface formats.

The basic data formats for an ENDF library have been developed in such a manner that few constraints are placed on using the data as input to the codes that generate any of the secondary libraries.

0.2.6 Testing

All ENDF/B evaluations go through at least some testing before being released as a part of the library. Phase 1 testing uses a set of utility codes[5] maintained by NNDC for checking and visual inspection by a reviewer to assure that the evaluation conforms to the current formats and procedures, takes advantage of the best recent data, and chooses format options suited to the physics being represented. Phase 2 uses calculations of data testing "benchmarks," when available, to evaluate the usefulness of the evaluation for actual applications.[6] [7] This checking and testing process is a critically important part of the ENDF system.

0.2.7 Documentation

The system is documented by a set of ENDF reports (see Section 0.7) published by the National Nuclear Data Center at Brookhaven National Laboratory. In addition, the current status of the formats, procedures, evaluation process, and testing program is contained in the Summary of the Meetings of the Cross Section Evaluation Working Group.

0.3 General Description of the ENDF System

The ENDF libraries are a collection of documented data evaluations stored in a defined computer-readable format that can be used as the main input to nuclear data processing programs. For this reason, the ENDF format has been constructed with the processing codes in mind. The ENDF format uses 80-character records. For historic reasons the parameters are defined in the old-fashioned form of FORTRAN variables (that is, integers start with

[3] D.E. Cullen, PREPRO 2007 - 2007 ENDF/B Pre-processing Codes, report IAEA-NDS-39, Rev. 13, March 2007

[4] R.E. MacFarlane, D.W. Muir, The NJOY Nuclear Data Processing System, Version 91, LA-12740-M (1994)

[5] C. L. Dunford, ENDF Utility Codes, "http://www.nndc.bnl.gov/nndcscr/endf/"

[6] Cross Section Evaluation Working Group Benchmark Specifications, ENDF-202, 1974 (last updated 1991).

[7] OECD/NEA: The International Criticality Safety Benchmark Evaluation Project (ICSBEP), "http://icsbep.inel.gov/".

the letters I, J, K, L, M, or N, and parameters starting with other letters represent real numbers). A complete list of all the parameters defined for the ENDF-6 format can be found in Appendix A (Glossary).

Each ENDF evaluation is identified by a set of key parameters organized into a hierarchy. Following is a list of these parameters and their definitions.

0.3.1 Library (NLIB, NVER, LREL, NFOR)

A ***library*** is a collection of material evaluations from a recognized evaluation group. Each of these collections is identified by an NLIB number. Currently defined NLIB numbers are given in Table 2. The NVER, LREL and NFOR parameters that describe the version, release number and format of the library are defined in Table 16.

0.3.2 Incident Particles and Data Types (NSUB)

The sub-library distinguishes between different incident particles and types of data using NSUB = 10*IPART+ITYPE. In this formula, IPART=1000*Z+A defines the incident particle; use IPART=0 for incident photons or no incident particle (decay data), use IPART=11 for incident electrons, and IPART=0 for photo-atomic or electro-atomic data. The sub-libraries allowed in ENDF-6 are listed in Table 3.

Sublibraries contain the data for different materials identified by MAT numbers. Each material evaluation contains data blocks referred to as "Files". For the precise definition of the material numbers and Files see Section 0.4.

0.3.2.1 Incident-Neutron Data (NSUB=10)

The procedures for describing neutron-induced reactions for ENDF-6 have been kept similar to the procedures used for previous versions so that current evaluations can be carried over, and in order to protect existing processing capabilities. The new features have most of their impact at high energies (above 5-10 MeV) or low atomic weight (^{2}H, ^{9}Be), and include improved energy-angle distributions, improved nuclear heating and damage capabilities, improved charged-particle spectral data, and the use of R-matrix or R-function resonance parameterization.

Each evaluation starts with a descriptive data and directory, File 1 (see Section 1.1). For fissionable isotopes, sections of File 1 may be present that describe the number of neutrons produced per fission and the energy release from fission.

A File 2 with resonance parameters is always given. For some materials, it may contain only the effective scattering radius, and for other materials, it may contain complete sets of resolved and/or unresolved resonance parameters.

A File 3 with tabulated cross sections is always given. The minimum required energy range is from the threshold or from 10^{-5} eV up to 20 MeV, but higher energies are allowed. There is a section for each important reaction or sum of reactions. The reaction MT-numbers for these sections are chosen based on the emitted particles as described in Section 0.4.3 (Reaction Nomenclature). For resonance materials in the resolved resonance energy range, the cross sections for the elastic, fission, and capture reactions are normally the sums of

Table 1: Key parameters defining the hierarchy of entries in an ENDF file.

Library	NLIB	a collection of evaluations from a specific evaluation group (*e.g.*, NLIB 0=ENDF/B, see Table 2 for details).
Version	NVER	one of the periodic updates to a library in ENDF format (*e.g.*, NVER=7 for ENDF/B-VII). A change of version may imply a change in format, standards, and/or procedures.
Release	LREL	library release number of an intermediate release containing minor updates and corrections of errors after a general release of a library. A release number is appended to the library/version name for each succeeding revision of the data set(*e.g.*, ENDF/B-VI.2 for Release 2 of the ENDF/B-VI library).
Sublibrary	NSUB	a set of evaluations for a particular data type, (*e.g.*, NSUB=4 for radioactive decay data, 10 for incident-neutron data, 12 for thermal neutron scattering data, *etc.*). (See Table 3 for the complete list of sub-libraries).
Format	NFOR	format in which the data is tabulated; tells the processing codes how to read the subsequent data records (*e.g.*, NFOR=6 for ENDF-6).
Material	MAT	integer designation for the target in a reaction sub-library, or the radioactive (parent) nuclide in a decay sub-library; see Section 0.4.1.
Mod	NMOD	"modification" flag; see Section 0.4.1.
File	MF	subdivision of material identified by (MAT) into logical units referred to as Files; each File contains data for a certain class of information (*e.g.*, MF=3 contains reaction cross sections, MF=4 contains angular distributions, *etc.*). MF runs from 1 to 99. (See Table 4 for a complete list of assigned MF numbers).
Section	MT	subdivision of a File identified by (MF) into sections; each section describes a particular reaction or a particular type of auxiliary data (*e.g.*, MT=102 contains capture data, *etc.*). MT runs from 1 to 999. (See Appendix B for a complete list of assigned MT numbers).

Table 2: Currently defined NLIB numbers

NLIB	Library Definition
0	**ENDF/B** - United States Evaluated Nuclear Data File
1	**ENDF/A** - United States Evaluated Nuclear Data File
2	**JEFF** - NEA Joint Evaluated Fission and Fusion File (formerly JEF)
3	**EFF** - European Fusion File (now part of JEFF)
4	**ENDF/B** High Energy File
5	**CENDL** - China Evaluated Nuclear Data Library
6	**JENDL** - Japan Evaluated Nuclear Data Library
21	**SG-23** - Fission product library of the Working Party on Evaluation Cooperation Subgroup-23 (WPEC-SG23)
31	**INDL/V** - IAEA Evaluated Neutron Data Library
32	**INDL/A** - IAEA Nuclear Data Activation Library
33	**FENDL** - IAEA Fusion Evaluated Nuclear Data Library
34	**IRDF** - IAEA International Reactor Dosimetry File
35	**BROND** - Russian Evaluated Nuclear Data File (IAEA version)
36	**INGDB-90** - Geophysics Data
37	**FENDL/A** - FENDL activation evaluations
41	**BROND** - Russian Evaluated Nuclear Data File (original version)

Table 3: Sub-library Numbers and Names

NSUB	IPART	ITYPE	Sub-library Names
0	0	0	Photo-Nuclear Data
1	0	1	Photo-Induced Fission Product Yields
3	0	3	Photo-Atomic Interaction Data
4	0	4	Radioactive Decay Data
5	0	5	Spontaneous Fission Product Yields
6	0	6	Atomic Relaxation Data
10	1	0	Incident-Neutron Data
11	1	1	Neutron-Induced Fission Product Yields
12	1	2	Thermal Neutron Scattering Data
113	11	3	Electro-Atomic Interaction Data
10010	1001	0	Incident-Proton Data
10011	1001	1	Proton-Induced Fission Product Yields
10020	1002	0	Incident-Deuteron Data
10030	1003	0	Incident-Triton Data
20030	2003	0	Incident-Helion (^{3}He) Data
20040	2004	0	Incident-Alpha data
...			

the values given in File 3 and the resonance contributions computed from the parameters given in File 2. An exception to this rule is allowed for certain derived evaluations (see LRP=2 in Section 1.1). In the unresolved resonance range, the self-shielded cross sections will either be sums of File 2 and File 3 contributions, as above, or File 3 values multiplied by a self-shielding factor computed from File 2 (see Sections 2.3.1, 2.4.17).

Distributions for emitted neutrons and other particles or nuclei are given using File 4, a combination of Files 4 and 5, or File 6. As described in more detail in Chapter 4, File 4 is used for simple two-body reactions (elastic, discrete inelastic). Files 4 and 5 are used for simple continuum reactions, which are nearly isotropic, have minimal pre-equilibrium component, and emit only one important particle. File 6 is used for more complex reactions that require energy-angle correlation, that are important for heating or damage, or that have several important products, which must be tallied.

If any of the reaction products are radioactive, they should be described further in File 8. This file indicates how the production cross section is to be determined (from File 3, 6, 9, or 10) and gives minimal information on the further decay of the product. Additional decay information can be retrieved from the decay data sub-library when required.

Note that yields of particles and residual nuclei are sometimes implicit; for example, the neutron yield from reaction A(n,2n) is two and the yield of the product A-1 is one. If File 6 is used, all yields are given explicitly. This is convenient for computing gas production and transmutation cross sections. Branching ratios (or relative yields) for the production of different isomeric states of a radionuclide may be given in File 9. Alternatively, radionuclide isomer-production cross sections can be given in File 10. In the latter case, it is possible to determine the yield by dividing by the corresponding cross section from File 3. File 9 is used in preference to File 10 for reactions described by resonance parameters (*e.g.*, radiative capture).

For compatibility with earlier versions, photon production and photon distributions can be described using File 12 (photon production yields), File 13 (photon production cross sections), File 14 (photon angular distributions), and File 15 (photon energy distributions). Note that File 12 is preferred over File 13 when strong resonances are present (capture, fission). Whenever possible, photons should be given with the individual reaction that produced them using File 12. When this cannot be done, summation MT numbers can be used in Files 12 or 13 as described in Section 0.4.3.8.

When File 6 is used to represent neutron and charged-particle distributions for a reaction, it should also be used for all other emitted particles like photons and recoils. This makes an accurate energy-balance check possible for the reaction. When emitted photons cannot be assigned to a particular reaction, they can be represented using summation MT numbers as described in Section 0.4.3.8.

Finally, covariance data are given in Files 30-40. Procedures for these files are given in Chpaters 30-40.

0.3.2.2 Thermal Neutron Scattering (NSUB=12)

Thermal neutron scattering data[8] are kept in a separate sub-library because the targets are influenced by their binding to surrounding atoms and their thermal motion; therefore, the physics represented[9] requires different formats than other neutron data. The data extend to a few eV for several molecules, liquids, solids, and gases. As usual, each evaluation starts with descriptive data and a directory file (see Section 1.1). The remaining data is included in File 7. Either the cross sections for elastic coherent scattering, if important, are derived from Bragg edges and structure factors, or cross sections for incoherent elastic scattering are derived from the bound cross section and Debye-Waller integral. Finally, scattering law data for inelastic incoherent scattering are given, using the S(α,β) formalism and the short-collision-time approximation.

0.3.2.3 Fission Product Yield Data

Data for the production of fission products are given in different sub-libraries according to the mechanism inducing fission. Currently, sub-libraries are defined for yields from spontaneous fission (NSUB=5), neutron-induced fission product yields (NSUB=11), photo-induced fission product yields (NSUB=1), proton-induced fission product yields (NSUB=10011) and other charged-particle induced fission product yields, where the NSUB value is defined as described in Section 0.3.2. Each material starts with a descriptive data and directory file (see Section 1.1). The remaining data is given in File 8, which contains two sections: independent yields, and cumulative yields. As described in Section 8.3, the format for these two sections is identical. Uncertainty data are self-contained in File 8.

0.3.2.4 Radioactive Decay Data (NSUB=4)

Evaluations of decay data for radioactive nuclides are grouped together into a sub-library. This sub-library contains decay data for all radioactive products (*e.g.*, fission products and activation products). Fission product yields and activation cross sections will be found elsewhere. Each material contains two, three, or four files, and starts with a descriptive data and directory file (see Section 1.1). For materials undergoing spontaneous fission, additional sections in File 1 give the total, delayed, and prompt fission neutron yields. In addition, the spectra of the delayed and prompt neutrons from spontaneous fission are given in File 5. The File 5 formats are the same as for particle-induced fission (see Section 5), and the distributions are assumed to be isotropic in the laboratory system. File 8 contains half-lives, decay modes, decay energies, and radiation spectra (see Section 8.4). Finally, covariance data for the spectra in File 5 may be given in File 35; covariance data of other parameters are self-contained in File 8.

[8] Used for incident neutrons, IPART=1 only.

[9] J.U. Koppel and D.H. Houston, Reference Manual for ENDF Thermal Neutron Scattering Data, General Atomic report GA-8774 (ENDF-269) (Revised and reissued by NNDC, July 1978).

0.3.2.5 Charged-Particle (NSUB≥10010) and Photo-Nuclear (NSUB=0) Sub-libraries

Evaluations for incident charged-particle and photo-nuclear reactions are grouped together into sub-libraries by projectile. As usual, each evaluation starts with a descriptive data and directory file (see Section 1.1). For particle-induced fission or photo-fission, File 1 can also contain sections giving the total, delayed, and prompt number of neutrons per fission, and the energy released in fission. Resonance parameter data (File 2) may be omitted entirely (see LRP=-1 in Section 1.1).

Cross sections are given in File 3. The MT numbers used are based upon the particles emitted in the reaction as described in Section 0.4.3. A special case is the elastic scattering of charged particles, which is discussed separately in Section 0.4.3.1. Explicit yields for all products (including photons) must be given in File 6. In addition, the charged-particle stopping power should be given. If any of the products described by a section of File 6 are radioactive, they should be described further in a corresponding section of File 8. This section gives the half-life, minimum information about the decay chain, and decay energies for the radioactive product. Further details, if required, can be found in the decay data sub-library.

Angular distributions or correlated energy-angle distributions can be given for all particles, recoil nuclei, and photons in File 6. It is also possible to give only the average particle energy for less important reactions, or even to mark the distribution "unknown" (see Section 6.2.1).

Finally, Files 30 through 40 may be used to describe the covariances for charged-particle and photo-nuclear reactions.

0.3.2.6 Photo-Atomic Interaction Data (NSUB=3)

Incident photon reactions with the atomic electrons[10] are kept in a separate sub-library. These data are associated with elements rather than isotopes. Each material starts with a descriptive data and directory file (see Section 1.1), as usual. In addition, the material may contain File 23 for photon interaction cross sections, and File 27 for atomic form factors.

0.3.2.7 Electro-Atomic Interaction Data (NSUB=113)

Incident electron reactions with the atomic electrons are also kept in a separate sublibrary. These data are again associated with elements rather than isotopes. Each material starts with a descriptive data and directory file (see Section 1.1), as usual. In addition, File 23 is given for the elastic, ionization, bremsstrahlung, and excitation cross sections, and File 26 is given for the elastic angular distribution, the bremsstrahlung photon spectra and energy loss, the excitation energy transfer, and the spectra of the scattered and recoil electrons associated with subshell ionization.

[10] D.E. Cullen, et al., EPDL97: the Evaluated Photon Data Library, '97 Version, UCRL–50400, Vol. 6, Rev. 5, September 1997.

0.3.2.8 Atomic Relaxation Data (NSUB=6)

The target atom can be left in an ionized state due to a variety of different types of interactions, such as photon or electron induced ionization, internal conversion, *etc.* This section provides the data needed to describe the relaxation of an ionized atom back to neutrality. This includes subshell energies, transition energies, transition probabilities, and other parameters needed to compute the X-ray and electron spectra due to atomic relaxation.

The materials are elements. Each material starts with a descriptive data and directory file (see Section 1.1), as usual. In addition, File 28 is given containing the relaxation data for all the subshells defined in the photo-atomic or electro-atomic sublibraries.

0.4 Contents of an ENDF Evaluation

For a given sub-library (NSUB) that defines the projectile and the type of data, the target material for a reaction evaluation or the radioactive nuclide for a decay evaluation is specified by the material (MAT) number. An evaluation for a material is further subdivided into data blocks called "Files", identified by the MF-number. Sections within individual Files are identified by the MT-numbers, which indicate the type of data represented by a section and the products resulting from the reaction.

0.4.1 Material (MAT, MOD)

A ***material*** may be a single nuclide, a natural element containing several isotopes, or a mixture of several elements (compound, alloy, molecule, *etc.*). A single isotope can be in the ground state or an excited (or isomeric) state. Each material in an ENDF library is assigned a unique identification number, designated by the symbol MAT, which ranges from 1 to 9999.[11]

The assignment of MAT numbers for ENDF/B libraries is made on a systematic basis assuming uniqueness of the four digit MAT number for a material. A material will have the same MAT number in each sub-library (decay data, incident neutrons, incident charged particles, *etc.*).

One hundred MAT numbers ($Z01$-$Z99$) have been allocated to each element Z, through Z = 98. Natural elements have MAT numbers $Z00$. The MAT numbers for isotopes of an element are assigned on the basis of increasing mass in steps of three, allowing for the ground state and two metastable states.[12] In the ENDF/B files, which are application oriented, the evaluations of neutron excess nuclides are of importance, since this category of nuclide is required for decay heat applications. Therefore, the lightest stable isotope is assigned the MAT number $Z25$ so that the formulation can easily accommodate all the neutron excess nuclides.

[11] The strategy for assigning MAT numbers for ENDF/B libraries is described here; other libraries may have different schemes.

[12] This procedure leads to difficulty for the nuclides of xenon, cesium, osmium, platinum, *etc.*, where more than 100 MAT numbers could be needed and some decay data where more than two isomeric states might be present.

For the special cases of elements from einsteinium to lawrencium (Z$\geq$ 99) MAT numbers 99xx are assigned, where xx = 30, 25, 20, 15, and 12 for elements 99 to 103 respectively; such a scheme covers all known nuclides with allowance for expansion.

For mixtures, compounds, alloys, and molecules, MAT numbers between 0001 and 0099 are assigned on a special basis (see Appendix C).

The above conventions are adopted in ENDF/B libraries and are recommended (but not mandatory) in other libraries in ENDF-6 format.

All versions of a data set (*i.e.*, the initial release, revisions, or total re-evaluations) are indicated using the material "modification" MOD number. For example, for the initial release of ENDF/B-VI, the modification flag for each material (MAT) and section (MT) carried over from previous versions is set to zero (MOD=0); for new evaluations they are set to one (MOD=1). Each time a change is made to a material, the modification flag for the material is incremented by one. The modification flag for each section changed in the revised evaluation is set equal to the new material modification number. If a complete re-evaluation is performed, the modification flag for every section is changed to equal the new material "modification" number.

As an example, consider the following. Evaluator X evaluates a set of data for ^{235}Uand transmits it to the NNDC. The Center assigns the data set a MAT number of 9228 subject to CSEWG's approval of the evaluation. This evaluation has "modification" flags equal to 1 for the material and for all sections. Should the evaluation of material 9228 subsequently be revised and released with CSEWG's approval, the material will be assigned MOD flag of 2. This material would have MOD flags of 2 on each revised section, but the unchanged sections will have MOD flags of 1.

0.4.2 ENDF Data Blocks (Files - MF)

A "File" in the ENDF nomenclature is a block of data in an evaluation that describes a certain data type. The list of allowed Files (MF) and a description of their usage in different sub-libraries is given in Table 4.

With respect to the earlier versions of the ENDF formats the following MF numbers have been retired: 16, 17, 18, 19, 20, 21, 22, 24, and 25.

The structure and the contents of the Files are described in details in the Chapters that follow.

0.4.3 Reaction Nomenclature (MT)

The following paragraphs explain how to choose MT numbers for particle-induced and photonuclear reactions in ENDF-6. A complete list of the definitions of the MT numbers can be found in Appendix B.

0.4.3.1 Elastic Scattering

Elastic scattering is a two-body reaction that obeys the kinematic equations given in Appendix E. The sections are labeled by MT=2 (except for photo-atomic data, see Chapter 23). For incident neutrons, the elastic scattering cross section is determined from File 3 together

Table 4: Definitions of File Types (MF)

MF	Description
1	General information
2	Resonance parameter data
3	Reaction cross sections
4	Angular distributions for emitted particles
5	Energy distributions for emitted particles
6	Energy-angle distributions for emitted particles
7	Thermal neutron scattering law data
8	Radioactivity and fission-product yield data
9	Multiplicities for radioactive nuclide production
10	Cross sections for radioactive nuclide production
12	Multiplicities for photon production
13	Cross sections for photon production
14	Angular distributions for photon production
15	Energy distributions for photon production
23	Photo- or electro-atomic interaction cross sections
26	Electro-atomic angle and energy distribution
27	Atomic form factors or scattering functions for photo-atomic interactions
28	Atomic relaxation data
30	Data covariances obtained from parameter covariances and sensitivities
31	Data covariances for nu(bar)
32	Data covariances for resonance parameters
33	Data covariances for reaction cross sections
34	Data covariances for angular distributions
35	Data covariances for energy distributions
39	Data covariances for radionuclide production yields
40	Data covariances for radionuclide production cross sections

with resonance contributions, if any, from File 2. The angular distribution of scattered neutrons is given in File 4.

For incident charged particles, the Coulomb scattering makes it impossible to define an integrated cross section, and File 3, MT=2 contains either a dummy value of 1.0 or a "nuclear plus interference" cross section defined by a particular cutoff angle. The rest of the differential cross section for the scattered particle is computed from parameters given in File 6, MT=2 (see Section 6.2.6).

0.4.3.2 Simple Single Particle Reactions

Many reactions have only a single particle and a residual nucleus (and possibly photons) in the final state. These reactions are associated with well-defined discrete states or a continuum of levels in the residual nucleus, or they may proceed through a set of broad levels that may be treated as a continuum. The MT numbers to be used are given in Table 5.

Table 5: Definitions of MT numbers of Simple Single Particle Reactions

Discrete	**Continuum**	**Discrete + Continuum**	**Emitted Particle**
50-90	91	4	n
600-648	649	103	p
650-698	699	104	d
700-748	749	105	t
750-798	799	106	^{3}He
800-848	849	107	α

By definition, the emitted particle is the lighter of the two particles in the final state.

If the reaction is associated with a discrete state in the residual nucleus, use the first column of numbers in Table 5. For example, neutron emission MT=50 leaves the residual nucleus in the ground state, MT=51 leaves it in the first excited state, MT=52 in the second, and so on. A similar convention applies to all other reactions. The elastic reaction uses MT=2 as described above and the emitted particle is of the same type as the incident particle; therefore, do not use MT=50 for incident neutrons, do not use MT=600 for incident protons, and so on. For incident neutrons, the discrete reactions are assumed to obey two-body kinematics (see Appendix E), and the angular distribution for the particle is given in File 4 or File 6 (except for MT=2). If possible, the emitted photons associated with discrete levels should be represented in full detail using the corresponding MT numbers in File 6 or File 12. For incident charged particles, the emitted particle must be described in File 6. A two-body law can be used for narrow levels, but broader levels can also be represented using energy-angle correlation. Photons associated with the particle should be given in the same section (MT) of File 6 when possible.

If the reaction is associated with a range of levels in the residual nucleus (*i.e.*, continuum), use the second column of MT numbers. For incident neutrons, Files 4 and 5 are allowed for compatibility with previous versions, but it may be necessary to use File 6 to obtain the desired accuracy. When Files 4 and 5 are used, photons should be given in File 12 using the same MT number if possible. For more complicated neutron reactions or incident charged particles, File 6 must be used for the particle and the photons.

The "sum" MT numbers (3rd column in Table 5) are used in File 3 for the sum of all the other reactions in that row, but they are not allowed for describing particle distributions in Files 4, 5, or 6. As an example, a neutron evaluation might contain sections with MF/MT=3/4, 3/51, 3/91, 4/51, and 6/91. A deuteron evaluation might contain sections with 3/103, 3/600, and 6/600 (the two sections in File 3 would be identical). For a neutron evaluation with no 600-series distributions or partial reactions given, MT=103-107 can appear by themselves; they are simply components of the absorption cross section.

In some cases, it is difficult to assign all the photons associated with a particular particle to the reactions used to describe the particle. In such cases, these photons can be described using the "sum" MT numbers in File 12 or 13 (for neutrons) or in File 6 (for other projectiles).

Some examples of simple single-particle reactions are listed in Table 6. Nomenclature z_n for the emitted particle implies particle "z" emission with residual in the n-th discrete level

state.

Table 6: Examples of simple single-particle reactions

Reaction	**MT**
^{9}Be(α,n$_0$)^{12}C	50
Fe(n,n$_c$)Fe	91
^{2}H(d,p$_0$)^{3}He	600
^{6}Li(t,d$_0$)^{7}Li	650
^{6}Li(t,d$_1$)^{7}Li	651

For the purposes of this manual, reactions are written as if all prompt photons have been emitted; that is, the photons do not appear explicitly in the reaction nomenclature. Therefore, no "*" is given on Li in the last example above that would signify the excited state of the nucleus.

0.4.3.3 Simple Multi-Particle Reactions

If a reaction has only two to four particles, a residual nucleus, and photons in the final state, and if the residual nucleus does not break up, it will be called a "simple multi-particle reaction." The MT numbers that can be used are listed in Table 7.

Table 7: Examples of simple multi-particle reactions

MT	**Emitted Particles**	**MT**	**Emitted Particles**
11	2nd	37	4n
16	2n	41	2np
17	3n	42	3np
22	nα	44	n2p
23	n3α	45	npα
24	2nα	108	2α
25	3nα	109	3α
28	np	111	2p
29	n2α	112	pα
30	2n2α	113	t2α
32	nd	114	d2α
33	nt	115	pd
34	n^{3}He	116	pt
35	nd2α	117	dα
36	nt2α		

For naming purposes, particles are always arranged in ZA order; thus, (n,np) and (n,pn) are summed together under MT=28. In addition, there must always be a residual particle. By definition, it is the particle or nucleus in the final state with the largest ZA. This means that the reaction d+t$\rightarrow$ n+α must be classified as the reaction ^{3}H(d,n)^{4}He (MT=50) rather

than the reaction ^{3}H(d,nα) (MT=22). The cross sections for these reactions will be found in File 3, as usual.

This list is not exhaustive, and new MT numbers can be added if necessary. However, some reactions are more naturally defined as "breakup" or "complex" reactions (see below).

For compatibility with previous versions, Files 4 and 5 are allowed in the incident-neutron sub-library. In this case, the particle described in Files 4 and 5 is the first one given under "Emitted Particles" above. At high neutron energies, the use of File 6 is preferred because it allows to describe energy-angle correlated distributions resulting from pre-equilibrium effects for more than one kind of particle. Using File 6 also makes it possible to give an energy distribution for the recoil nucleus and photons. These distributions are needed in calculating nuclear heating and radiation damage. If Files 4/5 are used, photons should be given in File 12 or 13 using the same MT number when possible. In some cases the photons cannot be assigned to individual reactions, in which case their lumped contribution can be described as the nonelastic cross section with MT=3, as described below.

For charged-particle sub-libraries, File 6 must be used for these reactions and should include recoils and photons. If the photons cannot be assigned to a particular reaction, the nonelastic MT=3 can be used as described below.

0.4.3.4 Breakup Reactions

A number of important reactions can be described as proceeding in two steps: first, one or several particles are emitted as in the simple reactions described above, then the remaining nuclear system either breaks up or emits another particle. In the nomenclature of ENDF-6, these are both called "breakup reactions." For ENDF/B-V, these reactions were represented using special MT numbers or "LR flags". For ENDF/B-VI, the preferred representation uses File 3 and File 6. The same MT numbers are used as for the simple reactions described above. The cross section goes in File 3 as usual, but a special LR flag is used to indicate that this is a breakup reaction (see below). The yield and angular distribution or energy-angle distribution for each particle emitted before breakup is put into File 6. In addition, yields and distributions for all the breakup products are allowed in File 6. For photo-nuclear and charged-particle sub-libraries, the photons are also given in File 6; but for neutron sub-libraries, the photons may be given in Files 6 or 12-15. The approach of using File 6 provides complete accounting of particle and recoil spectra for transport, heating, and damage calculations. It also provides a complete accounting of products for gas production and activation calculations. Finally, it does all of this without requiring a large list of new MT numbers.

Some examples of breakup reactions are listed in Table 8. Nomenclature z_n for the emitted particle implies particle "z" emission with residual in the n-th discrete level state.

By convention, the particles are arranged in Z, A order in each set of parentheses. This leads to ambiguity in the choice of the intermediate state. For example,two possibilities of representation exist for neutrons incident on a ^{12}C target:

^{12}C(n,n') ^{12}C $\rightarrow 3\alpha$

^{12}C(n,α) ^{9}Be $\rightarrow$ n+2α

and similarly, there are four possible representations for tritons incident on a ^{7}Li target:

Table 8: Examples of breakup reactions

Reaction	**MT**
^{3}H(t,n$_0$) ^{5}He $\rightarrow$ n+α	50
^{6}Li(d,n$_3$) ^{7}Be $\rightarrow$ ^{3}He+α	53
^{7}Li(n,n$_c$) ^{7}Li $\rightarrow$ t+α	91
^{7}Li(t,2n) ^{8}Be $\rightarrow$ 2α	16
^{7}Li(p,d$_1$) ^{6}Li $\rightarrow$ d+α	651
^{9}Be(a,n$_3$) ^{12}C $\rightarrow$ 3α	53
^{16}O(n,n$_6$) ^{16}O $\rightarrow$ α+^{12}C	56

^{7}Li(t,2n) ^{8}Be $\rightarrow$ 2α
^{7}Li(t,n) ^{9}Be $\rightarrow$ n+2α
^{7}Li(t,α) ^{6}He $\rightarrow$ 2n+α
^{7}Li(t,nα) ^{5}He $\rightarrow$ n+α

The evaluator must either choose one channel, partition the reaction between several channels, or use the "complex reaction" notation (see below). Care must be taken to avoid double counting.

In some cases, a particular intermediate state can break up by more than one path; for example:
^{6}Li(d,p$_4$) ^{7}Li $\rightarrow$ t+α E$_x$ = 7.47 MeV,
^{6}Li(d,p$_4$) ^{7}Li $\rightarrow$ n+^{6}Li.

If two channels are both given under the same MT number, File 6 is used to list the emitted particles and to give their fractional yields. The notation to be used for this type of reaction is:
^{6}Li(d,p$_4$)^{7}Li $\rightarrow$ X.
where "X" designates all reaction products.

Note that the Q-value calculated for the entire reaction is not well defined. Another option is to split the reaction up and use two consecutive MT numbers as follows:
^{6}Li(d,p$_4$) ^{7}Li $\rightarrow$ t+α Ex=7.47 MeV, MT=604,
^{6}Li(d,p$_5$) ^{7}Li $\rightarrow$ n+^{6}Li Ex=7.4701 MeV, MT=605.

The same proton distribution would be given for MT=604 and 605. The mass-difference Q-value is well defined for both reactions, but the level index no longer corresponds to real levels.

The choice between the "simple multi-particle" and "breakup" representations should be based on the physics of the process. As an example, an emission spectrum may show several peaks superimposed on a smooth background. If the peaks can be identified with known levels in one or more intermediate systems, they can be extracted and represented by breakup MT numbers. The remaining smooth background can often be represented as a simple multi-particle reaction.

As described above, the MT number for a simple reaction indicates which particles are emitted. However, complex breakup reactions emit additional particles. The identity of these additional particles can be determined from LR or File 6.

Table 9: Identification of additional particles in File 6

LR	Meaning
0	Simple reaction. Identity of the product is implicit in MT.
1	Complex or breakup reaction. The identity of all products is given explicitly in File 6.
22	α emitted (plus residual, if any)
23	3α emitted (plus residual, if any)
24	nα emitted (plus residual, if any)
25	2nα emitted (plus residual, if any)
28	p emitted (plus residual, if any)
29	2α emitted (plus residual, if any)
30	n2α emitted (plus residual, if any)
32	d emitted (plus residual, if any)
33	t emitted (plus residual, if any)
34	^{3}He emitted (plus residual, if any)
35	d2α emitted (plus residual, if any)
36	t2α emitted (plus residual, if any)
39	internal conversion
40	electron-positron pair formation

The values LR=22-36 are provided for compatibility with ENDF/B-V. Some examples of their use are given in Table 10

Table 10: Some examples of LR values

Reaction	MT	LR
^{6}Li(n,n$_1$) ^{6}Li $\rightarrow$ d+α	51	32
^{7}Li(n,n$_c$) ^{7}Li $\rightarrow$ t+α	91	33
^{10}B(n,n$_{12}$) ^{10}B $\rightarrow$ d+2α	62	35
^{12}C(n,n$_2$) ^{12}C $\rightarrow$ 3α	52	23
^{16}O(n,n$_1$) ^{16}O $\rightarrow$ e$^+$+e$^-$+^{16}O	51	40
^{16}O(n,n$_6$) ^{16}O $\rightarrow$ α+^{12}C	56	22

Note that the identity of the residual must be deduced from MT and LR. Only the first particle is described in File 4 and/or File 5; the only information available for the breakup products is the net energy that can be deduced from kinematics.

The use of LR=1 and File 6 is preferred for new evaluations because explicit yields and distributions can be given for all reaction products.

0.4.3.5 Complex Reactions

At high energies, there are typically many reaction channels open, and it is difficult to decompose the cross section into simple reactions. In such cases, the evaluation should use MT=5. This complex reaction identifier is defined as the sum of all reactions not given explicitly elsewhere in this evaluation. As an example, an evaluation might use only MT=2

and 5. Sections of File 6 with MT=5 and the correct energy-dependent yields would then represent the entire nonelastic neutron spectrum, the entire proton spectrum, and so on. A slightly more refined evaluation might use MT=2, 5, 51-66, and 600-609. In this case, MT=5 would represent all the continuum neutron and proton emission. The discrete levels would be given separately to represent the detailed angular distribution and two-body kinematics correctly. The notation used for complex reactions is, for example, ^{6}Li(d,X).

0.4.3.6 Radiative Capture

The radiative capture reaction is identified by MT=102. For neutron sublibraries, the only products are usually photons, and they are represented in Files 6 or 12-15. Note that File 6 or 12 must be used for materials with strong resonances. For charged-particle libraries, simple radiative capture reactions must be represented using File 3 and File 6. In addition, radiative capture followed by breakup is common for light targets; an example is d+t$\rightarrow$ γ+n+α, which is written as a breakup reaction ^{3}H(d,γ)^{5}He(nα) for the purposes of this format. This reaction is represented using MT=102 with the special breakup flag set in File 3. The gamma, neutron, and alpha distributions are all given in File 6.

0.4.3.7 Fission

The nomenclature used for fission is identical to that used in previous versions of the ENDF format.

Table 11: Definition of MT numbers related to fission

MT	Meaning	Description
18	(z,xf)	total prompt fission
19	(z,f)	first chance fission
20	(z,nf)	second chance fission
21	(z,2nf)	third chance fission
38	(z,3nf)	fourth chance fission
452	$\overline{\nu_T}$	total number of neutrons per fission
455	$\overline{\nu_d}$	number of delayed neutrons per fission
456	$\overline{\nu_p}$	number of prompt neutrons per fission
458		components of energy release in fission

Cross sections (File 3) can be given using either MT=18 or the combination of MT=19, 20, 21, and 38. In the latter case, MT=18 may be given and must contain the sum of the partial reactions.

0.4.3.8 Nonelastic Reaction for Photon Production

Whenever possible, the same MT number should be used to describe both the emitted particle and the photons. However, this is usually only possible for discrete photons from low-lying levels, radiative capture, or for photons generated from nuclear models. Any photons that cannot be assigned to a particular level or particle distribution can be given in

a section with the nonelastic summation reaction MT=3 in File 6, 12, or 13 (for neutrons) or in File 6 (for other projectiles). As described in Section 0.4.3.2, MT=4, 103, 104, 105, 106, and 107 can also be used as summation reactions for photon production in Files 12 and 13.

0.4.3.9 Special Production Cross Sections

A special set of production cross sections are provided, mostly for use in derived libraries. The list is given in Table 12.

Table 12: Special MT numbers for particle production

MT	Meaning
201	neutron production
202	photon production
203	proton production
204	deuteron production
205	triton production
206	^{3}He production
207	α production

Each one is defined as the sum of the cross section times the particle yield over all reactions (except elastic scattering) with that particle in the final state. The yields counted must include implicit yields from reaction names, LR flags, or residual nuclei in addition to explicit yields from File 6. As an example, for an evaluation containing the reactions (n,α) (MT=107), and (n,n′3α) (MT=91, LR=23), the helium production cross section would be calculated using

MT207 = MT107 + 3×MT91.

The cross section in File 3 is barns per particle (or photon). A corresponding distribution can be given using Files 4 and 5, or the distribution can be given using File 6 with the particle yield of 1.0. These MT numbers will ordinarily be used in File 3 of special gas production libraries.

0.4.3.10 Auxiliary MT Numbers

Several MT numbers are used to represent auxiliary quantities instead of cross sections. The values 151, 451, 452, 454, 455, 456, 457, 458, and 459 have already been mentioned. Additional values are defined in Table 13

The continuous-slowing-down parameters (MT=251-253) and the heat production cross sections (MT=301-450) are usually used in derived libraries only. A complete list of reaction MT numbers and auxiliary MT numbers is given in Appendix B.

0.4.3.11 Sum Rules for ENDF

A number of ENDF reaction types can be calculated from other reactions. Whenever one or more constituting reactions are present, the reaction defined by the summation rules is

Table 13: Auxiliary MT numbers

MT	Meaning
251	μ_L, average cosine of the angle for elastic scattering (laboratory system). Derived files only.
252	ξ, average logarithmic energy decrement for elastic scattering. Derived files only.
253	γ, average of the square of the logarithmic energy decrement, divided by $2 \times \xi$. Derived files only.
301-450	Energy release rate parameters (eV-barns) for the reaction obtained by subtracting 300 from this MT; *e.g.*, 301 is total kerma, 407 is kerma for (n,α), *etc.* Derived files only.
851-870	Special series used only in covariance files (MF=31-40) to give covariances for groups of reactions considered together (lumped partials). See Chpater 30.

redundant and must be consistent with the sum of the constituting reactions. The rules for these summations follow in Table 14.

Table 14: ENDF sum rules for cross sections

MT	$\sum$MT	Meaning
1	2, 3	Total cross sections (incident neutrons only)
3	4-5, 11, 16-18, 22-37, 41-42, 44-45	Non-elastic
4	50-91	Total of neutron level cross sections (z,n)
18	19-21, 38	Total fission
27	18, 101	Total absorption
101	102-117	Neutron disappearance
103	600-649	Total of proton level cross sections (z,p)
104	650-699	Total of deuteron level cross sections (z,d)
105	700-749	Total of triton level cross sections (z,t)
106	750-799	Total of ^{3}He level cross sections (z,^{3}He)
107	800-849	Total of alpha level cross sections (z,α)

Note: Reactions corresponding to MT 3, 4, 18, 27, 101, 103-107 are redundant when one or more of their constituting components are present. They must be computed and accounted for internally, when reconstructing cross sections by summation, even if they do not appear in the file explicitly.

0.5 Representation of Data

0.5.1 Definitions and Conventions

The data given in all sections always use the same set of units. These are summarized in Table 15.

Table 15: Summary of ENDF units

Quantity	**Units**
energies	electron-volts (eV)
angles	dimensionless cosines of the angle
cross sections	barns
temperatures	Kelvin
mass	units of the neutron mass
angular distributions	probability per unit-cosine
energy distributions	probability per electron-volt
energy-angle distributions	probability per unit-cosine per electron-volt
half life	seconds

The first record of every section contains a ZA number that identifies the specific material. ZA variants are also employed to identify projectiles and reaction products. In most cases, ZA is constructed by

$$\mathrm{ZA} = 1000.0 \times Z + A,$$

where Z is the atomic number and A is the mass number for the material. If the material is an element containing two or more naturally occurring isotopes in significant concentrations, A is taken to be 0.0. For mixtures, compounds, alloys, or molecules, special ZA numbers between 1 and 99 can be defined (see Appendix C).

A material, incident particle (projectile), or reaction product is also characterized by a quantity that is proportional to its mass relative to that of the neutron. Typically, these quantities are denoted as AWR, AWI, or AWP for a material, projectile, or product, respectively. For example, the symbol AWR is defined as the ratio of the mass of the material to that of the neutron.[13] Another way to say this is that "all masses are expressed in neutron units." For materials which are mixtures of isotopes, the abundance weighted average mass is used.

0.5.1.1 Atomic Masses Versus Nuclear Masses

Mass quantities for materials (AWR for all Z) and "heavy" reaction products (AWP for $Z > 2$) should be expressed in atomic units, *i.e.*, the mass of the electrons should be included. Mass quantities for incident particles (AWI) and "light" reaction products (AWP for $Z \leq 2$) should be expressed in nuclear mass units. For neutrons, this ratio is 1.00000. For charged particles likely to appear in ENDF files, see Appendix H.

0.5.2 Interpolation Laws

Many types of ENDF data are given as a table of values on a defined grid with an interpolation law to define the values between the grid points. Simple one-dimensional "graph paper"

[13] See Appendix H for neutron mass.

interpolation schemes, a special Gamow interpolation law for charged-particle cross sections, simple Cartesian interpolation for two-dimensional functions, and two non-Cartesian schemes for two-dimensional distributions are allowed.

0.5.2.1 One-dimensional Interpolation Schemes

Consider how a simple function $y(x)$, which might be a cross section, $\sigma(E)$, is represented. $y(x)$ is represented by a series of tabulated values, pairs of x and $y(x)$, plus a method for interpolating between input values. The pairs are ordered by increasing values of x. There will be NP values of the pair, x and $y(x)$ given. The complete region over which x is defined is broken into NR interpolation ranges. An interpolation range is defined as a range of the independent variable x in which a specified interpolation scheme can be used; *i.e.,* the same scheme gives interpolated values of $y(x)$ for any value of x within this range. To illustrate this, see Figure 1 and the definitions, below:

$x(n)$	is the nth value of x,
$y(n)$	is the nth value of y,
NP	is the number of pairs (x and y) given,
INT(m)	is the interpolation scheme identification number used in the mth range,
NBT(m)	is the value of n separating the mth and the $(m+1)^{th}$ interpolation ranges.

The list of allowed interpolation schemes is given in Table 16.

Table 16: Definition of Interpolation Types

INT	**Interpolation Scheme**
1	y is constant in x (constant, histogram)
2	y is linear in x (linear-linear)
3	y is linear in $\ln(x)$ (linear-log)
4	$\ln(y)$ is linear in x (log-linear)
5	$\ln(y)$ is linear in $\ln(x)$ (log-log)
6	special one-dimensional interpolation law, used for charged-particle cross sections only
11-15	method of corresponding points (follow interpolation laws of 1-5)
21-25	unit base interpolation (follow interpolation laws of 1-5)

Interpolation code, INT=1 (constant), implies that the function is constant and equal to the value given at the lower limit of the interval.

Note that where a function is discontinuous (for example, when resonance parameters are used to specify the cross section in one range), the value of x is repeated and a pair (x, y) is given for each of the two values at the discontinuity (see Figure 1).

A one-dimensional interpolation law, INT=6, is defined for charged-particle cross sections and is based on the limiting forms of the Coulomb penetrabilities for exothermic reactions

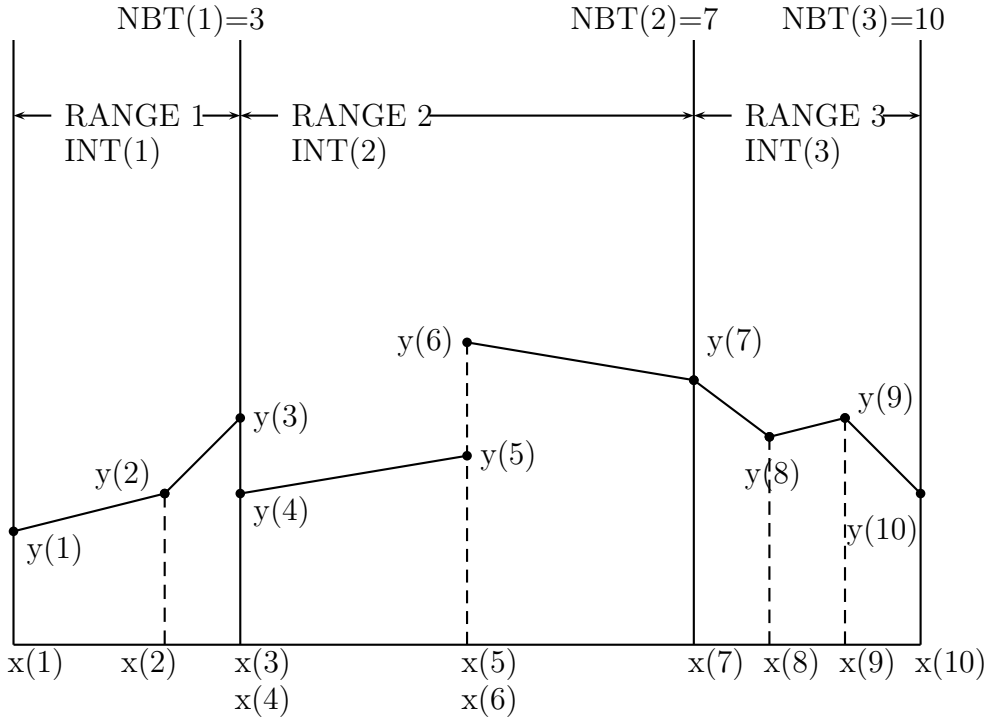

Figure 1: Interpolation of a tabulated one-dimensional function for a case with NP=10, NR=3.

at low energies and for endothermic reactions near the threshold. The expected energy dependence is:

$$\sigma = \frac{A}{E} \exp\left[-\frac{B}{\sqrt{E-T}}\right] \tag{1}$$

where

$T =$ zero for exothermic reactions with $Q > 0$ and

equal to kinematic threshold energy for endothermic reactions with $Q \leq 0$.

Note that this formula gives a concave upward energy dependence near $E = T$ that is quite different from the behavior of the neutron cross sections.

This formula can be converted into a two-point interpolation scheme using

$$B = \frac{\ln \frac{\sigma_2 E_2}{\sigma_1 E_1}}{\frac{1}{\sqrt{E_1 - T}} - \frac{1}{\sqrt{E_2 - T}}} \tag{2}$$

and

$$A = \exp\left[\frac{B}{\sqrt{E_1 - T}}\right] \sigma_1 E_1 \tag{3}$$

where E_1, σ_1 and E_2, σ_2 are two consecutive points in the cross-section tabulation.

This interpolation method should only be used for E close to T. At higher energies, non-exponential behavior will normally begin to appear, and linear-linear interpolation is more suitable.

0.5.2.2 Two-Dimensional Interpolation Schemes

Three schemes are provided for two-dimensional interpolation:

1. simple Cartesian interpolation, wherein one simply interpolates the function values along constant lines of initial and final energy values,
2. a method called unit-base transform, and
3. the method of corresponding energies.

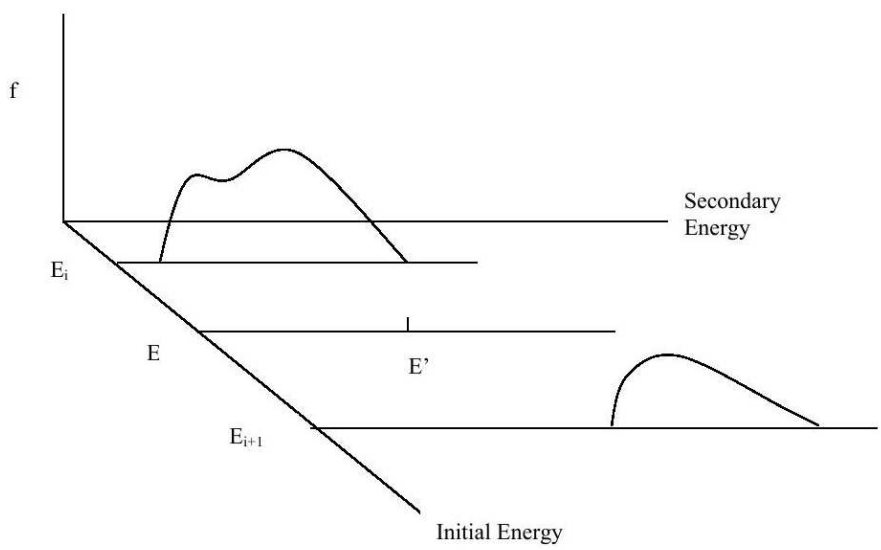

Figure 2: Interpolation between Two-Dimensional Panels.

Consider Figure 2. Here E is the initial energy and there are panels at and E_i and E_{i+1}. The panels describe the probabilities of scattering from these energies to other energies; *e.g.*, $f(E_i, E_i')$ and $f(E_{i+1}, E_{i+1}')$ are generally probability distributions that will integrate to unity, when they are integrated over all E'. These panels will be presented using the usual tabular schemes for arrays, or may be given in the form of an analytic expression.

For the case of simple Cartesian interpolation, intermediate values are determined by interpolating along lines of constant E and E' as noted earlier. Assume that all interpolation schemes are linear-linear in energy and that one wants to determine a value for a distribution at $E \in (E_i, E_{i+1})$. The equation for this is:

$$f(E, E') = f(E_i, E') + \frac{E - E_i}{E_{i+1} - E_i} \left[f(E_{i+1}, E') - f(E_i, E') \right]. \tag{4}$$

An examination of the above figure illustrates the major problem with Cartesian interpolation; viz., that the panel at E will have features from the lower panel at the low end, and from the upper panel at the high end. This, of course, is reasonable, but the resulting function will tend to have artificial peaks when the distributions shift as a function of energy, as is usually the case.

The unit-base transform was devised to try to reduce the non-physical characteristics of Cartesian interpolation. In this case, the data at the two panels surrounding E are transformed to a unit base where the new functions vary according to a variable x that ranges from 0 to 1.

$$x \equiv \frac{E' - E'_i}{E'_i(N) - E'_i(1)}. \tag{5}$$

In this case, $E'_i(1)$ is the energy of the first sink energy in the panel at E_i and $E'_i(N)$ is the last point. An exactly analogous equation is used to define the value of x at E_{i+1} and at E. From here, the interpolation is made using an expression such as shown in equation (4) except that it is made at a constant value of x. Special care must be taken to properly account for the integrals of the panel; i.e.,

$$\int dE' \; f(E') = \int dx \; g(x), \tag{6}$$

which requires:

$$f(E') \; dE' = g(x) \; dx, \tag{7}$$

or

$$g(x) = f(E') \left| \frac{dE'}{dx} \right|. \tag{8}$$

The latter radical is the Jacobian that is required for the transformation to the unit-base space and is determined from equation (5). In other words, when equation (4) is used, the interpolation is made at constant values of x and the function values must be multiplied by the Jacobians for the respective panels.

Two things can be noted about unit-base transform interpolation

(i) if the end points of two panels are the same, unit-base transform is exactly equivalent to Cartesian interpolation, and

(ii) the same interpolations can be made without transforming to unit-base space and transforming to the energy space at E.

The low energy value of the intermediate panel is simply:

$$E'_{low}(E) = E'_i(1) + \frac{E - E_i}{E_{i+1} - E_i}[E'_{i+1}(1) - E'_i(1)]. \tag{9}$$

A similar expression gives the high energy of the intermediate panel, and simply substitutes the top energies for the two panels in place of the bottom energies:

$$E'_{high}(E) = E'_i(N) + \frac{E - E_i}{E_{i+1} - E_i}[E'_{i+1}(M) - E'_i(N)]. \tag{10}$$

Here we have assumed the upper panel has M points. The Jacobian that should be used with the value from the bottom panel is

$$\left| \frac{dE'(E_i)}{dE'(E)} \right|$$

and is determined from equation (11) shown below. The secondary energy at E_i that corresponds to an E' at E is calculated from:

$$E'_i(E') = E'_i(1) + \frac{E' - E'_{low}}{E'_{high} - E'_{low}} \left[E'_i(N) - E'_i(1)\right]. \tag{11}$$

Here we have dropped the (E) arguments from the E' values at E for clarity. An analogous expression determines the secondary energy at the upper panel, and also the Jacobian for this panel. When the two values are interpolated at these two secondary energies and multiplied by their respective Jacobians, the values are simply interpolated using equation (4), or another appropriate expression, if the interpolation scheme is not linear in energy).

The Method of Corresponding Energies (MCE) is a scheme that was designed to circumvent one of the major problems associated with the unit-base transform approach; viz., that the unit-base transform depends directly on the way the end points of the successive distributions are taken. The MCE approach splits the integrals of distributions into equal integral bins and then interpolates linearly between corresponding bins. (The limits of these bins are the "corresponding energies".) This is a more physical approach than either Cartesian or unit-base transform interpolation and tends to emphasize the significant portions of the distributions. Perhaps a better way of saying this is that it tends to de-emphasize the insignificant portions of the distributions. For example, if 10 equal integral bins are to be used for the interpolation, the energies where the panels integrate to a tenth of the total integral are determined. Then the energies where the panels integrate to two-tenths of the total integral are determined, etc., until 10 sets of energy boundaries are defined for the bins in all panels. The interpolations between corresponding bins of successive panels are then performed using the unit-base transform approach.

It is important to note that that unit-base transform and MCE will require Jacobians to multiply the function values at successive panels, because a variable transformation is involved, while Cartesian interpolation is all done in real energy space, so that the unmodified function values are used.

0.6 General Description of Data Formats

An ENDF "tape" is built up from a small number of basic structures called "records," such as TPID, TEND, CONT, TAB1, and so on. These "records" normally consist of one or more 80-character FORTRAN records. It is also possible to use binary mode, where each of the basic structures is implemented as a FORTRAN logical record. The advantage of using

these basic ENDF "records" is that a small library of utility subroutines can be used to read and write the records in a uniform way.

0.6.1 Structure of an ENDF Data Tape

The structure of an ENDF data tape (file) is illustrated schematically in Fig. 0.3. The tape contains a single record at the beginning that identifies the tape. The major subdivision between these records is by ***material*** (identified by the MAT number). The data for a material is divided into ***files***, and each file (identified by the MF number) contains the data for a certain class of information. A file is subdivided into ***sections***, each one containing data for a particular reaction type (identified by the MT number). Finally, a section is divided into records. Every record on a tape contains three identification numbers: MAT, MF, and MT. These numbers are always in increasing numerical order, and the hierarchy is MAT, MF, MT. The end of a section, file, or material is signaled by special records called SEND, FEND, and MEND, respectively.

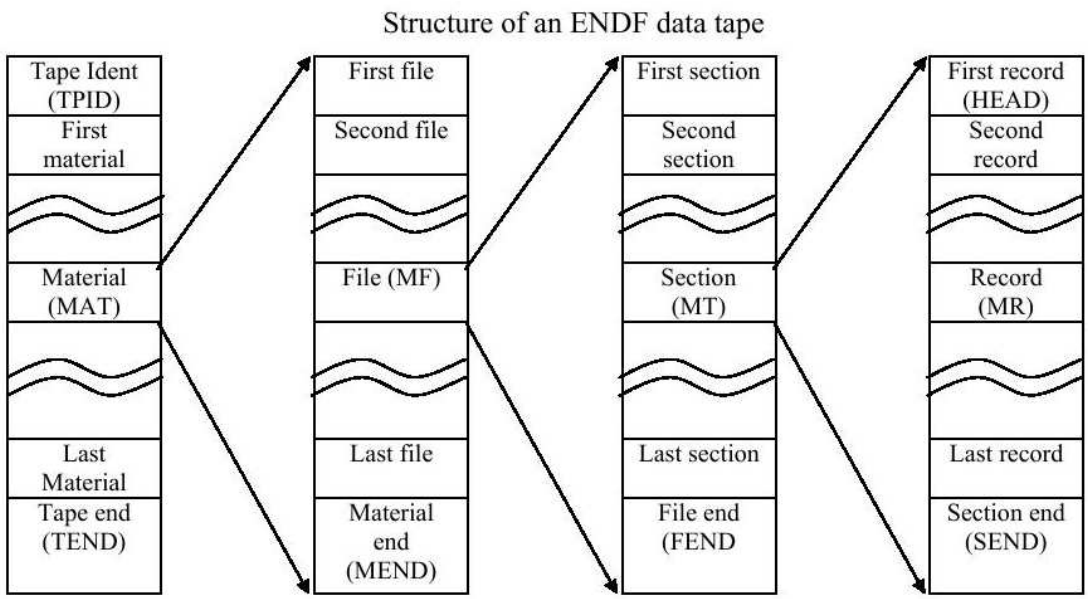

Figure 3: Structure of an ENDF data tape.

0.6.2 Symbol Nomenclature

An attempt has been made to use an internally consistent notation based on the following rules.

1. Symbols starting with the letter I, J, K, L, M, or N are integers. All other symbols refer to floating-point (real numbers).

2. The letter I or a symbol starting with I refers to an interpolation code (see Section 0.5.2).
3. Letters J, K, L, M, or N when used alone are indices.
4. A symbol starting with M is a control number. Examples are MAT, MF, MT.
5. A symbol starting with L is a test number.
6. A symbol starting with N is a count of items.

All numbers are given in fields of 11 columns. In character mode, floating-point numbers should be entered in one of the following forms:

±`1.234567`±`n`

±`1.23456`±`nn`, where `nn` ≤ 38

depending on the size of the exponent. Both of these forms can be read by the "E11.0" format specification of FORTRAN. However, a special subroutine must be used to output numbers in the above format. If evaluations are produced using numbers written by "1PE11.5" (that is, `1.2345Enn`, the numbers will be standardized into 6 or 7 digit form, but the real precision will remain at the 5 digit level.

0.6.3 Types of Records

All records on an ENDF tape are one of six possible types, denoted by TEXT, CONT, LIST, TAB1, TAB2, and INTG. The CONT record has six special cases called DIR, HEAD, SEND, FEND, MEND, and TEND. The TEXT record has the special case TPID. Every record contains the basic control numbers MAT, MF, and MT, as well as the sequence number NS. The definitions of the other fields in each record will depend on its usage as described below.

The sequence number of a record is a remnant of the past when the data were physically stored on paper cards that could get shuffled by accident. Nowadays NS serves merely as an additional parameter for checking the integrity of an evaluated library. The following conventions apply:

- the counter NS is reset for every section in the file. It starts with 1 and is incremented by 1 on every record up to the SEND record.
- SEND records (identified by MT=0) have NS=99999 by definition.
- FEND, MEND and TEND records have NS=0.

0.6.3.1 TEXT Records

This record is used either as the first entry on an ENDF tape (TPID), or to give the comments in File 1. It is indicated by the following shorthand notation

```
[MAT, MF, MT/ HL] TEXT
```

where HL is 66 characters of text information. The TEXT record can be read with the following FORTRAN statements

```
      READ(LIB,10)HL,MAT,MF,MT,NS
 10   FORMAT(A66,I4,I2,I3,I5)
```

0.6.3.2 CONT Records

The smallest possible record is a control (CONT) record. For convenience, a CONT record is denoted by

```
[MAT,MF,MT/C1,C2,L1,L2,N1,N2]CONT
```

The CONT record can be read with the following FORTRAN statements

```
      READ(LIB,10)C1,C2,L1,L2,N1,N2,MAT,MF,MT,NS
 10   FORMAT(2E11.0,4I11,I4,I2,I3,I5)
```

The actual parameters stored in the six fields C1, C2, L1, L2, N1, and N2 will depend on the application for the CONT record.

0.6.3.3 HEAD Records

The HEAD record is the first in a section and has the same form as CONT, except that the C1 and C2 fields always contain ZA and AWR, respectively.

0.6.3.4 END Records

The SEND, FEND, MEND, and TEND records use only the three control integers, which signal the end of a section, file, material, or tape, respectively. In binary mode, the six standard fields are all zero. In character mode, the six are all zero as follows

```
[MAT,MF, 0/  0.0,  0.0,   0,   0,   0,   0] SEND
[MAT, 0, 0/  0.0,  0.0,   0,   0,   0,   0] FEND
[  0, 0, 0/  0.0,  0.0,   0,   0,   0,   0] MEND
[ -1, 0, 0/  0.0,  0.0,   0,   0,   0,   0] TEND
```

0.6.3.5 DIR Records

The DIR records are described in more detail in Section 1.1.1. The only difference between a DIR record and a standard CONT record is that the first two fields in the DIR record are blank in character mode.

0.6.3.6 LIST Records

This type of record is used to list a series of numbers B1, B2, B3, *etc.* The values are given in an array B(n), and there are NPL of them. The shorthand notation for the LIST record is

[MAT,MF,MT/ C1, C2, L1, L2, NPL, N2/ B_n] LIST

The LIST record can be read with the following FORTRAN statements

```
      READ(LIB,10)C1,C2,L1,L2,NPL,N2,MAT,MF,MT,NS
 10   FORMAT(2E11.0,4I11,I4,I2,I3,I5)
      READ(LIB,20)(B(N),N=1,NPL)
 20   FORMAT(6E11.0)
```

The maximum for NPL varies with use (see Appendix G).

0.6.3.7 TAB1 Records

These records are used for one-dimensional tabulated functions such as $y(x)$. The data needed to specify a one-dimensional tabulated function are the interpolation tables NBT(N) and INT(N) for each of the NR ranges, and the NP tabulated pairs of $x(n)$ and $y(n)$. The shorthand representation is:

[MAT,MF,MT/ C1, C2, L1, L2, NR, NP/x_{int}/$y(x)$]TAB1

The TAB1 record can be read with the following FORTRAN statements

```
      READ(LIB,10)C1,C2,L1,L2,NR,NP,MAT,MF,MT,NS
 10   FORMAT(2E11.0,4I11,I4,I2,I3,I5)
      READ(LIB,20)(NBT(N),INT(N),N=1,NR)
 20   FORMAT(6I11)
      READ(LIB,30)(X(N),Y(N),N=1,NP)
 30   FORMAT(6E11.0)
```

The limits on NR and NP vary with use (see Appendix G). The limits must be strictly observed in primary evaluations in order to protect processing codes that use the simple binary format. However, these limits can be relaxed in derived libraries in which resonance parameters have been converted into detailed tabulations of cross section versus energy. Such derived libraries can be written in character mode or a non-standard blocked-binary mode.

0.6.3.8 TAB2 Records

The next record type is the TAB2 record, which is used to control the tabulation of a two-dimensional function $y(x, z)$. It specifies how many values of z are to be given and how to interpolate between the successive values of z. Tabulated values of $y_l(x)$ at each value of z_l are given in TAB1 or LIST records following the TAB2 record, with the appropriate value of z in the field designated as C2. The shorthand notation for TAB2 is

[MAT,MF,MT/ C1, C2, L1, L2, NR, NZ/ Z_{int}]TAB2,

The TAB2 record can be read with the following FORTRAN statements

```
      READ(LIB,10)C1,C2,L1,L2,NR,NZ,MAT,MF,MT,NS
 10   FORMAT(2E11.0,4I11,I4,I2,I3,I5)
      READ(LIB,20)(NBT(N),INT(N),N=1,NR)
 20   FORMAT(6I11)
```

For example, a TAB2 record is used in specifying angular distribution data in File 4. In this case, NZ in the TAB2 record specifies the number of incident energies at which angular distributions are given. Each distribution is given in a LIST or TAB1 record.

0.6.3.9 INTG records

INTG, or INTeGer, records are used to store a correlation matrix in integer format. The shorthand notation is

```
[MAT, MF, MT / II, JJ, KIJ ] INTG
```

where II and JJ are position locators, and KIJ is an array whose dimension is specified by the number of digits NDIGIT to be used for representing the values. NDIGIT can have any value from 2 to 6; the corresponding dimensions (NROW) are 18, 13, 11, 9, and 8 respectively. The INTG record can be read with the following FORTRAN statements

```
      PARAMETER (NROW=18)
      DIMENSION KIJ(NROW)
      IF(NDIGIT.EQ.2) READ(LIB,20) II,JJ,(KIJ(K),K=1,18),MAT,MF,MT,NS
      IF(NDIGIT.EQ.3) READ(LIB,30) II,JJ,(KIJ(K),K=1,13),MAT,MF,MT,NS
      IF(NDIGIT.EQ.4) READ(LIB,40) II,JJ,(KIJ(K),K=1,11),MAT,MF,MT,NS
      IF(NDIGIT.EQ.5) READ(LIB,50) II,JJ,(KIJ(K),K=1, 9),MAT,MF,MT,NS
      IF(NDIGIT.EQ.6) READ(LIB,60) II,JJ,(KIJ(K),K=1, 8),MAT,MF,MT,NS
   20 FORMAT (2I5,1X,18I3,1X,I4,I2,I3,I5)
   30 FORMAT (2I5,1X,13I4,3X,I4,I2,I3,I5)
   40 FORMAT (2I5,1X,11I5,   I4,I2,I3,I5)
   50 FORMAT (2I5,1X, 9I6,1X,I4,I2,I3,I5)
   60 FORMAT (2I5,    8I7,   I4,I2,I3,I5)
```

See File 32, LCOMP=2, for details regarding the use of this format.

0.7 ENDF Documentation

1. **BNL 8381**, ENDF - *Evaluated Nuclear Data File Description and Specifications*, January 1965, H.C. Honeck.

2. **BNL 50066 (ENDF 102)**, ENDF/B - *Specifications for an Evaluated Nuclear Data File for Reactor Applications*, May 1966, H.C. Honeck. Revised July 1967 by S. Pearlstein.

3. **BNL 50274 (ENDF 102)**, Vol. I - *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, October 1970, M.K. Drake, Editor.

4. **LA 4549 (ENDF 102)**, Vol. II - *ENDF Formats and Procedures for Photon Production and Interaction Data*, October 1970, D.J. Dudziak.

5. **BNL-NCS-50496 (ENDF 102)**, *ENDF102 Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF*, October 1975, Revised by D. Garber, C. Dunford, and S. Pearlstein.

6. **ORNL/TM-5938 (ENDF-249)**, *The Data Covariance Files for ENDF/B-V*, July 1977, F. Perey.

7. **BNL-NCS-50496 (ENDF 102)**, Second Edition, *ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF/B-V*, October 1979, Edited by R. Kinsey. Revised by B.A. Magurno, November 1983.

8. **BNL-NCS-28949 (Supplement ENDF 102)**, Second Edition, *Supplement to the ENDF/B-V Formats and Procedures Manual for Using ENDF/B-IV Data*, November 1980, S. Pearlstein.

9. **BNL-NCS-44945 (ENDF-102)**, Revision 10/91, *ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6*, October 1991, Edited by P. F. Rose and C. L. Dunford.

Chapter 1

File 1: GENERAL INFORMATION

File 1 is the first part of any set of evaluated cross-section data for a material. Each material must have a File 1 that contains at least one section. This required section provides a brief documentation of how the data were evaluated and a directory that summarizes the files and sections contained in the material. In the case of fissionable materials, File 1 may contain up to five additional sections giving fission neutron and photon yields and energy release information. Each section has been assigned an MT number (see below), and the sections are arranged in order of increasing MT number. A section always starts with a HEAD record and ends with a SEND record. The end of File 1 (and all other files) is indicated by a FEND record. These record types are defined in detail in Section 0.6.

1.1 Descriptive Data and Directory (MT=451)

This section is always the first section of any material and has two parts:

1. a brief documentation of the cross-section data, and
2. a directory of the files and sections used for this material.

In the first part, a brief description of the evaluated data set is given. This information should include the significant experimental results used to obtain the evaluated data, descriptions of any nuclear models used, a clear specification of all the MT numbers defined to identify reactions, the history of the evaluation, and references. The descriptive information is given as a series of records, each record containing up to 66 characters.

The first three records of the descriptive information contain a standardized presentation of information on the material, projectile, evaluators, and modification status. The following quantities are defined for MF=1, MT=451:

ZA,AWR Standard material charge and mass parameters (see Section 0.5.1).

LRP Flag indicating whether resolved and/or unresolved resonance parameters are given in File 2:
LRP=−1, no File 2 is given (not allowed for incident neutrons);

LRP=0, no resonance parameter data are given, but a File 2 is present containing the effective scattering radius;
LRP=1, resolved and/or unresolved parameter data are given in File 2 and cross sections computed from them must be added[1] to background cross sections given in File 3;
LRP=2, parameters are given in File 2, but cross sections derived from them are not to be added to the cross sections in File 3. The option LRP=2 is to be used for derived files only and is typical in the so-called PENDF files, in which the cross sections are already reconstructed from the resonances parameters and written in File 3.

LFI Flag indicating whether this material fissions:
LFI=0, this material does not fission;
LFI=1, this material fissions.

NLIB Library identifier (*e.g.* NLIB= 0 for ENDF/B). Additional values have been assigned to identify other libraries using ENDF format. See Section 0.3.1 for details.

NMOD Modification number for this material:
NMOD=0, evaluation converted from a previous version;
NMOD=1, new or revised evaluation for the current library version;
NMOD$\geq$ 2, for successive modifications.

ELIS Excitation energy of the target nucleus relative to 0.0 for the ground state.

STA Target stability flag:
STA=0, stable nucleus;
STA=1 unstable nucleus. If the target is unstable, radioactive decay data should be given in the decay data sub-library (NSUB=4).

LIS State number of the target nucleus. The ground state is indicated by LIS=0.

LISO Isomeric state number. The ground state is indicated by LISO=0. LIS is greater than or equal to LISO.

NFOR Library format.
NFOR=6 for all libraries prepared according to the specifications given in this manual.

AWI Mass of the projectile in neutron mass units. For incident photons or decay data sub-libraries, use AWI=0.

EMAX Upper limit of the energy range for evaluation.

LREL Library release number; for example, LREL=2 for the ENDF/B-VI.2 library.

[1] In the unresolved region, it is also possible to compute self-shielding factors from File 2 and multiply them by complete unshielded cross section given in File 3. See Chapter 2 for details

NSUB Sub-library number. See Section 0.4 for a description of sub-libraries.

NVER Library version number; for example, NVER=7 for version ENDF/B-VII.

TEMP Target temperature (Kelvin) for data that have been generated by Doppler broadening. For derived data only; use TEMP=0.0 for all primary evaluations.

LDRV Special derived material flag that distinguishes between different evaluations with the same material keys (*i.e.*, MAT, NMOD, NSUB):
LDRV=0, primary evaluation:
LDRV$\geq$ 1, special derived evaluation (for example, a dosimetry evaluation using sections (MT) extracted from the primary evaluation).

NWD Number of records with descriptive text for this material. Each record contains up to 66 characters.

NXC Number of records in the directory for this material. Each section (MT) in the material has a corresponding line in the directory that contains MF, MT, NC, and MOD. NC is a count of the number of records in the section (not including SEND), and MOD is the modification flag (see below).

ZSYMAM Character representation of the material defined by the atomic number, chemical symbol, atomic mass number, and metastable state designation in the form Z-cc-AM with
Z, right justified in col. 1 to 3,
- (hyphen) in col. 4,
cc, two-character chemical name left justified in col. 5 and 6,
- (hyphen) in col. 7,
A, right justified in col. 8 to 10 or blank,
M for the indication of a metastable state in col. 11,
for example, `1-H -  2, 40-Zr- 90, 95-Am-242M`, *etc.*

ALAB Mnemonic for the originating laboratory(s) left adjusted in col. 12-22.

EDATE Date of evaluation given in the form "`EVAL-DEC74`" in col. 23-32.

AUTH Author(s) name(s) left adjusted in col. 34-66.

REF Primary reference for the evaluation left adjusted in col. 2-22.

DDATE Original distribution date given in the form "`DIST-DEC74`" in col. 23-32.

RDATE Date and number of the last revision to this evaluation in col. 34-43 in the form "`REV2-DEC74`", where "2" in column 37 is the release number and must be equal to LREL. The term "revision" (IREV), which appeared in earlier editions of this manual, was synonymous with "release" (LREL) and has been dropped in favor of the more-frequently used term "release".

ENDATE Master File entry date in the form *yyyymmdd* right adjusted in col. 56-63. The Master File entry date is assigned by NNDC for ENDF/B libraries.

HSUB Identifier for the library contained on three successive records is useful for visual inspection of the files and is followed strictly in the ENDF/B libraries. The first record contains four dashes starting in col. 1, directly followed by the library type (NLIB) and version (NVER). For example,
"`---- ENDF/B-VI`", followed by `MATERIAL XXXX` starting in col. 23 where XXXX is the MAT number, and REVISION 2 (starting in col. 45 only if required) where "2" is the revision number IREV.
The second record contains five dashes starting in col. 1, and followed by the sub-library identifier (see Table 3). For example,
"`----- DECAY DATA`",
"`----- PHOTO-ATOMIC INTERACTION DATA`" or
"`----- INCIDENT NEUTRON DATA`"
The third record contains six dashes starting in col. 1 and followed by `ENDF-6` where "6" is the library format type (NFOR).

Note: the three HSUB records can be generated by the utility program, STANEF.

MF$_n$ ENDF file number of the nth section.

MT$_n$ ENDF reaction designation of the nth section.

NC$_n$ Number of records in the nth section. This count does not include the SEND record.

MOD$_n$ Modification indicator for the nth section. The value of MOD$_n$ is equal to NMOD if the corresponding section was changed in this revision. MOD$_n$ must always be less than or equal to NMOD.

1.1.1 Formats

The structure of this section is

```
[MAT, 1,451/    ZA,   AWR,   LRP,    LFI, NLIB,  NMOD]HEAD
[MAT, 1,451/  ELIS,   STA,   LIS,   LISO,    0,  NFOR]CONT
[MAT, 1,451/   AWI,  EMAX,  LREL,      0, NSUB,  NVER]CONT
[MAT, 1,451/  TEMP,   0.0,  LDRV,      0,  NWD,   NXC]CONT
[MAT, 1,451/ZSYMAM,  ALAB, EDATE,   AUTH             ]TEXT
[MAT, 1,451/   REF, DDATE, RDATE, ENDATE             ]TEXT
[MAT, 1,451/  HSUB                                   ]TEXT
      ------------------------------------
      continue for the rest of the NWD descriptive records
      ------------------------------------
[MAT, 1,451/ blank, blank,   MF1,    MT1,  NC1,  MOD1]CONT
[MAT, 1,451/ blank, blank,   MF2,    MT2,  NC2,  MOD2]CONT
      ------------------------------------
      ------------------------------------
[MAT, 1,451/ blank, blank, MFNXC,  MTNXC,NCNXC,MODNXC]CONT
[MAT, 1,  0/    0.0,  0.0,     0,      0,    0,     0]SEND
```

1.1.2 Procedures

Note that the parameters NLIB, LREL, NVER, NSUB, MAT, NMOD, LDRV, and sometimes TEMP define a unique set of "keys" that identifies a particular evaluation or "material" in the ENDF system. These keys can be used to access materials in a formal data base management system if desired.

The flag LRP indicates whether resolved and/or unresolved resonance parameter data are to be found in File 2 (Resonance Parameters) and how these data are to be used with File 3 to compute the net cross section. For incident neutrons, every material will have a File 2. If LRP=0, the file contains only the effective scattering radius; the potential cross section corresponding to this scattering radius has already been included in the File 3 cross sections. If LRP=1, File 2 contains resolved and/or unresolved resonance parameters. Cross sections or self-shielding factors computed from these parameters are to be combined with any cross sections found in File 3 to obtain the correct net cross section. For other sub-libraries (decay data, incident photons, incident charged particles, fission product yields), File 2 can be omitted (use LRP=-1). A number of processing codes exist which reconstruct resonance-region cross sections from the parameters in File 2 and output the results in ENDF format. Such a code can set LRP=2 and copy the original File 2 to its output ENDF tape. Other processing codes using such a tape will know that resonance reconstruction has already been performed, but the codes will still have easy access to the resonance parameters if needed. The LRP=2 option is not allowed in primary evaluations.

The flag LFI indicates that this material fissions in the context of the present sub-library. In this case, a section specifying the total number of neutrons emitted per fission, $\overline{\nu}(E)$, *must* be given as MF=1, MT=452. Sections *may* also be given that specify the number of delayed neutrons per fission (MT=455) and the number of prompt neutrons per fission (MT=456), and that specify the components of energy release in fission (MT=458).

The flag LDRV indicates that this material was derived in some way from another evalu-

ation; for example, it could represent an activation reaction extracted from a more complete evaluation, it could be part of a gas production library containing production cross sections computed from more fundamental reactions, it could represent a reconstructed library with resonance parameters expanded into detailed point-wise cross sections, and so on.

The data in the descriptive section must be given for every material. The first three records are used to construct titles for listings, plots, *etc.*, and the format should be followed closely. The remaining records give a verbal description of the evaluated data set for the material. The description should mention the important experimental results upon which the recommended cross sections are based, the evaluation procedures and nuclear models used, a brief history and origin of the evaluation, important limitations of the data set, estimated uncertainties and covariances, references, and any other remarks that will assist the user in understanding the data. For incident neutron evaluations, the 2200 m/s cross sections contained in the data should be tabulated, along with the infinite dilution resonance integrals for capture and fission (if applicable). For charged-particle and high-energy reactions, the meaning of each MT should be carefully explained using the notation of Section 0.4.3.

1.2 Number of Neutrons per Fission, $\overline{\nu}$, (MT=452)

If the material fissions (LFI=1), then a section specifying the average *total* number of neutrons per fission, $\overline{\nu}$ (MT=452), must be given. This format applies to both particle induced and spontaneous fission, each in its designated sub-library. Values of $\overline{\nu}$ may be tabulated as a function of energy or in the form of coefficients provided for the following polynomial expansion:

$$\overline{\nu}(E) = \sum_{\mathrm{n=1}}^{\mathrm{NC}} C_n E^{n-1} \tag{1.1}$$

where

$\overline{\nu}(E)$ the average total (prompt plus delayed) number of neutrons per fission produced by neutrons of incident energy E (eV),

C_n the nth coefficient, and

NC the number of terms in the polynomial.

MT=452 for an energy-dependent neutron multiplicity cannot be represented by a polynomial expansion when MT=455 and MT=456 are utilized in the file.

1.2.1 Formats

The structure of this section depends on whether values of $\overline{\nu}(E)$ are tabulated as a function of energy or represented by a polynomial. The following quantities are defined:

LNU Test that indicates what representation of $\overline{\nu}(E)$ has been used:
LNU=1, polynomial representation;
LNU=2, tabulated representation.

NC Count of the number of terms used in the polynomial expansion. (NC$\leq$ 4).

C_n Coefficients of the polynomial. There are NC coefficients given.

NR Number of interpolation ranges used to tabulate values of $\overline{\nu}(E)$. (See Section 0.5.2)

NP Total number of energy points used to tabulate $\overline{\nu}(E)$.

$\mathbf{E}_{\text{int}}$ Interpolation scheme (see Section 0.5.2 for details).

$\overline{\nu}(E)$ Average number of neutrons per fission.

If **LNU=1**, the structure of the section is

```
[MAT, 1, 452/  ZA, AWR,  0, LNU,  0,  0]HEAD           (LNU=1)
[MAT, 1, 452/ 0.0, 0.0,  0,   0, NC,  0/ C1, C2, ...CNC]LIST
[MAT, 1,   0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

If **LNU=2**, the structure of the section is

```
[MAT, 1, 452/  ZA, AWR,  0, LNU,  0,  0]HEAD    (LNU=2)
[MAT, 1, 452/ 0.0, 0.0,  0,   0, NR, NP/E_int,ν̄(E)]TAB1
[MAT, 1,   0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

1.2.2 Procedures

If a polynomial representation (LNU=1) is used to specify $\overline{\nu}(E)$, this representation is valid over any range in which the fission cross section is specified (as given in Files 2 and 3). The polynomial fit of $\overline{\nu}(E)$ must be limited to a third-degree polynomial (NC$\leq$4). If such a fit does not reproduce the recommended values of $\overline{\nu}(E)$, a tabulated form (LNU=2) should be used.

If tabulated values of $\overline{\nu}(E)$ are specified (LNU=2), then pairs of energy-$\overline{\nu}$ values are given. Values of $\overline{\nu}(E)$ must be given that cover the entire energy range over which the fission cross section is given in Files 2 and/or 3.

The values of $\overline{\nu}(E)$ given in this section are for the average total number of neutrons produced per fission event. When the number of delayed neutrons from fission $\overline{\nu}_d$ are also present in the file (MT=455), the presence of the number of prompt neutrons per fission $\overline{\nu}_p$ is mandatory (MT=456) and the sum of the two must be consistent with the total $\overline{\nu}(E)$. In this case, only LNU=2 representation is allowed for MT=452.

For spontaneous fission, the polynomial representation (LNU=1) with NC=1 is used to describe the total number of neutrons per fission and $C_1 = \overline{\nu}$. There is no energy dependence.

1.3 Delayed Neutron Data, $\overline{\nu}_d$, (MT=455)

This section describes the delayed neutrons resulting from either particle induced or spontaneous fission. The average total number of delayed neutron precursors emitted per fission, $\overline{\nu}_d$, is given, along with the decay constants, λ_i, for each precursor family. The fraction of $\overline{\nu}_d$ generated for each family is given in File 5 (Chapter 5 of this report). The energy distributions of the neutrons associated with each precursor family are also given in File 5.

For particle-induced fission, the total number of delayed neutrons is given as a function of energy in tabulated form (LNU=2). The energy dependence is specified by tabulating $\overline{\nu}_d(E)$ at a series of neutron energies using the same format as for MT=452. For spontaneous fission LNU=1 is used with NC=1 and $C_1 = \overline{\nu}_d$ as for MT=452.

The total number of delayed neutron precursors emitted per fission event at incident energy E is given in this file and is defined as the sum of the number of neutrons emitted for each of the precursor families,

$$\overline{\nu}_d = \sum_{\mathrm{i=1}}^{\mathrm{NNF}} \overline{\nu}_i(E), \tag{1.2}$$

where NNF is the number of precursor families. The fraction of the total, $P_i(E)$, emitted for each family is given in File 5 (see Chapter 5) and is defined as:

$$P_i(E) = \frac{\overline{\nu}_i(E)}{\overline{\nu}_d(E)} \tag{1.3}$$

1.3.1 Formats

The following quantities are defined.

LNU Test indicating which representation is used:
LNU=1 means that polynomial expansion is used;
LNU=2 means that a tabulated representation is used.

LDG Flag indicating energy dependence of delayed-group constants:
LDG=0 means that decay constants are energy-independent;
LDG=1 means that decay constants are energy-dependent.

NE Number of energies at which the delayed-group constants are given.

NC Number of terms in the polynomial expansion (NC$\leq$ 4).

NR Number of interpolation ranges used (NR$\leq$ 20).

NP Total number of energy points used in the tabulation of $\overline{\nu}(E)$

$\mathbf{E}_{\mathrm{int}}$ Interpolation scheme (see Section 0.5.2)

$\overline{\nu}_d(E)$ Total average number of delayed neutrons formed per fission event.

NNF Number of precursor families considered.

$\lambda_i(E)$ Decay constant (sec^{-1}) for the ith precursor. (May be constant)

$\alpha_i(E)$ Delayed-group abundances.

The structure when values of $\overline{\nu}_d$ are tabulated (LNU=2) and the delayed-group constants are energy-independent (LDG=0) is

```
[MAT, 1,455/  ZA, AWR, LDG, LNU,   0,  0]HEAD    (LDG=0, LNU=2)
[MAT, 1,455/ 0.0, 0.0,   0,   0, NNF,  0/ λ1,λ2,...λNNF]LIST
[MAT, 1,455/ 0.0, 0.0,   0,   0,  NR, NP/ Eint, ν̄d(E)]TAB1
[MAT, 1,  0/ 0.0, 0.0,   0,   0,   0,  0]SEND
```

The structure when values of $\overline{\nu}_d$ are tabulated (LNU=2) and the delayed-group constants are energy-dependent (LDG=1) is

```
[MAT, 1,455/  ZA, AWR, LDG, LNU,  0,  0]HEAD (LDG=1, LNU=2)
[MAT, 1,455/ 0.0, 0.0,   0,   0, NR, NE/ Eint]TAB2
[MAT, 1,455/ 0.0,  E1,   0,   0, NNF*2, 0/
   λ1(E1), α1(E1), λ2(E1), α2(E1),  ...λNNF(E1), αNNF(E1)]LIST
   ------------------------------------
   ------------------------------------
[MAT, 1,455/ 0.0, ENE,   0,   0, NNF*2, 0/
   λ1(ENE), α1(ENE), λ2(ENE), α2(ENE),  ...λNNF(ENE), αNNF(ENE)]LIST
[MAT, 1,455/ 0.0, 0.0, 0, 0, NR, NP/Eint, ν̄d(E)]TAB1
[MAT, 1,  0/ 0.0, 0.0, 0, 0,  0,  0]SEND
```

The structure when values of $\overline{\nu}_d$ are defined by a polynomial expansion (LNU=1) and the delayed-group constants are energy-independent (LDG=0), the structure of the section is [2]

```
[MAT, 1,455/  ZA, AWR, LDG, LNU,   0,  0]HEAD (LDG=0, LNU=1)
[MAT, 1,455/ 0.0, 0.0,   0,   0, NNF,  0/
   λ1, λ2,...  λNNF]LIST
[MAT, 1,455/ 0.0, 0.0,   0,   0,   1,  0/ ν̄d]TAB1
[MAT, 1,  0/ 0.0, 0.0,   0,   0,   0,  0]SEND
```

The structure when values of $\overline{\nu}_d$ are defined by a polynomial expansion (LNU=1) and the delayed-group constants are energy dependent (LDG=1), the structure of the section is:

```
[MAT, 1,455/  ZA, AWR, LDG, LNU,  0,  0]HEAD (LDG=1, LNU=1)
[MAT, 1,455/ 0.0, 0.0,   0,   0, NR, NE/ Eint]TAB2
[MAT, 1,455/ 0.0,  E1,   0,   0, NNF*2, 0/
   λ1(E1), α1(E1), λ2(E1), α2(E1),  ...λNNF(E1), αNNF(E1)]LIST
   ------------------------------------
   ------------------------------------
[MAT, 1,455/ 0.0, ENE,   0,   0, NNF*2, 0/
   λ1(ENE), α1(ENE), λ2(ENE), α2(ENE),  ...λNNF(ENE), αNNF(ENE)]LIST
[MAT, 1,455/ 0.0, 0.0,   0,   0, NR, NP/Eint, ν̄d(E)]TAB1
[MAT, 1,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

[2] Mandatory format option for spontaneous fission.

1.3.2 Procedures

When tabulated values of $\overline{\nu}_d(E)$ are specified, as is required for particle-induced fission in Section 1.2, they should be given for the same energy range as that used to specify the fission cross section.

The probabilities of producing the precursors for each family and the energy distributions of neutrons produced by each precursor family are given in File 5 (Chapter 5 of this report). If parameters are incident-particle energy-dependent (LDG=1), the delayed-group abundances are also given in File 1 (MT=455). It is extremely important that the same precursor families be given in File 5 as are given in File 1 with the same abundances, and the ordering of the families should be the same in both files. It is recommended that the families be ordered by decreasing half-lives ($\lambda_1 < \lambda_2 < \ldots < \lambda_{\mathrm{NNF}}$).

For spontaneous fission, the polynomial form (LNU=1) is used with only one term (NC=1, $C_1=\overline{\nu}_d$).

If MT=455 is used, then MT=456 must also be present, in addition to MT=452.

1.4 Number of Prompt Neutrons per Fission, $\overline{\nu}_p$, (MT=456)

If the material fissions (LFI=1), a section specifying the average number of prompt neutrons per fission, $\overline{\nu}_p$, (MT=456) can be given using formats identical to MT=452. For particle-induced fission, $\overline{\nu}_p$ is given as a function of energy. The prompt $\overline{\nu}$ for spontaneous fission can also be given using MT=456, but there is no energy dependence.

1.4.1 Formats

The following quantities are defined:

LNU Indicates what representation of $\overline{\nu}_p(E)$ has been used:
LNU=1, polynomial representation has been used;
LNU=2, tabulated representation.

NC Count of the number of terms used in the polynomial expansion. (NC$\leq$ 4)

NR Number of interpolation ranges used to tabulate values of $\overline{\nu}_p(E)$. (See Section 0.6.3.7)

NP Total number of energy points used to tabulate $\overline{\nu}_p(E)$.

$\mathbf{E}_{\mathrm{int}}$ Interpolation scheme (see Section 0.5.2)

$\overline{\nu}_p(E)$ Average number of prompt neutrons per fission.

If LNU=2, (tabulated values of $\overline{\nu}$), the structure of the section is:

```
[MAT, 1,456/  ZA, AWR,  0, LNU,  0,  0] HEAD   (LNU=2)
[MAT, 1,456/ 0.0, 0.0,  0,   0, NR, NP/ E_int, /ν̄_p(E)]TAB1
[MAT, 1,  0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

If LNU=1 (spontaneous fission) the structure of the section is:

```
[MAT, 1,456/  ZA, AWR,  0, LNU,  0, 0]HEAD   (LNU=1)
[MAT, 1,456/ 0.0, 0.0,  0,   0,  1, 0/ ν̄_p]LIST}
[MAT, 1,  0/ 0.0, 0.0,  0,   0,  0, 0]SEND
```

1.4.2 Procedures

If tabulated values of $\overline{\nu}_p(E)$ are specified (LNU=2), then pairs of energy-$\overline{\nu}$ values are given. Values of $\overline{\nu}_p(E)$ should be given that cover any energy range in which the fission cross section is given in File 2 and/or File 3. The values of $\overline{\nu}_p(E)$ given in this section are for the average number of prompt neutrons produced per fission event. The energy independent $\overline{\nu}_p$ for spontaneous fission is given using LNU=1 with NC=1 and $C_1=\overline{\nu}_p$ as described for MT=452.

If MT=456 is specified, then MT=455 must also be specified as well as MT=452.

1.5 Components of Energy Release Due to Fission (MT=458)

The energy released in fission is carried by fission products, neutrons, gammas, betas (+ and -), and neutrinos and anti-neutrinos. The term *fission products* refers to all charged particles that are emitted promptly, since for energy-deposition calculations, all such particles have short ranges and are usually considered to lose their energy locally. Neutrons and gammas transport their energy elsewhere and need to be considered separately. In addition, some gammas and neutrons are delayed, and in a shut-down assembly, one needs to know the amount of energy tied up in these particles and the rate at which it is released from the metastable nuclides or precursors. The neutrino energy is lost completely in most applications, but is part of the Q-value. As far as the betas are concerned, prompt betas, being charged, deposit their energy locally like the fission products, and their prompt energies are included with the fission product energy.

This format recognises nine specific components for fission energy release. The nomenclature used to define these nine energy release terms is:

ET Sum of all the partial energies that follow. This sum is the total energy release per fission and equals the Q-value.

EFR Kinetic energy of the fission products (following prompt neutron emission from the fission fragments).

ENP Kinetic energy of the prompt fission neutrons.

END Kinetic energy of the delayed fission neutrons.

EGP Total energy released by the emission of prompt γ rays.

EGD Total energy released by the emission of delayed γ rays.

EB Total energy released by delayed β's.

ENU Energy carried away by neutrinos.

ER Total energy less the energy of the neutrinos (`ET - ENU`); equal to the pseudo-Q-value in File 3 for MT=18.

NPLY Order of the polynomial expansion of the energy-components.

The total energy release due to fission is an incident-energy dependent quantity, as are many, if not all, of the constituent terms.

There are two formats available to represent these energy dependencies. From the work of Sher and Beck (Reference 1), the energy dependence is given as:

$$E_i(E_{\text{inc}}) = E_i(0) - \delta E_i(E_{\text{inc}}) \tag{1.4}$$

where:

$E_i(E_{\text{inc}})$ is the fission energy release for each of the nine components;

$E_i(0)$ is a constant, one for each of the nine fission energy release terms. These constants and their uncertainties are specified via the `NPLY=0` format option, defined in Section 1.5.1;

$\delta E_i(E_{\text{inc}})$ is a function that allows for the definition of the energy-dependence of this fission energy component. These functions can not be determined based upon the data given in the evaluated file; rather, unique functions are defined for the various fission energy release terms as follows:

$$\begin{aligned}
\delta\text{ET} &= -1.057\ E_{\text{inc}} + 8.07\,[\overline{\nu}(E_{\text{inc}}) - \overline{\nu}(0)] \\
\delta\text{EB} &= 0.075 E_{\text{inc}} \\
\delta\text{EGD} &= 0.075 E_{\text{inc}} \\
\delta\text{ENU} &= 0.100 E_{\text{inc}} \\
\delta\text{EFR} &= 0 \\
\delta\text{ENP} &= -1.307 E_{\text{inc}} + 8.07\,[\overline{\nu}(E_{\text{inc}}) - \overline{\nu}(0)] \\
\delta\text{EGP} &= 0
\end{aligned}$$

However, a recent study of relevant experimental data, supplemented with model calculations, by Madland (Reference 2) has shown that δEFR and δEGP terms are not zero, but instead have definite dependencies upon the incident neutron energy E_{inc}. This means that the remaining δ values above are accounting for these dependencies in addition to their own dependencies. In short, the calculations of individual energy release values are suspect even though the total energy release, ET, is substantially correct. Madland concludes that the energy dependence for the various fission energy release terms may be accurately represented with simple polynomial expansions in incident neutron energy. As such, the energy dependencies are completely defined by specifying the coefficients of NPLYth order polynomials:

$$E_i(E_{\text{inc}}) = c_0 + c_1 E_{\text{inc}} + c_2 E_{\text{inc}}^2 + \ldots$$

The polynomial expansion coefficients and their uncertainties are specified via the NPLY$\neq$0 option in Section 1.5.1 With the Madland representation, the complete energy release may be determined solely from the data tabulated by the evaluator, without regard to the various functional forms defined above.

1.5.1 Formats

The structure of this section always starts with a HEAD record and ends with a SEND record. The section contains no subsections and only one LIST record. The structure of a section takes one of two forms. When NPLY=0, the format is:

```
[MAT, 1,458/  ZA,  AWR,   0,      0,    0,    0]HEAD
[MAT, 1,458/ 0.0,  0.0,   0, NPLY=0,N1=18, N2=9/
             EFR, ΔEFR, ENP, ΔENP, END, ΔEND,
             EGP, ΔEGP, EGD, ΔEGD, EB,  ΔEB,
             ENU, ΔENU, ER,  ΔER,  ET,  ΔET]LIST
[MAT, 1,  0/ 0.0,  0.0,   0,    0,    0,    0]SEND
```

where the Δ terms represent the uncertainties on the preceeding quantity. The data are used in conjunction with the Sher and Beck formulas from Section 1.5 to determine the energy release.

For the polynomial expansion represntation, NPLY represents the highest polynomial order needed to define any of the energy release components. The size of the list record is 18×(NPLY+1). The first 18 values are nine pairs of c_0 and Δc_0 terms, followed by nine pairs of c_1 and Δc_1 terms, and continuing through the maximum polynomial order.

```
[MAT, 1,458/  ZA,  AWR,   0,    0,     0,            0]HEAD
[MAT, 1,458/ 0.0,  0.0,   0,    NPLY,  18*(NPLY+1), 9*(NPLY+1)/
             c_0^EFR, Δc_0^EFR, c_0^ENP, Δc_0^ENP, c_0^END, Δc_0^END
             c_0^EGP, Δc_0^EGP, c_0^EGD, Δc_0^EGD, c_0^EB , Δc_0^EB
             c_0^ENU, Δc_0^ENU, c_0^ER , Δc_0^ER , c_0^ET , Δc_0^ET
             c_1^EFR, Δc_1^EFR, c_1^ENP, Δc_1^ENP, c_1^END, Δc_1^END
             c_1^EGP, Δc_1^EGP, c_1^EGD, Δc_1^EGD, c_1^EB , Δc_1^EB
             c_1^ENU, Δc_1^ENU, c_1^ER , Δc_1^ER , c_1^ET , Δc_1^ET
[MAT, 1,  0/ 0.0,  0.0,   0,    0,     0,    0]SEND
```

As with the NPLY=0 option, the Δ terms represent the uncertainties on the preceeding quantities, respectively.

1.5.2 Procedures

This section should be used for fertile and fissile isotopes only. Consistency should be maintained between the Q-values in File 3, the energies calculated from File 5 and 15 and the energies calculated from the data given here. Note that ER equals the pseudo-Q-value for fission (MT=18) in File 3.

Other components are not so readily determined or checked. When the NPLY=0 option is used, the procedure should be that File 5 and File 15 data take precedent, whenever possible. That is, "prompt" fission neutron energy calculated from File 5 spectra for MT=18 should be put into File 1; the same holds true for the delayed neutron spectra given in File 5, MT=455. The "prompt" gamma energy calculated from File 15 (MT=18 for fission) should be put into File 1; these are the prompt gammas due to the fission process. When NPLY$\neq$0, the nature of the polynomial fitting process may yield small differences between the values calculated from the polynomial coefficients and the values calculated using the spectral data from Files 5 and 15.

These quantities should be calculated at the lowest energy given in the Files for MT=18 except for fissile isotopes for which the thermal spectra should be used. For fertile materials, the spectrum given at threshold would be appropriate. Note that the File 5 spectra for MT=18 should be used with $\overline{\nu}$ prompt (not $\overline{\nu}$ total) for the fission neutrons. MT=455 in File 5 contains the delayed fission neutron spectra.

In many reactor applications, the time dependent energy deposition rates are required rather than the components of the total energy per fission which are the values given in this MT. Time-dependent energy deposition parameters can be obtained from the group spectra in File 5 (MT=455) for delayed neutrons. Codes such as CINDER, RIBD, and ORIGEN must be used, however, to obtain more detailed information on the delayed neutrons and all time-dependent parameters for the betas and the gammas due to the fission process.

The time-integrated energies for delayed neutrons, delayed gammas, and delayed betas as calculated from the codes listed above may not always agree with the energy components given in File 1. The File 1 components must sum to ET (the total energy released per fission).

In heating calculations, the energy released in all nuclear reactions besides fission, principally the gamma-energy released in neutron radiative capture, enters analogously to the various fission energy components. Thus the (n,γ) energy-release would be equal to the Q-value in File 3, MT=102, for the capturing nuclide. The capture gammas can be prompt or delayed, if branching to isomeric states is involved, and this is relevant to various fission- and burnup-product calculations. The "sensible energy" in a heating calculation is the sum of ER, defined previously, plus the energy released in all other reactions.

1.6 Delayed Photon Data (MT=460)

This section describes the delayed photon source function resulting from either particle induced or spontaneous fission. The delayed gamma source function is defined as the number of gammas emitted per unit time after the fission event, per unit energy for a fixed incident energy:

$$S_\gamma(E, E_\gamma, t) + \frac{d^2 n_\gamma}{dt\ dE_\gamma}(E, E_\gamma, t). \tag{1.5}$$

Here E is the energy of the fission-inducing projectile, E_γ is the energy of the emitted photon, t is the time following fission at which the photon is emitted, and $d^2n_\gamma/dt\ dE_\gamma$ is the number of photons emitted per fission per second per eV. The source function may be given either in a discrete or continuous representation.

In the discrete representation (LO=1), the source function is given as a series of tables of photon multiplicities, $y_i(E)$, in File 12 with LO=1, with their associated time dependences:

$$S_\gamma(E, E_\gamma, t) = \sum_{i=1}^{\mathrm{NG}} \delta(E_\gamma - E_i)\ y_i(E)\ T_i. \tag{1.6}$$

The continuous representation (LO=2) is similar in spirit to the delayed neutron data (MT=455). In this representation, one must give the photon multiplicities in File 12 and the fraction of photons emitted at each energy, $f_i(E \leftarrow E_\gamma)$, in an MF=15 table, for each precursor family. The time dependence of each precursor family is given as a list of time constants:

$$S_\gamma(E, E_\gamma, t) = \sum_{i=1}^{\mathrm{NNF}} y_i(E)\ f_i(E \leftarrow E_\gamma)\ \lambda_i \exp(-t\lambda_i) \tag{1.7}$$

Only the precursor family time constants are stored in MF=1.

1.6.1 Formats

1.6.1.1 Discrete Representation (LO=1)

The following quantities are defined:

NG	The number of discrete photons.
NR, NP, $\mathbf{t}_{\mathrm{int}}$	Standard TAB1 parameters.
E_i	Energy of the ith photon (eV).
$T_i(t)$	Time dependence of the ith photons multiplicity (sec-1).

The structure of the time dependence data block is:

```
[MAT,1,460/  ZA, AWR, LO, 0, NG,  0]HEAD     (LO=1)
[MAT,1,460/  E1, 0.0,  1, 0, NR, NP/t_int/ T_1(t)]TAB1
[MAT,1,460/  E2, 0.0,  2, 0, NR, NP/t_int/ T_2(t)]TAB1
            ----------------------
[MAT,1,460/ E_NG, 0.0, NG, 0, NR, NP/t_int/ T_NG(t)]TAB1
[MAT,1,  0/ 0.0, 0.0,  0, 0,  0,  0]SEND
```

1.6.1.2 Continuous Representation (LO=2)

The following quantities are defined:

NNF The number of precursor families considered.

λ_i Decay constant (sec^{-1}) for the ith precursor.

The structure of this data block is:

```
[MAT,1,460/ ZA, AWR, LO, 0,   0, 0]HEAD     (LO=2)
[MAT,1,460/0.0, 0.0,  0, 0, NNF, 0/
           λ_1, λ_2, ---------- λ_NNF]LIST
[MAT,1,  0/0.0, 0.0,  0, 0,   0, 0] SEND
```

1.6.2 Procedures

1.6.2.1 Discrete Representation (LO=1)

The photon multiplicity is given in File 12 with LO=1 in File 12 set. Each discrete photon in File 12 must have an associated time dependence table specified in File 1. It is recommended that the photon multiplicities be given in the same order as the photons that are listed in File 1.

1.6.2.2 Continuous Representation (LO=2)

The probability of producing precursors for each family and the energy distributions of photons produced by each precursor family are given in Files 12 and 15. It is extremely important that the same precursor families be given in Files 12 and 15 as in File 1 (MT=460) and the ordering of families should be the same in all files. It is recommended that all families be ordered by decreasing half-lives ($\lambda_1 < \lambda_2 < \cdots < \lambda_{\text{NNF}}$).

References for Chapter 1

1. R. Sher and C. Beck, Electric Power Research Institute report, EPRI-NP-1771 (1981).
2. D.G. Madland, Nucl.Phys. **A772** (2006) 113-137.

Chapter 2

File 2: RESONANCE PARAMETERS

2.1 General Description

The primary function of File 2 is to contain data for both resolved and unresolved resonance parameters. It has only one section, with the reaction type number MT=151. A File 2 is required for incident-neutron evaluations, but it may be omitted in other cases. The use of File 2 is controlled by the parameter LRP (see section 1.1):

LRP=-1 No File 2 is given. Not allowed for incident neutrons.

LRP= 0 No resonance parameters are given except for the scattering radius AP.

AP is included for the convenience of users who need an estimate of the potential scattering cross section. It is not used to calculate a contribution to the scattering cross section, which in this case is represented entirely in File 3.

LRP= 1 Resonance contributions for the total, elastic, fission, and radiative capture cross sections are to be computed from the resonance parameters and added to the corresponding cross sections in File 3[1].

The File 2 resonance contributions should also be added to any lumped reactions included in File 3. For SLBW or MLBW (see below), any other competing reaction in the resonance range must be given in their entirety in File 3 under the corresponding MT number or as the background in the total cross section. The effects of the competing reactions on the resonance reactions are included using a single competitive width, Γ_x. This width is given

[1] In the unresolved resonance region, the evaluator may, optionally, specify a different procedure, which uses the unresolved resonance parameters in File 2 solely for the purpose of computing an energy-dependent self-shielding factor. This option is governed by a flag, LSSF, defined in Section 2.3.1, and discussed in Section 2.4.17. When this option is specified, File 3 is used to specify the entire infinitely-dilute cross section, and the function of File 2 is to specify the calculation of self-shielding factors for shielded pointwise or multigroup values.

explicitly in the unresolved resonance region, and implicitly in the resolved region; in the latter case, it is permissible for the total width to exceed the sum of the partials. The difference is the competitive width:

$$\Gamma_x = \Gamma - (\Gamma_n + \Gamma_\gamma + \Gamma_f)$$

For the Reich-Moore or Adler-Adler formalisms, competitive reactions are not used. For the R-Matrix Limited Format (LRF=7, see below), competitive reactions are included as separate channels.

LRP= 2 Resonance parameters are given in File 2 but are not to be used in calculating cross sections, which are assumed to be represented completely in File 3. This option is usually used in derived libraries to flag that the cross sections had already been reconstructed, but the source resonance parameters are stil available, if needed.

The resonance parameters for a ***material*** are obtained by specifying the parameters for each ***isotope*** in the ***material***. The data for the various ***isotopes*** are ordered by increasing ZAI values (charge-isotopic mass number). The resonance data for each isotope may be divided into several incident neutron energy ranges, given in order of increasing energy. The energy ranges for an isotope should not overlap; each may contain a different representation of the cross sections.

In addition to these parameterized resonance ranges, the full energy range of the evaluated data file may contain one or two ranges, in which the cross sections are given in pointwise form. Comments on these ranges follow:

1. The low energy region (LER) is one in which the cross sections are tabulated as smooth functions of energy. Doppler effects must be small enough so that the values essentially correspond to zero degrees Kelvin. For light elements, *i.e.*, those whose natural widths far exceed their Doppler widths and hence undergo negligible broadening, the entire energy range can often be represented in this way. For heavier materials, this region can sometimes be used below the lowest resolved resonances. With a good multilevel resonance fit, the LER can often be omitted entirely, and this is preferred. An important procedure for the LER is described in Section 2.4.6 item 4.

2. The resolved resonance region (RRR) is one in which resonance parameters for individual resonances are given. Usually this implies that experimental resolution is good enough to "see" the resonances, and to determine their parameters by area or shape analysis, but an evaluator may choose to supply fictitious resolved parameters if he so desires. If the evaluator does this, the resonances must have physically-allowed quantum numbers, and be in accord with the statistics of level densities (Appendix D, Section D.2.2). A File 3 background may be given. The essential point is that resonance self-shielding can be accounted for by the user for each resonance individually.

3. The unresolved resonance region (URR) is that region in which the resonances still do not actually overlap, so that self-shielding is still important, but experimental

resolution is inadequate to determine the parameters of individual resonances. In this situation, self-shielding must be handled on a statistical basis. A File 3 may be given. The interpretation of this cross section depends on the flag LSSF (see Sections 2.3.1 and 2.4.17). It may be interpreted either as a partial background cross section, to be added to the File 2 contribution, as in the resolved resonance region or it may be interpreted as the entire dilute cross section, in which case File 2 is to be used solely to specify the self-shielding appropriate to this energy region. It is important to choose the boundary between the RRR and the URR so that the statistical assumptions underlying the unresolved resonance treatments are valid. This problem is discussed further in Section 2.4.

4. The high-energy region (HER) starts at still higher energies where the resonances overlap and the cross sections smooth out, subject only to Ericson fluctuations. The boundary between the URR and HER should be chosen so that self-shielding effects are small in the HER.

File 3 may contain "background cross sections" in the resonance ranges resulting from inadequacies in the resonance representation (*e.g.*, SLBW), the effects of resonances outside the energy range, the average effects of missed resonances, or competing cross sections, which are not accounted for explicitly. If these background cross sections are non-zero, there must be double energy points in File 3 corresponding to each resonance range boundary (except 10^{-5}eV). See Section 2.4 for a more complete discussion of backgrounds.

Several representations are allowed for specifying resolved resonance parameters. The flag, LRF, indicates the representation used for a particular energy range:

LRF=1 Single-level Breit-Wigner; (no resonance-resonance interference; one single-channel inelastic competitive reaction is allowed). Use of this format is discouraged for new evaluations, which should use the Reich-Moore approximation (LRF=3 or 7).

LRF=2 Multilevel Breit-Wigner (resonance-resonance interference effects are included in the elastic scattering and total cross sections; one single-channel inelastic competitive reaction is allowed). Use of this format is discouraged for new evaluations, which should use the Reich-Moore approximation (LRF=3 or 7).

LRF=3 Reich-Moore (multilevel multi-channel R-matrix; no competitive reactions allowed).

It is possible to define partial widths Γ_{ls_1J} and Γ_{ls_2J} with two different values of the channel spin, as is required when both the target spin and the orbital angular momentum are greater than zero. This is accomplished by setting the resonance spin parameter AJ to a positive value for the larger channel spin ($s = I + 1/2$), and negative for the smaller channel spin ($s = I - 1/2$). (See definition of AJ in Section 2.2.1.) Older ENDF files have not used this feature, but instead have only positive AJ; in this case, all resonances of a given l, J are assumed to have the same channel spin.

For a given resonance, the only rigorously conserved quantities are J (total angular momentum) and π (total parity). Nevertheless, this format assumes that both l (orbital angular momentum) and s (channel spin) are also conserved quantities.

The LRF=3 format permits only a limited subset of Reich-Moore evaluations, but is adequate for some situations.

LRF=4 Adler-Adler (level-level and channel-channel interference effects are included in all cross sections via "effective" resonance parameters; usually applied to low-energy fissionable materials; no competitive reactions).

LRF=5 This option is no longer available.

LRF=6 This option is no longer available.

LRF=7 R-Matrix Limited format, which contains all the generality of LRF=3 plus unlimited numbers and types of channels.

Preferred formalisms for evaluation are discussed in Section 2.4.15. Further discussion of the above formalisms is contained in the Procedures Section 2.4.

Each resonance energy range contains a flag, LRU, that indicates whether it contains resolved or unresolved resonance parameters. LRU=1 means resolved, LRU=2 means unresolved.

Only one representation is allowed for the unresolved resonance parameters, namely average single-level Breit-Wigner. However, several options are permitted, designated by the flag LRF. With the first option, LRF=1, only the average fission width is allowed to vary as a function of incident neutron energy. The second option, LRF=2, allows the following average parameters to vary: level spacing, fission width, reduced neutron width, radiation width, and a width for the sum of all competitive reactions.

The data formats for the various resonance parameter representations are given in Sections 2.2.1 (resolved) and 2.3.1 (unresolved). Formulae for calculating cross sections from the various formalisms are given in Appendix D.

The following quantities have definitions that are the same for all resonance parameter representations:

NIS Number of isotopes in the material (NIS$\leq$10).

ZAI (Z,A) designation for an isotope.

NER Number of resonance energy ranges for this isotope.

ABN Abundance of an isotope in the material. This is a number fraction, not a ***weight*** fraction, nor a ***percent***.

LFW Flag indicating whether ***average fission widths*** are given in the unresolved resonance region for this isotope:

LFW=0, average fission widths ***are not*** given;

LFW=1, average fission widths ***are*** given.

NER Number of resonance energy ranges for isotope.

EL Lower limit for an energy range[2].

EH Upper limit for an energy range[3].

LRU Flag indicating whether this energy range contains data for resolved or unresolved resonance parameters:

LRU=0, only the scattering radius is given (LRF=0, NLS=0, LFW=0);

LRU=1, resolved resonance parameters are given.

LRU=2, unresolved resonance parameters are given.

LRF Flag indicating which representation has been used for the energy range. The definition of LRF depends on the value of LRU:

If **LRU=1** (resolved parameters), then:

LRF=1, single-level Breit-Wigner (SLBW);

LRF=2, multilevel Breit-Wigner (MLBW);

LRF=3, Reich-Moore (RM);

LRF=4, Adler-Adler (AA);

LRF=5, no longer available;

LRF=6, no longer available;

LRF=7, R-Matrix Limited (RML).

If LRU=2 (unresolved parameters), then:

LRF=1, only average fission widths are energy-dependent;

LRF=2, average level spacing, competitive reaction widths, reduced neutron widths, radiation widths, and fission widths are energy-dependent.

NRO Flag designating possible energy dependence of the scattering radius:

NRO=0, radius is energy independent;

NRO=1 radius expressed as a table of energy, radius pairs.

[2]These energies are the limits to be used in calculating cross sections from the parameters. Some resolved resonance levels, e.g., bound levels, will have resonance energies outside the limits.

NAPS Flag controlling the use of the two radii, the ***channel radius*** a and the ***scattering radius*** AP.

For NRO=0 (AP energy-independent), if:

NAPS=0 calculate a from Equation (D.0) given in Appendix D, and read AP as a single energy-independent constant on the subsection's second CONT record that defines the range; use a in the penetrabilities P_l and shift factors S_l, and AP in the hard-sphere phase shifts ϕ_l;

NAPS=1 do not use Equation (D.0); use AP in the penetrabilities and shift factor as well as in the phase shifts.

For NRO=1 (AP energy-dependent), if:

NAPS=0 calculate a from the above equation and use it in the penetrabilities and shift factors. Read AP(E) as a TAB1 quantity in each subsection and use it in the phase shifts;

NAPS=1 read AP(E) and use it in all three places, P_l, S_l, ϕ_l;

NAPS=2 read AP(E) and use it in the phase shifts. In addition, read the single, energy-independent quantity "AP, see following, and use it in P_l and S_l, overriding the above equation for a.

File 2 contains a single section (MT=151) containing subsections for each energy range of each isotope in the material.

Two versions of the File 2 format structure are presented here. The first one (sometimes denoted as a *special case*), is merely a particular instance of the general case with particular values NER=1, LRU=0, and NRO=0. No resonance parameters are given, only the scattering radius is specified (such material is not permitted to have multiple isotopes or an energy-dependent scattering radius). The structure of File 2, for this special case is

```
[MAT, 2,151/  ZA, AWR,  0,  0, NIS,   0]HEAD (NIS=1)
[MAT, 2,151/ ZAI, ABN,  0,LFW, NER,   0]CONT (ZAI=ZA,ABN=1,LFW=0,NER=1)
[MAT, 2,151/  EL,  EH,LRU,LRF, NRO,NAPS]CONT (LRU=0,LRF=0,NRO=0,NAPS=0)
[MAT, 2,151/ SPI,  AP,  0,  0, NLS,   0]CONT (NLS=0)}
[MAT, 2,  0/ 0.0, 0.0,  0,  0,   0,   0]SEND
[MAT, 0,  0/ 0.0, 0.0,  0,  0,   0,   0]FEND
```

The second version is a general case with given resonance parameters. The structure of File 2 for this general case is as follows:

```
[MAT, 2,151/  ZA, AWR,   0,   0, NIS,    0]HEAD
[MAT, 2,151/ ZAI, ABN,   0, LFW, NER,    0]CONT  (isotope)
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
     <Subsection for the first energy range
     <for the first isotope (depends on LRU and LRF)>
            ...
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
     <Subsection for the second energy range>
     <for the first isotope>
           ...
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT (range)
     <Subsection for the last energy range>
     <for the last isotope for this material>
           ...
[MAT, 2,  0/ 0.0, 0.0,   0,   0,   0,    0]SEND}
```

The data are given for all ranges for a given isotope, and then for all isotopes. The data for each range start with a CONT (range) record; those for each isotope, with a CONT (isotope) record. The specifications for the subsections that include resonance parameters are given in Sections 2.2.1 for the resolved region and Section 2.3.1 for the unresolved region. A multi-isotope material is permitted to have ***some***, but not all, isotopes specified by a scattering radius only. The structure of a ***subsection*** for such an isotope is:

```
[MAT, 2,151/ SPI,   AP,   0,   0, NLS,    0]CONT   (NLS=0)}
```

and as above LFW=0, NER=1, LRU=0, LRF=0, NRO=0, and NAPS=0 for this isotope.

In the case that NRO≠0, the "range" record preceding each subsection is immediately followed by a record giving the energy dependence of the scattering radius, AP.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / AP(E)]TAB1

If NAPS is 0 or 1 the value of AP on the next record of the subsection should be set to 0.0. If NAPS is 2, it should be set equal to the desired value of the channel radius.

2.2 Resolved Resonance Parameters (LRU=1)

2.2.1 Formats

Several different resonance formalisms are allowed to represent the resolved resonance parameters. Formulae for the various quantities, and further comments on usage, are given in Appendix D. The flag LRU=1, given in the second CONT record, indicates that resolved resonance parameters are given for a particular energy range. Another flag, LRF, in the same record specifies which resonance formalism has been used.

The following quantities are defined for use with all formalisms:

SPI Spin, I, of the target nucleus.

AP Scattering radius in units of 10^{-12}cm. For LRF=1 through 4, it is assumed to be independent of the channel quantum numbers.

NLS Number of l-values (neutron orbital angular momentum) in this energy region.

LRF=1 through 4, a set of resonance parameters is given for each l-value.

LRF=5 and 6, NLS is the number of l-values required to converge the calculation of the scattering cross section (see Sections 2.4.19 and 2.4.20). Another cutoff, NLSC, is provided for converging the angular distributions. For the limit on NLS see Appendix G.

AWRI Ratio of the mass of a particular isotope to that of a neutron.

QX Q-value to be added to the incident particle's center-of-mass energy to determine the channel energy for use in the penetrability factor. The conversion to laboratory system energy depends on the reduced mass in the exit channel. For inelastic scattering to a discrete level, the Q-value is minus the level excitation energy. QX=0.0 if LRX=0.

L Value of l.

LRX Flag indicating whether this energy range contains a competitive width:

LRX=0 no competitive width is given, and $\Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f$ in the resolved resonance region, while $\langle \Gamma_x \rangle = 0$ in the unresolved resonance region; LRX must be 0 for LRF=3, 4 and 7;

LRX=1 a competitive width is given, and is an inelastic process to the first excited state. In the resolved region, it is determined by subtraction, $\Gamma_x = \Gamma - [\Gamma_n + \Gamma_\gamma + \Gamma_f]$

This parameter is irrelevant for LRF=7.

NRS Number of resolved resonances for a given l-value. For the limit on NRS see Appendix G.

ER Resonance energy (in the laboratory system).

AJ The absolute value of AJ is the floating-point value of J (the spin, or total angular momentum, of the resonance).

When two channel spins are possible, if the sign of AJ is negative, the lower value for the channel spin is implied; if positive, the higher value is implied. When AJ is zero, only one value of channel spin is possible so there is no ambiguity; the channel spin s is equal to the orbital angular momentum l.

GT Resonance total width, Γ, evaluated at the resonance energy ER.

GN Neutron width Γ_n evaluated at the resonance energy ER.

GG Radiation width, Γ_γ, a constant.

GF Fission width, Γ_f, a constant.

GX Competitive width, Γ_x, evaluated at the resonance energy ER.

It is not given explicitly for LRF=1 or 2 but is to be obtained by subtraction, GX = GT –(GN+ GG + GF), if LRX≠0.

a ***Channel*** radius, in 10^{-12} cm. An uppercase symbol is not defined because it is not an independent library quantity. Depending on the value of NAPS, it is either calculated from the equation given earlier (and in Appendix D), or read from the position usually assigned to the ***scattering radius*** AP.

2.2.1.1 SLBW and MLBW (LRF=1 or 2)

The structure of a ***subsection*** is:

```
[MAT, 2,151/ 0.0, 0.0,  0,  0,  NR, NP/ E_int /AP(E)]TAB1 (if NRO ≠0)
[MAT, 2,151/ SPI,  AP,  0,  0, NLS,  0]CONT
    Use AP=0.0, if AP(E) is supplied and NAPS=0 or 1.
[MAT, 2,151/ AWRI,  QX,     L,   LRX, 6*NRS,    NRS
             ER1,   AJ1,    GT1,   GN1,    GG1,   GF1,
             ER2,   AJ2,    GT2,   GN2,    GG2,   GF2,
             ERNRS, AJNRS, GTNRS, GNNRS, GGNRS, GFNRS] LIST
```

The LIST record is repeated until each of the NLS l-values has been specified in order of increasing l. The values of ER for each l-value are given in increasing order.

The use of either of the Breit-Wigner formats is discouraged for new evaluations. The recommended format is the R-Matrix Limited Format (LRF=7).

2.2.1.2 Reich-Moore (LRF=3)

The following additional quantities are defined:

LAD Flag indicating whether these parameters can be used to compute angular distributions.

LAD=0 do not use

LAD=1 can be used if desired. Do ***not*** add to file 4.

NLSC Number of l-values which must be used to converge the calculation with respect to the incident l-value in order to obtain accurate elastic angular distributions. See Sections D.1.5 and D.1.6 (NLSC≥NLS).

APL l-dependent scattering radius. If zero, use APL=AP.

GFA First partial fission width, a constant.

GFB Second partial fission width, a constant.

GFA and GFB are signed quantities, their signs being determined by the relative phase of the width amplitudes in the two fission channels. In this case, the structure of a subsection is similar to LRF=1 and 2, but the total width is eliminated in favor of an additional partial fission width. GFA and GFB can both be zero, in which case, Reich-Moore reduces to an R-function.

The structure for a subsection is:

```
[MAT, 2,151/ 0.0,0.0,   0,  0,    NR,   NP/E_int/AP(E)]TAB1 (if NRO≠ 0)
[MAT, 2,151/ SPI, AP, LAD,  0,   NLS, NLSC]CONT
[MAT, 2,151/AWRI,APL,   L,  0, 6*NRS,  NRS/
            ER_1, AJ_1, GN_1, GG_1,  GFA_1, GFB_1,
            ER_2, AJ_2, GN_2, GG_2,  GFA_2, GFB_2,
           --------------------------------
         ER_NRS,AJ_NRS,GN_NRS,GG_NRS,GFA_NRS,GFB_NRS]LIST
```

The LIST record is repeated until each of the NLS l-values has been specified in order of increasing l. The values of ER for each l-value are given in increasing order.

2.2.1.3 Adler-Adler (LRF=4)

For the case of LRF=4 additional quantities are defined:

LI Flag to indicate the kind of parameters given:

LI=1, total widths only

LI=2, fission widths only

LI=3, total and fission widths

LI=4, radiative capture widths only

LI=5, total and capture widths

LI=6, fission and capture widths

LI=7, total, fission, and capture widths.

NX Number of sets of background constants given. There are six constants per set. Each set refers to a particular cross section type. The background correction for the ***total*** cross section is calculated by using the six constants in the manner following .

σ_T Background

$$= C \Big/ \sqrt{E}\,(AT_1 + AT_2/E + AT_3/E^2 + AT_4/E^3 + BT_1E + BT_2E^2)$$

where $C = \pi\lambda\!\!\!^{-2} = \pi/k^2$ and k is defined in Appendix D.

The background terms for the ***fission*** and ***radiative capture*** cross sections are calculated in a similar manner.

NX=2, background constants are given for the total and capture cross sections.

NX=3, background constants are given for the total, capture, and fission cross sections.

NJS Number of sets of resolved resonance parameters (each set having its own J-value) for a specified l.

NLJ Number of resonances for which parameters are given, for a specified AJ and L.

AT_1, AT_2, AT_3, AT_4, BT_1, BT_2 Background constants for the total cross section.

AF_1, AF_2, AF_3, AF_4, BF_1, BF_2 Background constants for the fission cross section.

AC_1, AC_2, AC_3, AC_4, BC_1, BC_2 Background constants for the radiative capture cross section.

DET_r [3]Resonance energy, (μ), for the total cross section. Here and below, the subscript r denotes the rth resonance.

DEF_r Resonance energy, (μ), for the fission cross section.

DEC_r Resonance energy, (μ), for the radiative capture cross section.

DWT_r Value of $\Gamma/2$, (v), for the total cross section.

DWF_r Value of $\Gamma/2$, (v), for the fission cross section.

DWC_r Value of $\Gamma/2$, (v), for the radiative capture cross section.

GRT_r Symmetrical total cross section parameter, G_r^T.

GIT_r Asymmetrical total cross section parameter, H_r^T.

GRF_r Symmetrical fission parameter, G_r^f.

GIF_r Asymmetrical fission parameter, H_r^f.

GRC_f Symmetrical capture parameter, G_r^γ.

[3]Note: DETr=DEFr=DECr and DWTr=DWFr=DWCr. The redundancy is an historical carryover.

GIC$_r$ Asymmetrical capture parameter, H_r^γ.

The structure of a subsection for LRF=4 depends on the value of NX (the number of sets of background constants). For the most general case (NX=3) the structure is

```
[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_int / AP(E)] TAB1
```

optional record for energy-dependent scattering radius.

```
[MAT, 2,151/  SPI,  AP,   0,   0,   NLS,   0] CONT
[MAT, 2,151/ AWRI, 0.0,  LI,   0,  6*NX,  NX
              AT1,  AT2,  AT3, AT4,  BT1, BT2,
              AF1, --------------------, BF2,
              AC1, --------------------, BC2] LIST
[MAT, 2,151/ 0.0, 0.0,    L,   0,   NJS,   0] CONT(l)
[MAT, 2,151/  AJ, 0.0,    0,   0,12*NLJ, NLJ/
            DET1, DWT1, GRT1, GIT1, DEF1, DWF1,
            GRF1, GIF1, DEC1, DWC1, GRC1, GIC1,
            DET2, DWT2, GIC2, --------------
            DET3,---------------------------
            --------------------------------
            ------------------------, GICNLJ] LIST
```

The last LIST record is repeated for each J-value (there will be NJS such LIST records). A new CONT (l) record will be given which NJS LIST records will follow. Note that if NX=2 then the quantities AF_1 through BF_2 will not be given in the first LIST record. Also, if LI$\neq$7 then certain of the parameters for each level may be set to zero, *i.e.*, the fields for parameters not given (depending on LI) will be set to zero.

The format has no provision for giving Adler-Adler parameters for the scattering cross section. The latter is obtained by subtracting the capture and fission cross sections from the total.

Although the format allows separation of the resonance parameters into J-subsets, no use is made of J in the Adler-Adler formalism. There is no analog to the resonance-resonance interference term of the MLBW formalism. Such interference is represented implicitly by the asymmetric terms in the fission and capture cross sections.

2.2.1.4 General R-Matrix (LRF=5)

The format is no longer available in ENDF-6.

2.2.1.5 Hybrid R-function (LRF=6)

The format is no longer available in ENDF-6.

2.2.1.6 R-Matrix Limited Format (LRF=7)

In the R-matrix scattering theory, a channel is defined by the two particles inhabiting that channel and by the quantum numbers for the combination. The two particles are hereafter

referred to as a particle-pair (PP), and are defined by their properties: neutron (or other particle) plus target nuclide (in ground or excited state), with individual identifiers such as mass, spin, parity, and charge. The additional quantum numbers defining the channel include orbital angular momentum l, channel spin s and associated parity, and total spin and parity J^{π} .

NOTE: This format is NOT restricted to one neutron (entrance) channel and two exit channels. There may be several entrance channels and a multitude of exit channels. Charged-particle exit channels are not excluded.

The term "spin group" may be used to define the set of resonances with the same channels and quantum numbers. For any given spin group, only total spin and parity are constant; there may be several entrance channels and/or several reaction channels (and, hence, several values of l or s, etc.) contributing to the spin group.

The "R-Matrix Limited" (RML) format was designed to accommodate the features of R-Matrix theory as implemented in analyses codes being used for current evaluations. In this format, relevant parameters appear only once. Particle-pairs are given first: the masses, spins and parities, and charges for the two particles are specified, as well as the Q-value and the MT value (which defines whether this particle-pair represents elastic scattering, fission, inelastic, capture, etc.). Two particle-pairs will always be present: gamma + compound nucleus, and neutron + target nucleus in ground state. Other particle-pairs are included as needed.

The list of resonance parameters is ordered by J^{π}, which (as stated above) is the only conserved quantity for any spin group. For each spin group, the channels are first specified in the order in which they will occur in the list of resonances. For each channel, the particle-pair number and the values for l and s are given, along with the channel radii.

Formats for the basic RML subsection

Additional quantities are defined (or, in some cases, re-defined):

KRM Flag to specify which formulae for the R-matrix are to be used.

KRM = 1 for single-level Breit-Wigner,

KRM = 2 for multilevel Breit-Wigner,

KRM = 3 for Reich Moore,

KRM = 4 for full R-matrix. (Others may be added at a later date.)

KRL Flag is zero for non-relativistic kinematics, 1 for relativistic.

NJS Number of values of J^{π} to be included.

NPP Total number of particle-pairs.

IA Spin (and parity, if non-zero) of one particle in the pair (the neutron or projectile, if this is an incident channel).

IB Spin of the other particle in the pair (target nuclide, if this is an incident channel). IB is set to zero and ignored if the first particle is a photon.

PA Parity for first particle in the pair, used only in the case where IA is zero and the parity is negative. (Value = +1.0 if positive, –1.0 if negative.)

PB Parity for second particle, used if IB= 0 and parity is negative.

MA Mass of first particle in the pair (in units of neutron mass).

MB Mass of second particle (in units of neutron mass).

ZA Charge of first particle.

ZB Charge of second particle.

QI Q-value for this particle-pair. (See Section 3.3.2 for details)

PNT Flag if penetrability is to be calculated;

PNT= 1 - calculate penetrability;

PNT=–1 - do not calculate penetrability;

PNT= 0 - assign value depending on the MT number. The default for capture (MT=102) or fission (MT=19) is PNT=–1; the default for other MT numbers is PNT=+1.

SHF Flag if shift factor is to be calculated (default = not):

SHF= 1 calculate the shift factor;

SHF=–1 do not calculate the shift factor.

MT Reaction type associated with this particle-pair; see Appendix B.

AJ Floating point value of J (spin); sign indicates parity.

PJ Parity (used only if AJ = 0.0).

NCH Number of channels for the given J^π.

IPP Particle-pair number for this channel (written as floating-point number).

L Orbital angular momentum (floating-point value).

CH Channel spin (floating-point value).

BND Boundary condition for this channel (needed when SHF=+1)

APE Effective channel radius (scattering radius), used for calculation of phase shift only. Units are 10^{-12} cm.

APT True channel radius (scattering radius), used for calculation of penetrability and shift factors. Units are 10^{-12} cm.

KBK Non-zero if background R-matrix exists; see Subsect. 2.2.1.7.2. (Often set to zero)

KPS Non-zero if non-hard-sphere phase shift are to be specified. (Often set to zero)

NRS Number of resonances for the given J^π.

NX Number of lines required for all resonances for the given J^π, assuming each resonance starts on a new line; equal to (NCH/6+1)*NRS. If there are no resonances for a spin group, then NX = 1.

ER Resonance energy in eV.

IFG Flag
IFG=0 - GAM is the channel width in eV,
IFG=1 - GAM is the reduced-width amplitude in $\mathrm{eV}^{1/2}$.

GAM Channel width in eV or reduced-width amplitude in $\mathrm{eV}^{1/2}$.

NOTE: For IFG = 0, the input quantity GAM is the width at the energy of the resonance; it is calculated from reduced width amplitudes through equation (D.45) of Appendix D.1.7, with E set to E_λ. For negative-energy dummy resonances, the convention is that the input quantity is the width evaluated at the absolute value of the resonance energy. In all cases, if the value GAM given in File 2 for the partial width is negative, the standard convention is assumed: the negative sign is to be associated with the reduced width amplitude $\gamma_{\lambda c}$ rather than with $\Gamma_{\lambda c}$ (since $\Gamma_{\lambda c}$ is always a positive quantity). More specifically, $\Gamma_{\lambda c} = |GAM|$ and $\gamma_{\lambda c} = \mathrm{sign(GAM)} \times \sqrt{|\mathrm{GAM}|/2\mathrm{P}}$, with P evaluated at the energy of the resonance.

If IFG =1, the input quantity is the reduced width amplitude $\gamma_{\lambda c}$.

The formats are as follows:

```
[MAT,2,151/ 0.0, 0.0, IFG, KRM, NJS, KRL ]CONT
```

(The following record provides all particle-pair descriptions. For KRM=1,2, or 3, the first particle-pair is the gamma plus compound nucleus pair.)

```
[MAT,2,151/0.0,   0.0,     NPP,     0, 12*NPP,  2*NPP/
          MA1,    MB1,     ZA1,   ZB1,    IA1,    IB1,
           Q1,   PNT1,    SHF1,   MT1,    PA1,    PB1,
          MA2,    MB2,     ZA2,   ZB2,    IA2,    IB1,
           Q2,   PNT2,    SHF2,   MT2,    PA2,    PB1,
          -------------------------------------------
       MANPP,  MBNPP,  ZANPP, ZBNPP, IANPP, IBNPP,
        QNPP, PNTNPP, SHFNPP, MTNPP, PANPP, PBNPP]LIST
```

(The following record provides the channel descriptions for one spin group. This record and the next one are repeated together, once for each of the NJS spin groups.)

```
[MAT,2,151/  AJ,    PJ,     KBK,      KPS,    6*NCH,     NCH/
           IPP1,    L1,     SCH1,     BND1,     APE1,     APT1,
           IPP2,    L2,     SCH2,     BND2,     APE2,     APT2,
           ----------------------------------------------
         IPPNCH, LNCH, SCHNCH, BNDNCH, APENCH, APTNCH]LIST
```

(The following record gives the values for resonance energy and widths for each resonance in this spin group.)

```
[MAT,2,151/ 0.0,     0.0,      0,      NRS,     6*NX,      NX/
            ER1,   GAM1,1,   GAM2,1,    GAM3,1,   GAM4,1,   GAM5,1,
          GAM6,1, ------------------------- GAMNCH,1,
            ER2,   GAM1,2,   GAM2,2,    GAM3,2,   GAM4,2,   GAM5,2,
          GAM6,2, ------------------------- GAMNCH,2,
            ----------------------------------------------
         ERNRS, GAM1,NRS, GAM2,NRS, GAM3,NRS, GAM4,NRS, GAM5,NRS,
       GAM6,NRS, ------------------------ GAMNCH,NRS          ]LIST
```

(If the number of resonances is zero for a spin group, then NRS=0 but NX=1 in this record.)

Other records may be included here, as described below. If KBK is greater than zero, a "background R-matrix" is given. If KPS is greater than zero, tabulated values exist for phase shifts. If KBK=0 and KPS=0, no additional records are needed.

The above two records, beginning with "channel descriptions," are repeated until each of the NJS J^π spin groups has been fully specified.

Formats for optional extensions to the RML

The formats described above are sufficient for most evaluations currently (2003) available (using KRM=3, KBK=0, and KPS=0). For the sake of generality, and to accommodate expected future developments in R-matrix analysis codes, additional capabilities are included in the RML format.

Different R-Matrix formulations (KRM = 1,2,4)

Equations given in Appendix D.1.7 are relevant to the Reich-Moore approximation to R-Matrix theory. The format, however, can also be used for single-level Breit-Wigner (KRM = 1), multilevel Breit-Wigner (KRM = 2), R-Matrix without approximations (KRM = 4). Equations for KRM = 1 or 2 will be written up if/when the need arises. Equations for KRM = 4 are identical to those given in Appendix D.1.7 with the elimination of the imaginary term in the denominator of equation (6), and the inclusion of each gamma-channel on a equal basis with all other channels.

Background R-matrix (KBK > 0):

As described in Appendix D.1.7.5, a background R-Matrix can be defined in a variety of different methods.

For KBK=0, Option 0 is used everywhere (that is, for all channels for this spin group) for the background R-Matrix. No additional formats are required and no additional records need to be written; the dummy resonances are included along with the physical resonances in the list record described above.

For KBK > 0, one LIST record (and two TAB1 records, for tabulated values) is included for each channel of the current spin group, a total of NCH records. The particular option to be used for the channel is identified by parameter **LBK**. The formats for the four options are as follows:

Option 0. Dummy resonances (**LBK**=0)
No additional information is conveyed in this record, other than LBK=0. No terms are added to the R-matrix for this channel.

```
[MAT,2,151/ 0.0, 0.0,   0,   0, LBK,   1/
            0.0, 0.0, 0.0, 0.0, 0.0, 0.0]LIST
```

Option 1. Tabulated complex function of energy (**LBK**=1)
Notation:

RBR Value of real part of tabulated function

RBI Value of imaginary part of tabulated function

```
[MAT,2,151/ 0.0, 0.0,   0,   0, LBK,   1/
            0.0, 0.0, 0.0, 0.0, 0.0, 0.0]LIST
[MAT,2,151/ 0.0, 0.0,   0,   0,  NR,  NP/ E_int / RBR(E) ]TAB1
[MAT,2,151/ 0.0, 0.0,   0,   0,  NR,  NP/ E_int / RBI(E) ]TAB1
```

(Recall that NR and NP are parameters, which define the interpolation scheme for TAB1 records, as defined in Section 0.6.3.7. Energy values given by E_{int} are in units of eV.)

Option 2. SAMMY's logarithmic parameterization (**LBK**=2)
Notation (See equation (D.76) of Section D.1.7.5 for the meanings of these quantities):

R0 $\overline{R}_{com,c}$

S0 $\overline{s}_{com,c}$

R1 $\overline{R}_{lin,c}$

S1 $\overline{s}_{lin,c}$

R2 $\overline{R}_{q,c}$

EU E_c^{up}

ED E_c^{down}

```
[MAT,2,151/ ED, EU,  0,  0, LBK,   1/
            R0, R1, R2, S0,  S1, 0.0]LIST
```

Option 3. Fröhner's parameterization (**LBK**=3)
Notion (See equations (D.77) and D.78) in Section D.1.7.5 for the meanings of these quantities):

R0 $\overline{R}_c$

S0 $\overline{s}$

GA Γ_γ

EU E_c^{up}

ED E_c^{down}

```
[MAT,2,151/ ED, EU,  0,   0, LBK,   1/
            R0, S0, GA, 0.0, 0.0, 0.0]LIST
```

Tabulated phase shifts (KPS=1)

When phase shifts are calculated externally (from optical model potentials, for example), rather than generated from the usual hard-sphere phase shift formulae, then the phase shifts must be presented in tabular form.

If parameter KPS is equal to 0, all phase shifts are calculated from the hard-sphere phase shift formulae (see Table D.1 for non-Coulomb and Appendix D.1.7 for a discussion on Coulomb hard-sphere phase shifts).

For KPS>0, one LIST record (and two TAB1 records, for tabulated values) are included for each channel of the current spin group, a total of NCH records. The particular option to be used for the channel is identified by parameter LPS. The formats for the two options are as follows:

Option 0. Hard-sphere phase shifts (**LPS**=0)

No additional information is conveyed in this record, other than LPS=0.

```
[MAT,2,151/ 0.0, 0.0,   0,   0, LPS,   1/
            0.0, 0.0, 0.0, 0.0, 0.0, 0.0]LIST
```

Option 1. Phase shift is a tabulated complex function of energy (**LPS**=1)

Notation:

PSR Value of the real part of the tabulated phase shift

PSI Value of the imaginary part of the tabulated phase shift

```
[MAT,2,151/ 0.0, 0.0,   0,   0, LPS,   1/
            0.0, 0.0, 0.0, 0.0, 0.0, 0.0]LIST
[MAT,2,151/ 0.0, 0.0,   0,   0,  NR,  NP/Eint/ PSR(E) ]TAB1
            0.0, 0.0,   0,   0,  NR,  NP/Eint/ PSI(E) ]TAB1
```

(Recall that NR and NP are parameters, which define the interpolation scheme for TAB1 records, as defined in Secttion 0.6.3.7. Energy values given by Ei_{nt} are in units of eV.)

2.3 Unresolved Resonance Parameters (LRU=2)

2.3.1 Formats

Only the SLBW formalism for unresolved resonance parameters is allowed (see Appendix D for pertinent formulae). However, several options are available for specifying the energy-dependence of the parameters, designated by the flag LRF. Since unresolved resonance parameters are averages of resolved resonance parameters over energy, they are constant with respect to energy throughout the energy-averaging interval. However, they are allowed to vary from interval to interval, and it is ***this*** energy-dependence, which is referred to above and in the following paragraphs.

The parameters depend on both l (neutron orbital angular momentum) and J (total angular momentum). Each width is distributed according to a chi-squared distribution with a certain number of degrees of freedom. This number may be different for neutron and fission widths and for different (l,J) channels.

The following quantities are defined for use in specifying unresolved resonance parameters (LRU=2):

SPI Spin of the target nucleus, I.

AP Scattering radius in units of 10^{-12} cm. No channel quantum number dependence is permitted by the format.

LSSF Flag governing the interpretation of the File 3 cross sections.

- LSSF=0 File 3 contains partial "background" cross sections, to be added to the average unresolved cross sections calculated from the parameters in File 2.
- LSSF=1 File 3 contains the entire dilute cross section for the unresolved resonance region. File 2 is to be used solely for the calculation of the self-shielding factors, as discussed in Section 2.4.17.

NE Number of energy points at which energy-dependent widths are tabulated. For the limit on NE see Appendix G.

NLS Number of l-values. For the limit on NLS see Appendix G.

ES$_i$ Energy of the ith point used to tabulate energy-dependent widths.

L Value of l.

AWRI Ratio of the mass of a particular isotope to that of the neutron.

NJS Number of J-states for a particular l-state. For the limit on NJS see Appendix G.

AJ Floating-point value of J (the spin, or total angular momentum of the set of parameters).

D Average level spacing for resonances with spin J. (D may be energy-dependent if LRF=2).

AMUX Number of degrees of freedom used in the competitive width distribution. (Assuming it is inelastic, 1.0≤AMUX≤2.0, determined by whether the spin of the first excited state is zero or not.)[4]

AMUN Number of degrees of freedom in the neutron width distribution. (1.0 ≤AMUN≤ 2.0)

AMUG Number of degrees of freedom in the radiation width distribution. (At present AMUG = 0.0. This implies a constant value of Γ_γ.)

AMUF Number of degrees of freedom in the fission width distribution. (1.0 ≤AMUF≤ 4.0)

MUF Integer value of the number of degrees of freedom for fission widths. (1 ≤MUF≤ 4)

INT Interpolation scheme to be used for interpolating between the ***cross sections*** obtained from average resonance parameters. ***Parameter interpolation*** is discussed in the Procedures Section 2.4.2.

GN0 Average reduced neutron width. It may be energy-dependent if LRF=2.

GG Average radiation width. It may be energy-dependent if LRF=2.

GF Average fission width. It may be energy-dependent if LRF=1 or 2.

GX Average competitive reaction width, given only when LRF=2, in which case it may be energy-dependent.

The structure of a ***subsection***[5] depends on whether LRF=1 or LRF=2. If LRF=1, only the fission width is given as a function of energy. If LRF=1 and the fission width is not given (indicated by LFW=0), then the simplest form of a subsection results. If LRF=2, energy-dependent values may be given for the level density, competitive width, reduced neutron width, radiation width, and fission width. Three sample formats are shown below (all LRU=2).

Case A
LFW=0 (fission widths not given)
LRF=1 (all parameters are energy-independent).
The structure of a subsection is:

[4]See Appendix D.2.2.6.

[5]The structure of a section was defined previously, and covers both resolved resonance and unresolved resonance subsections.

```
[MAT, 2,151/  SPI,    AP,    LSSF,     0,    NLS,   0] CONT
[MAT, 2,151/ AWRI,   0.0,       L,     0,  6*NJS, NJS/
              D1,   AJ1,    AMUN1,   GNO1,   GG1, 0.0,
              D2,   AJ2,    AMUN2,   GNO2,   GG2, 0.0,
              --------------------------------------
             DNJS, AJNJS, AMUNNJS, GNONJS, GGNJS, 0.0] LIST
```

The LIST record is repeated until data for all l-values have been specified. In this example, AMUG is assumed to be zero, and there is no competitive width.

Case B

LFW=1 (fission widths given)
LRF=1 (only fission widths are energy-dependent; the rest are energy-independent).
The structure of a subsection is:

```
[MAT, 2,151/ SPI,  AP, LSSF, 0, NE, NLS]CONT
              ES1,  ES2, ES3, ------------
             ------------------------- ESNE]LIST
[MAT, 2,151/AWRI, 0.0,    L,   0,  NJS,   0]CONT
[MAT, 2,151/ 0.0, 0.0,    L, MUF, NE+6,   0/
              D,  AJ, AMUN, GNO,  GG,  0.0,
              GF1, GF2, GF3,--------------
             ------------------------- GFNE]LIST
```

The last LIST record is repeated for each J-value (there will be NJS such LIST records). A new CONT(l) record will then be given which will be followed by its NJS LIST records until data for all l-values have been specified (there will be NLS sets of data).

In the above section, no provision was made for INT, and interpolation is assumed to be linear-linear. AMUG is assumed to be zero, AMUF equals MUF, and there is no competitive width.

Case C

LFW=0 or 1 (does not depend on LFW).
LRF=2 (all energy-dependent parameters).
The structure of a subsection is:

```
[MAT, 2,151/  SPI,  AP,  LSSF,     0,    NLS,    0]CONT
[MAT, 2,151/ AWRI, 0.0,     L,     0,    NJS,    0]CONT
[MAT, 2,151/   AJ, 0.0,   INT,     0, 6*NE+6,   NE/
              0.0, 0.0,  AMUX,  AMUN,   AMUG, AMUF,
              ES1,  D1,   GX1,  GNO1,    GG1,  GF1,
              ES2,  D2,   GX2,  GNO2,    GG2,  GF2,
              ------------------------------
             ESNE, DNE, GXNE, GNONE, GGNE, GFNE] LIST
```

The LIST record is repeated until all the NJS J-values have been specified for a given l-value. A new CONT(l) record is then given, and all data for each J-value for that l-value are given. The structure is repeated until all l-values have been specified. This example permits the specification of all four degrees of freedom.

2.4 Procedures for the Resolved and Unresolved Resonance Regions

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2.4.1 Abbreviations

UR(R)	unresolved resonance (region)
RR(R)	resolved resonance (region)
RRP	resolved resonance parameter(s)
URP	unresolved resonance parameter(s)
SLBW	single-level Breit-Wigner
MLBW	multilevel Breit-Wigner
MLAG	multilevel Adler-Gauss
UCS	unresolved cross section(s)

2.4.2 Interpolation in the Unresolved Resonance Region (URR)

For energy-dependent formats (LRF=2, or LRF=1 with LFW=1), the recommended procedure is to interpolate on the ***cross sections*** derived from the unresolved resonance parameters (URP). This is a change from the ENDF/B-III and IV procedure, which was to interpolate on the parameters. The energy grid should be fine enough so that the cross

sections at intermediate energy values can be computed with sufficient accuracy using this procedure. Normally, three to ten points per decade will be required to obtain reasonable accuracy. Some evaluations prepared for earlier versions of ENDF/B do not meet these standards. In such cases, if two adjacent grid points differ by more than a factor of three, the processing code should add additional intermediate energy points at a spacing of approximately ten-per-decade and compute the cross sections at the intermediate points using parameter interpolation. Additional cross sections can then be obtained by cross section interpolation in the normal way.

For many isotopes, there is not sufficient information for a full energy-dependent evaluation. In these cases, the evaluator may provide a single set of unresolved resonance parameters based on systematics or extrapolation from the resolved range (see LRF=1, LFW=0). Such a set implies a definite energy-dependence of the unresolved cross sections due to the slowly-varying wave number, penetrability, and phase shift factors in the SLBW formulas. It is incorrect to calculate cross sections at the ends of the URR, and then to compute intermediate cross sections by cross section interpolation. Instead, the processing code should generate a set of intermediate energies using a spacing of approximately ten-per-decade and then compute the cross sections on this grid using the single set of parameters given in the file. Additional intermediate values are then obtained by linear cross section interpolation as in the energy-dependent case.

It is recommended that evaluators provide the URP's on a mesh dense enough that the difference in results of interpolating on either the parameters or the cross sections be small. A 1% maximum difference would be ideal, but 5% is probably quite acceptable.

Finally, even if the evaluator provides a dense mesh, the user may end up with different numbers than the evaluator "intended". This is particularly true when genuine structure exists in the cross section and the user chooses different multigroup breakpoints than those in the evaluation. There is no solution to this problem, but the dense mesh procedure minimizes the importance of the discrepancy.

In order to permit the user to determine what "error" he is incurring, it is recommended that evaluators state in the documentation what dilute, unbroadened average cross sections they intended to represent by the parameters in File 2. Note that the self-shielding factor option specified by the flag LSSF (Sections 2.3.1 and 2.4.17) greatly reduces the impact of this interpolation ambiguity.

2.4.3 Unresolved Resonances in the Resolved Resonance Range

As discussed in Section 2.4.4, the boundary between the resolved and unresolved resonance regions should be chosen to make the statistical assumptions used in the URR valid. This creates problems in evaluating the resonance parameters for the RRR.

Problem 1: At the upper end of the resolved range, the smaller resonances will begin to be missed. An equivalent contribution could be added to the background in File 3. This contribution will not be self-shielded by the processing codes, so it cannot be allowed to become "significant". A better procedure is to supply fictitious resolved resonance parameters, based on the statistics of the measured ones, checking that the average cross section agrees with whatever poor-resolution data are available.

If both procedures are employed, care should be taken not to distort the statistics of the underlying parameter distributions.

Problem 2: Because d-wave resonances are narrower than p-waves, which are narrower than s-waves, everything else being equal, the point at which p-waves will be instrumentally unresolved can be expected to be lower in energy than for s-waves, and lower still for d-waves. Thus the unresolved region for p-waves will usually overlap the resolved region for s-waves, and similarly for d-waves. Current procedure does not permit representing this effect explicitly; one cutoff-point must serve for all l-values.

The remedies are the same as above, either putting known or estimated resonances into the background in the URR, or putting fictitious estimated resonances into the RRR. The latter is preferred because narrow resonances tend to self-shield more than broad ones, hence the error incurred by treating them as unshielded File 3 background contributions is potentially significant.

2.4.4 Energy Range Boundary Problems

There may be as many as four different kinds of boundaries under current procedures which permit multiple RRR's:

1. between a low-energy File 3 representation (range 1) and EL for the RRR (range 2),
2. between successive RR ranges,
3. between the highest RRR and the URR,
4. between EH for the URR and the high-energy File 3 representation.

Discontinuities can be expected at each boundary. At item 1, a discontinuity will occur if range 1 and range 2 are not consistently Doppler-broadened. In general, only an identical kernel-broadening treatment will produce continuity, *i.e.*, only if the range-1 cross sections are broadened from the temperature at which they were measured, and range-2 is broadened from absolute zero. A kernel treatment of range 1, or no broadening at all, will be discontinuous with a ψ-χ treatment of range 2. This effect is not expected to be serious at normal reactor temperatures and presumably, the CTR and weapons communities are cognizant of the Doppler problem. In view of these problems, a double energy point will not usually produce exact continuity in the complete cross section, (file 2 + file 3), unless evaluator and user employ identical methods throughout.

Discontinuities will occur between successive RRR's, unless the evaluator takes pains to adjust the "outside" resonances for each RRR to produce continuity at absolute zero. If the unbroadened cross sections in two successive RRR's are broadened separately, the discontinuity will be preserved, and possibly enhanced. These discontinuities are not believed to be technologically significant.

A discontinuity at item 3 is unavoidable, because the basic representation has changed. However if the RRR cross sections are group-averaged or otherwise smoothed, the discon-

tinuity[6] should be reasonably small. A discontinuity greater than 10 or 15% obtained with a suitable averaging interval indicates that the evaluator might want to reconsider his parameterization of the poor-resolution data. Some materials have large genuine fluctuations in the URR, and for these the 10-15% figure is not applicable. A double energy point will normally occur at this boundary, but will not eliminate the discontinuity.

Discontinuity at item 4 should be small, since both the URR and the high-energy range represent rather smooth cross sections, and the opportunity for error ought to be small. Anything over 5% or so should be viewed with suspicion.

The upper and lower energy limits of any energy range indicate the energy range of validity of the given parameters for calculating cross sections. Outside this energy range the cross sections must be obtained from the parameters given in another energy range and/or from data in file 3.

The lower energy limit of the URR should be chosen to make the statistical assumptions used in this range valid. The basic requirement is that there be "many" resonances in an energy-averaging interval, and that the energy-averaging interval be narrow with respect to slowly-varying functions of E such as wave number and penetrability. As an example, assume that the energy-averaging interval can extend 10% above and below the energy point, that the average resonance spacing is 1 eV, and that "many" is 100. Then the lowest reasonable energy for the URR would be about 500 eV, as given by 0.2 E=100×1. Some implications of this choice for the RRR-URR boundary were discussed in Section 2.4.3.

It is sometimes necessary to give parameters whose energies lie ***outside*** a specified energy range in order to compute the cross section for neutron energies that are ***within*** the energy range. For example, the inclusion of bound levels may be required to match the cross sections at low energies, and resonances will often be needed above EH to compensate the opposite, positive, bias at the high energy end.

For materials that contain more than one isotope, it is recommended that the lower energy limit of the resolved resonance region be the same for all isotopes. If resolved and/or unresolved resonance parameters are given for only ***some*** of the naturally occurring isotopes, then AP should be given for the others.

If more than one energy range is used, the ranges must be contiguous and not overlap.

Overlapping of the resolved and unresolved ranges is not allowed for any one isotope, but it can occur in an evaluation for an element or other mixture of different isotopes. In fact, it is difficult to avoid since the average resonance spacing varies widely between even-even and even-odd isotopes. Such evaluations are difficult to correctly self-shield. A kernel broadening code must first subtract the infinitely-dilute unresolved cross section, broaden the pointwise remainder, then add back the unresolved component. A multigroup averaging code that uses pointwise cross sections must first subtract the infinitely-dilute unresolved cross section to find the pointwise remainder, and then add back a self-shielded unresolved cross section computed for a background cross section which includes a contribution from the pointwise remainder.

[6] This refers to the discontinuity between the average cross section in the RRR, and the dilute (unshielded) pointwise cross section in the URR, which has been generated from the URR parameters. If the self-shielding factor option has been chosen (LSSF=1, Section 2.3.1), File 3 will contain the entire dilute cross section and no File 2 unresolved region calculation will be needed to ascertain the discontinuity.

2.4.5 Numerical Integration Procedures in the URR

The evaluation of effective cross sections in the URR can involve Doppler effects, flux-depression, and resonance-overlap as well as the statistical distributions of the underlying resonance parameters for a mixture of materials.

The previous ENDF recommendation for doing the complicated multi-dimensional integrations was the Greebler-Hutchins (GH) scheme [Reference 1], basically a trapezoidal integration. For essentially the same computing effort, a more sophisticated weighted-ordinate method can be used and it has been shown that the scheme in MC^2-II [Reference 2] produces results differing by up to several percent from GH. The MC^2-II subroutine[7], is the recommended procedure.

The M. Beer [Reference 3], analytical method has also been suggested, and is quite elegant, but unfortunately will not treat the general heterogeneous case.

2.4.6 Doppler-broadening of File 3 Background Cross Sections

1. In principle, the contribution to each cross section from File 3 should be Doppler-broadened, but in practice, many codes ignore it. It is therefore recommended that the evaluator keep file 3 contributions in the RRR and URR small enough and/or smooth enough so that omission of Doppler-broadening does not "significantly" alter combined File 2 plus File 3 results up to 3000 K. Unfortunately, the diversity of applications of the data in ENDF files makes the word "significantly" impossible to define.

2. A possible source of structured File 3 data is the representation of multilevel or MLBW cross sections in the SLBW format, the difference being put into File 3. This difference is a series of residual interference blips and dips, which may affect the between-resonance valleys and possibly the transmission in thick regions or absorption rates in lumped poisons, shields, blankets, *etc.* Users of the SLBW formalism should consider estimating these effects for significant regions. A possible remedy is available in the Multilevel Adler-Gauss form of MLBW. (See Section 2.4.12). If the resonance-resonance interference term in MLBW is expanded in partial fractions, it becomes a single sum of symmetric and asymmetric SLBW-type terms. Two coefficients occur which require a single sum over all resonances for each resonance, but these sums are weakly energy-dependent and lend themselves to approximations that could greatly facilitate the use of ψ and χ functions with MLBW.

3. An "in-principle" correct method for constructing resonance cross sections is:

   (a) Use a Solbrig kernel [Reference 4] to broaden File 2 to the temperature of File 3, since the latter may be based on room-temperature or other nonzero ^{0}K data.

   (b) Add File 2 and File 3.

   (c) Sollbrig-broaden the result to operating temperature.

[7] This subroutine was provided by H. Henryson, II (ANL).

Using a Gaussian kernel instead of Sollbrig incurs a small error at low energies, unless it is misused, in which case the error can be large. Using ψ and χ functions introduces further errors. In fact, the Sollbrig kernel already approximates the true motion of the target molecules by a free-gas law, but anything more accurate is quite difficult to handle.

4. Some heavy element evaluations use a File 3 representation below the resolved resonance region. Often these cross sections are room-temperature values, so that if they are later broadened assuming they are zero-degrees Kelvin, they get broadened twice.

   A simple way to reduce the impact of this procedure without altering the representation of the data is to calculate the cross sections from the resonance parameters, ***broadened to room temperature***, and carry the calculation down through the low-energy region. Subtract these broadened values from the file 3 values and leave only the ***difference*** in file 3. Then extend the lower boundary of the resonance region to the bottom of the file. Now the "double-broadening" problem affects only the (small) residual file 3 and not the entire cross section.

   Note that subtracting off a ***zero degree*** resonance contribution would accomplish nothing.

2.4.7 Assignment of Unknown J-Values

In all multilevel resonance formalisms except Adler-Adler, the J-value determines which resonances interfere with each other. Usually, J is known only for a few resonances, and measurers report $2g\Gamma_n$ for the others. If this number is assumed to be Γ_n, one incurs an error of uncertain magnitude, depending on how different is the factor g

$$g = \frac{2J+1}{2\,(2I+1)}$$

from $l/2$, how large Γ_n is relative to the other partial widths, and how important resonance-resonance interference is.

It is recommended that evaluators assign J-values to each resonance, in proportion to the level density factor $2J+l$. To reduce the amount of interference, the J-values of strong neighboring resonances, which would produce the largest interference effects, can be chosen from different families.

In the past, some evaluations have put $J = I$, the target nucleus spin, for resonances with unknown J-values. This corresponds to putting $g = 1/2$, rather than its true value. Mixing of the $J = I$ resonances with the physically correct $I \pm 1/2$ families can result in negative scattering cross sections, or distortions of the potential scattering term, depending on what formalism is used and how it is evaluated. For this reason, such $J = I$ resonances must not be used.

In the amplitude-squared form of the MLBW scattering cross section,

$$\sigma_{nn} = \sum_{lsJ} g_J \left| A^{lsJ}_{\text{pot}} + A^{lsJ}_{\text{resonance}} \right|^2$$

the use of $J = I$ resonances will destroy the equivalence between this form and the "squared" form of MLBW in Appendix D since the sum on lsJ does not go over physically-correct values.

An exception to the prohibition against $J = I$ is the case where no J-values are known, since if ***all*** resonances are assigned $J = I$, the MLBW scattering cross section will be non-negative.

2.4.8 Competitive Width in the Resonance Region

2.4.8.1 Resolved Region

Procedures for the Resolved Resonance Region are contained in Section D.3.1 of Appendix D.

2.4.8.2 Unresolved Region

Procedures for the Unresolved Resonance Region are contained in Section D.3.2 of Appendix D. Users are directed to the discussion of the total cross section in Appendix D, Section D.3.3, since, as pointed out by H. Henryson, II, in connection with MC^2 procedures, a possibility for erroneous calculations exists.

2.4.9 Negative Cross Sections in the Resolved Resonance Region

To avoid negative cross sections, new evaluations should use only the rigorous formulations such as Reich-Moore (LRF=3) or R-Matrix Limited (LRF=7). However, resonance parameters coded in other formats may be encountered in some old evaluations.

2.4.9.1 In the SLBW Formalism:

Capture and fission use the positive symmetric Breit-Wigner shape and are never negative. Scattering involves an asymmetric term which goes negative for $E <$ER and can cause negative cross sections. A single resonance, or a series of well-separated resonances, will usually not produce negative cross sections, but when two or more resonances "cooperate", their negative tails can combine to produce negative values. In nature, these do not exist; the negative tails are compensated by either the positive tails of lower-lying resonances or multilevel interference effects. However, in evaluated data files the resonances are usually given only down to "E=0", a quite arbitrary point from the standpoint of the compound nucleus, so that "negative-energy" resonances are needed to compensate the negativity bias.

Although the negative ***scattering*** cross sections themselves can usually be classed as an inconvenience, their effect in distorting the ***total*** cross section, which governs neutron penetration, can be more serious. Perhaps more important is the fact that even when the cross section remains positive, it is still often too low due to the same effect and this bias again affects the total cross section and calculated absorption rates. To compensate this bias, the evaluator should put in either a series of negative energy resonances with reasonable size and spacing ("picket fence", or reflect the positive-energy ones around E=0)

or a few large fictitious ones ("barber poles"), or a compensating background in File 3 (*e.g.*, see Reference 5).

To compensate interior-region negativity requires a multilevel treatment of which MLBW is the simplest. Although there is no ***guarantee*** that MLBW cross sections will be more accurate than SLBW, they ***are*** guaranteed to be non-negative (but see next section) and are generally to be preferred over SLBW.

A similar bias occurs at the upper end of the resolved resonance range, where it is less noticeable because it is a positive bias, and most calculations are not as sensitive to this region as they are to the low-energy end. The remedy is the same extra resonances above the RRR, or compensation in file 3. The latter remedy requires a negative file 3 contribution, which is physically acceptable, but produces undesirable side-effects in some processing codes, hence the extra-resonance remedy is preferred. It is probably safe to say that there is never a compelling reason to use the SLBW formula for the calculation of pointwise scattering cross sections. If one is doing a calculation that is sophisticated enough to warrant the use of pointwise cross sections, then a multilevel formalism is certainly justifiable. If one is merely deriving multigroup cross sections, then the other approximations involved justify the use of any reasonable "fix" for the negative scattering, such as simply setting $\sigma_S = 0$ when it goes negative. Such a procedure should usually be accompanied by a corresponding increase in the ***total*** cross section.

2.4.9.2 In the MLBW Formalism:

Capture and ***fission*** use the SLBW formulas and are positive. Scattering uses a formula, which can be written as an absolute square and as such is non-negative. The use of J=I resonances (Section 2.4.7) can destroy the correspondence between the absolute-square form and the expanded form given in Appendix D and result in negative scattering cross sections. Despite its non-negativity, MLBW still produces biased cross sections at both ends of the RRR unless compensating extra resonances or File 3 contributions are included above and below. The evaluator should generally correct for this effect.

2.4.9.3 In the R-matrix, Reich-Moore, and R-function Formalisms:

These are again based on an absolute square and cannot be negative. However, they can be biased and extra resonances, background R-values, or File 3 contributions should be provided. If conversion of Reich-Moore to Adler format produces negative cross sections, dummy parameters should be provided to eliminate them.

2.4.9.4 In the Adler-Adler Formalism:

Although the formulae are derived from an absolute square and are in principle non-negative, in practice the parameters are chosen to fit measured data, so that the physical and mathematical constraints among the parameters, which prevent negative cross sections, are lost, and any of the cross sections can be negative. If the Adler formalism is used for evaluations, negativity should be checked for. The end-effect bias exists in this formalism also and should be checked for in the scattering and total cross sections by comparing with experiment.

2.4.10 Negative Cross Sections in the Unresolved Resonance Region

R. Prael, while at ANL, reported a difficulty with SLBW resonance ladders created by VIM from the unresolved resonance parameters in Mo (MAT l287), namely that the negative File 3 ***capture*** background sometimes caused negative capture cross sections in the resonance valleys. The evaluator intended the background to compensate for an excess of capture in the average unresolved capture cross section, but did not anticipate the problem that would arise when the parameters were used in a different context. One remedy is to drop out the negative File 3 background and adjust $< \Gamma_\gamma >$ on whatever energy mesh is needed to produce agreement with the dilute poor-resolution data.

The creation of SLBW ladders from average parameters can be expected to produce the same kind of end-effect bias and frequent negative scattering cross sections found in the resolved resonance region. Again, the scattering cross section per se may not be important, but the biased total cross section may adversely affect calculated reaction rates.

2.4.11 Use of Two Nuclear Radii

The current ENDF formats defines two different nuclear radii:

a) the scattering radius, AP, and

b) the channel radius, a.

The scattering radius is also referred to as "the effective scattering radius" and "the potential scattering radius". The channel radius is also referred to as "the hard-sphere radius", or "the nuclear radius". The former is the quantity defined as AP (for a^+ or $\hat{}a$) in File 2, which must be given even if no resonance parameters are given. The nuclear radius is defined in Appendix D, equation (D.14).

The channel radius is a basic quantity in R-matrix theory, where the internal and external wave-functions are joined and leads to the appearance of hard-sphere phase shifts defined in terms of it. The necessity to relax the definition and permit two radii can be thought of as a "distant-level effect", sometimes not explicit in R-matrix discussions.

The original ENDF formats made provision for an AM, or "A-minus", although it was always required that evaluators put AM=0, to signify that it was equal in value to AP. In the current formats, AM is eliminated, but one can anticipate that more sophisticated evaluation techniques may eventually force the reinstatement of not only AM, but a more general dependence of the scattering radius on the channel quantum numbers, especially as higher energies become important.

In theory, the scattering radius depends on all the channel quantum numbers, and in practice it is common to find that different optical model parameters are required for different l-values (s, p, d,...) and for different J-values ($p^{1/2}$, $p^{3/2}$, ,,,). This implies that one would require a different scattering radius for each of these states.

For the special case of s-waves, only two J-values are possible, namely $I \pm 1/2$, commonly denoted J_+ and J_-. This is the origin of the terminology a_+ and a_-.

Up through ENDF/B-V, the recommended ENDF procedure was to use the above equation for the channel radius in the penetrabilities $P_l(ka)$ and the shift factors $S_l(ka)$, but to use the scattering radius to calculate the hard-sphere phase shifts $\phi_l(ka)$.

Since the phase-shifts define the potential scattering cross section, the evaluator had the freedom to fit AP to a measured cross section while still leaving undisturbed those codes that use the $A^{1/3}$ formula to calculate the channel radius.

In the ENDF-6 format, new parameters NRO and NAPS are available to give the evaluator more flexibility for the SLBW, MLBW, and RM formalisms, by allowing the evaluator to use AP everywhere and to make AP energy-dependent (Section 2.1).

The full flexibility of channel-dependent radii is provided for the RML format.

2.4.12 The Multilevel Adler-Gauss Formula for MLBW

Appendix D gives (implicitly) for the MLBW formalism the equations:

$$\sigma_{n,\gamma}^{\mathrm{MLBW}}(E) \equiv \sigma_{n,\gamma}^{\mathrm{SLBW}}(E) \,, \tag{2.1}$$

$$\sigma_{n,f}^{\mathrm{MLBW}}(E) \equiv \sigma_{n,f}^{\mathrm{SLBW}}(E) \,, \tag{2.2}$$

$$\sigma_{n,n}^{\mathrm{MLBW}}(E) \equiv \sigma_{n,n}^{\mathrm{SLBW}}(E) + \sum_{l=0}^{\mathrm{NLS}-1} \sigma_{n,n,\mathrm{RRI}}^{l}(E) \tag{2.3}$$

where RRI labels the resonance-resonance-interference term for a given l-value:

$$\frac{\pi}{k^2} \sum_J g_J \sum_{r=2}^{\mathrm{NR}_J} \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left[(E-E'_r)(E-E'_s)+\Gamma_r\Gamma_s/4\right]}{\left[(E-E'_r)^2+(\Gamma_r/2)^2\right]\left[(E-E'_s)^2+(\Gamma_s/2)^2\right]} \tag{2.4}$$

As most users are aware, this double sum over resonances can eat prodigious amounts of computer time unless handled very tactfully. Thus, for a 200-resonance material, there are $\approx$ 40,000 cross terms, of which only 20,000 need to be evaluated because the expression is symmetric in r and s.

It has been noted many times in the past that partial fractions can reduce Equation (2.3) to a form with only a single Breit-Wigner denominator. DeSaussure, Olsen, and Perez (Reference 5) have written it compactly as:

$$\sigma_{n,n,\mathrm{RRI}}^{l}(E) = \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{G_r\Gamma_r + 2H_r(E-E'_r)}{(E-E'_r)^2+(\Gamma_r/2)^2} \tag{2.5}$$

$$\text{where} \qquad G_r = \frac{1}{2} \sum_{s=1, s\neq r}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{ns}(\Gamma_r+\Gamma_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2}$$

$$H_r = \sum_{s=1, s\neq r}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{ns}(E'_r-E'_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2}$$

The authors give the special case for I=l=0, but it is valid for any set of quantum numbers. Thus an existing SLBW code can be converted to MLBW by adding $G_r\Gamma_r$ to the symmetric part of the SLBW formula, $\Gamma_{nr}^2 \cos 2\phi_l - 2\Gamma_{nr}(\Gamma_r - \Gamma_{nr}) \sin^2 \phi_l$, and $2H_r$ to the coefficient of $(E - E_r')$ in the asymmetric part, $2\Gamma_{nr} \sin 2\phi_l$.

Since G_r and H_r are weakly energy-dependent, via the penetrabilities and shift factors, they lend themselves to approximations that can sharply reduce computing time compared to the form with the "double" Breit-Wigner denominator. In fact, if the resonances are all treated as s-wave (shifts of zero, penetrabilities of $\sqrt{E}$), and the total widths are taken as constant, then G_r/k^2 and H_r/k^2 become independent of the neutron energy and consume a negligible amount of computing time so that MLBW and SLBW become equivalent in that respect.

The amplitude-squared form of MLBW, defined by equations (D.19) to (D.21), also reduces computing time.

2.4.13 Notes on the Adler-Adler Formalism

Questions concerning the ENDF treatment of the Adler formalism are enumerated below[8], together with recommended procedures for handling them:

1. The resonance energy μ and total half-width ν are the same for each reaction for a given resonance in the Adler formalism, but, for the October l970 version of ENDF-l02, the formulae on page D7, and the format descriptions of pages 7.9 and Nl2 permit different values for the total, fission, and capture cross sections.

   This is a misreading of the formalism; the remedy is to constrain the equalities $\mathrm{DET}_N = \mathrm{DEF}_N = \mathrm{DEC}_N$ and $\mathrm{DWT}_N = \mathrm{DWF}_N = \mathrm{DWC}_N$. The formulas for capture and fission should also have the phases eliminated in Appendix D.

2. The Adler formalism, as applied by the Adlers, breaks the resolved resonance region up into sub-regions, and each is analyzed separately. This avoids problems with contributions from distant resonances, but requires that the polynomial background be tailored to each sub-region. However, the ENDF formats allow only one resolved resonance energy region, so this procedure cannot be used.

   If a single set of polynomial background constants is insufficient, additional background can be put into File 3, point-by-point.

3. The ENDF formats formerly permitted incomplete specification of the cross sections. The allowed values of LI were 5 (total and capture widths); 6 (fission and capture); and 7 (total, fission, and capture). LI=6 leaves the scattering (and total) undefined and LI=5 is deficient for fissile elements. LI=6 is now restricted to ENDF/A, and LI=5 should be used only for non-fissile elements.

4. The nomenclature for the G's and H's is not entirely consistent among different authors. The Adlers use for the total cross section the definitions:

[8] The following is a condensation and updating of the Appendix in the June, l974, Minutes of the Resonance Region Subcommittee.

$$G_t = \alpha \cos(2ka) + \beta \sin(2ka);$$

$$H_t = \beta \cos(2ka) - \alpha \sin(2ka);$$

and then the combination:

$$\nu G_t + (\mu - E) H_t.$$

For the reaction cross sections there are no phases, and they write:

$$\nu G_c + (\mu - E) H_c \quad \text{(capture)};$$

$$\nu G_f + (\mu - E) H_f \quad \text{(fission)};$$

G and H are properly designated as "symmetrical" and "asymmetrical" parameters. This manual changes α to G_t and β to H_t, viz:

$$\nu[G_t \cos(2ka) + H_t \sin(2ka)] + (\mu - E)[H_t \cos(2ka) - G_t \sin(2ka)]$$

These G_t's and H_t's are no longer symmetrical and asymmetrical, but are referred to that way. The precedent for this nomenclature is probably Reference 6.

DeSaussure and Perez, in their published tables of G and H, incorporate the Adler's constant c into their definition, but otherwise leave the formalism unchanged.

Users and evaluators should adhere to the definitions in this manual.

5. The flag NX, which tells what reactions have polynomial background coefficients given, should be tied to LI, so that the widths and backgrounds are given for the same reactions, *i.e.*, use NX=2 with LI=5 (total and capture), and NX=3 with LI=7 (total, capture, and fission). Since no NX is defined for LI=6 (fission and capture), one is forced to use NX=3 with the background total coefficients set equal to zero, but this now occurs only in ENDF/A, if at all.

2.4.14 Multi-Level Versus Single-Level Formalisms in the Resolved and Unresolved Resonance Regions

2.4.14.1 In the Resolved Resonance Region:

The SLBW formalism may be adequate for resonance treatments that do not require actual pointwise scattering cross sections, as, *e.g.*, multigroup slowing-down codes. Because of the frequent occurrence of negative scattering cross sections, when two or more resonance-potential interference terms overlap, SLBW should not be used to compute pointwise scattering cross sections. Instead, the MLBW formalism may be used, although MLBW is not a true multilevel formalism, but a limit which is valid if Γ/D is small.

The Reich-Moore reduced R-matrix formalism is a true multilevel formalism, and is recommended for all evaluations. All of its cross sections are non-negative, and its only significant drawbacksare the difficulty of determining a suitable R^{∞} to represent distant-level effects, and of determining the parameters of negative-energy resonances.

The Adler form of the Kapur-Peierls formalism is also a true multilevel treatment, but in actual applications the parameters are determined by fitting data and the theoretical constraints among them are lost, so that any Adler cross section can be negative.

The simplest true multilevel formalism is the reduced R-function, in which all channels except elastic scattering have been eliminated. It sometimes makes an adequate evaluation tool for non-fissile elements up to the threshold for inelastic scattering, since below that the eliminated channels are (usually) simply radiative capture. It can be corrected for distant-level effects by substituting optical-model phase shifts for the hard-sphere ones which occur in the formalism, and by introducing an appropriate R^{∞}. It can be carried above the inelastic threshold by augmenting it with the use of SLBW formulas for the reactions other than elastic scattering, since such reactions often show negligible multilevel effects. For structural and coolant materials, either Reich-Moore or R-Matrix Limited can be used. The latter provides more detail in describing competitive reactions, plus angular distributions, and allows treating resonances with both l >0 and I>0.

Multichannel multilevel fitting is also feasible for light elements, and permits the simultaneous use of non-neutron data leading to the same compound nucleus. Due to the complexity of such calculations, they may be presented in ENDF libraries as file 3 pointwise cross sections, although the R-matrix Limited format can handle this case.

2.4.14.2 In the Unresolved Resonance Region:

In principle, if the statistical distributions of the resolved resonance parameters are known, any formalism can be used to construct fictitious cross sections in the unresolved region. At the present time, only the SLBW formalism is allowed in ENDF, for the reason that no significant multilevel effect has been demonstrated, when SLBW is properly handled.

If resolved region statistics are used without adjustment to poor resolution data, then large multilevel/single-level differences can result, but there is no simple way to determine which is better. If both are adjusted to yield the same average cross sections, and for fissile materials, the same capture-to-fission ratio, then the remaining differences are within the statistical and measurement errors inherent in the method. The above comments on multilevel effects in the unresolved resonance region are based on the work of DeSaussure and Perez [Reference 7].

As noted in Section 2.4.l2, the use of SLBW to construct resonance profiles in the unresolved region will result in the defects associated with this formalism elsewhere, and is not recommended. This application calls for MLBW or better, and the SLBW scheme should be used only for constructing average cross sections where the negative scattering effects will combine with the other approximations and presumably be "normalized out" somewhere along the line.

2.4.15 Preferred Formalisms for Evaluating Data

Unless there is strong reason to do otherwise, the R-Matrix Limited format (LRF=7) should be used for reporting results of new evaluations, as it is the most comprehensive of the current formats.

1. Light nuclei: Use multilevel, multichannel R-matrix. Present either as pointwise cross sections in file 3, or as R-matrix parameters using LRF=7.

2. Materials with negligible or moderate multilevel effects, and no multichannel interference: Reich-Moore or MLBW. These are equivalent in computing time and all require kernel broadening, although MLBW lends itself to the ψ, χ approximation discussed in Section 2.4.12. However, RM and RML provide the angular distribution of elastically-scattered neutrons, which MLBW does not.

3. Materials with strong multilevel effects, but no multichannel interference: Reich-Moore or R-Matrix Limited. The structural materials do not exhibit channel-channel interference, but have level-level interference that is too strong for an MLBW treatment.

4. Materials with observable channel-channel interference: Reich-Moore or R-matrix Limited. In the past, only low-energy fissionable materials have shown channel-channel interference, and this is unlikely to change. Reich-Moore evaluations can be converted to Adler format for presentation in ENDF. The reason why Reich-Moore is preferred to Adler-Adler as the basic evaluation tool is that it has less flexibility and is therefore better able to distinguish between various grades of experimental data. However, it requires kernel broadening whereas Adler-Adler uses ψ and χ, making the latter more convenient to broaden. Unfortunately some of this convenience is lost in practice because there is no simple equivalence between Adler-Adler and SLBW (see Section 2.4.8). With modern computers and modern computer codes, the slight advantage offered by kernel broadening is no longer an important issue.

5. Materials with channelchannel interference and one or more competitive reactions: R-matrix, using the format LRF=7 to present the parameters.

2.4.16 Degrees of Freedom for Unresolved Resonance Parameters

A resonance in the system (neutron plus a target of mass A) corresponds to a quasi-stationary state in the compound nucleus $A+1$. Such a resonance can decay in one or more ways, each described as a channel. These are labeled by the identity of the emitted particle (two-body decay), the spins I and i of the residual nucleus and the emitted particle, and the orbital angular momentum l of the pair. To uniquely specify the channel, two more quantum numbers are needed, since the magnetic quantum numbers can be eliminated for unpolarized particles.

It is common to give the channel spin, s, which is the vector sum of I and i, plus $\overrightarrow{J} = \overrightarrow{s} + \overrightarrow{l}$, since this facilitates the isolation of the l-dependence of all channel quantities.

The important point is that the same set of three ingredient angular momenta, I, i, and l, will give rise to a number of different channels, according to the rules for coupling angular momenta. The resonance will decay into each of these channels, with a probability that is governed by a real number $\gamma_{\alpha IiJls}$, the reduced width amplitude, where α gives the identity of the emitted particle, the state of excitation of the daughter nucleus, *etc.* The partial width for the channel is:

$$\Gamma_{\alpha IiJls} = 2P_{\alpha IiJls}\gamma^2_{\alpha IiJls}. \tag{2.6}$$

The penetrabilities depend only on l, and are given in Appendix D for uncharged particles. For charged particles, their Coulomb analogs can be found in texts on the subject, and for gamma rays one uses $\sqrt{\Gamma_\gamma}$ rather than Γ and P.

If the collection of channel quantum numbers $(\alpha IiJls)$ is denoted by c, then the total width for the level is $\Gamma = \sum_c \Gamma_c$. [$\sum_c$ means a sum over all channels]. The argument from statistical compound nucleus theory is that the Γ_c's are random variables, normally distributed with zero mean and equal variance. The population referred to is the set of Γ_c's for a given channel and all the levels (or resonances). It follows that the total width is distributed as a chi-squared distribution with N degrees of freedom, since this is the statistical consequence of squaring and adding N normal variates. For $N = l$, this is the Porter-Thomas distribution. In determining the behavior of any quantity that is going to be averaged over resonances, it is necessary to know the way in which the widths are distributed, hence the inclusion of these degrees of freedom in ENDF.

1. The neutron width is governed by AMUN, which is specified for a particular l value. Usually, only the lowest allowed l value will be significant in any decay, although the formats would allow giving both s and d-wave widths for the same resonance. Since there is only one J value for a given resonance, and we label the widths by one l value, there can be at most two channels for neutrons ($i = 1/2$), labeled by the channel spin values $s = I \pm 1/2$. If $I = 0$, there is only one channel, $s = i = 1/2$; hence the restriction,

   $$1.0 \leq \text{AMUN} \leq 2.0.$$

   AMUN is the quantity $\mu_{l,J}$, discussed in Section D.2.2.2.

   Although there is no supporting evidence, it is assumed that the average partial widths for each channel spin are equal, and that $\langle\Gamma_n\rangle$ is the sum of two equal average partial widths. In Appendix D this factor of two is absorbed into the definition of $\langle\Gamma_n\rangle$, through the use of a multiplicity, which is the number of channel spins, 1 or 2.

2. The competitive width is currently restricted to inelastic scattering, which has the same behavior as elastic scattering, measured from a different "zero channel energy," hence

   $$1.0 \leq \text{AMUX} \leq 2.0$$

   Note that one should not set AMUX = 0 out of ignorance of its true value, as suggested in previous versions of ENDF-l02. This implies a constant from resonance to resonance, since the chi-squared distribution approaches a delta function as N$\rightarrow \infty$. An inelastic

reaction can be expected to proceed through a small number of channels and hence to fluctuate strongly from level to level.

Specifically, AMUX = μ_{lJ}, where J is the spin of the resonance, and $\overrightarrow{l}$ is the orbital angular momentum of the inelastically scattered neutron. Since the daughter nucleus may have a spin $\overrightarrow{I}$ different from the target spin I, $\overrightarrow{l}$ may be different from l, and the number of channel spin values μ_{lJ} may be different from $\mu_{\overrightarrow{l}J}$.

3. For the radiative capture process, AMUG should be set equal to zero. Radiative capture proceeds through many channels and it is not worthwhile deciding if AMUG is 30 or 40. (If some nucleus has selection rules that restrict radiative decay to a few channels, then a different value of AMUG might be appropriate.)

4. The fission value should be given as 1.0≤AMUF≤4.0 and the value zero would be incorrect. These small values violate the previous discussion of (Wigner-type) channels and obey instead statistics governed by fission barrier tunneling (Bohr-channels). The actual value of AMUF is determined by comparison between calculated and measured cross sections.

   The degrees of freedom are constant throughout the unresolved resonance region.

2.4.17 Procedures for the Unresolved Resonance Region

This number of energy points at which the parameters are given must be be sufficient to reproduce the gross structure in the unresolved cross sections. The limit on the maximum number of points is given in Appendix G. Within a given isotope the same energy grid must be used for all J and l-values. The grids may be different for different isotopes. Unresolved resonance parameters should be provided for neutron energy regions where temperature-broadening or self-shielding effects are important. It is recommended that the unresolved resonance region extend up to at least 20 keV.

If the flag LSSF (Section 2.3.1) is set equal to one, the evaluator can specify the gross structure in the unresolved range on as fine an energy grid as he desires, subject only to the overall limitation on the number of points in File 3 (see Appendix G). Under this option, File 3 represents the entire cross section at infinite dilution in the unresolved resonance region, and no File 2 contribution is to be added to it. Instead, File 2 is to be used to compute a "slowly-varying" self-shielding factor that may be applied to the "rapidly-varying" File 3 values. The self-shielding factor is defined as the ratio of File 2 average shielded cross section to the average unshielded value computed from the same parameters. This ratio is to be applied as a multiplicative factor to the values in File 3.

If LSSF is set equal to zero, File 3 will be interpreted in the same way as a resolved-region File 3, *i.e.*, it will represent a partial background cross section to be added to the average cross section, dilute or shielded that is computed from File 2.

The self-shielding factor procedure has certain advantages over the "additive" procedure:

1. The energy-variation of the dilute cross section in the unresolved region can be more accurately specified, without the limitation on the number of points imposed in File 2.

2. The energy grids in File 2 and File 3 are basically uncoupled, so that the File 2 grid can be made coarser and easier to process.

3. In principle, the results can be more accurate, since File 2 can be devoted entirely to representing changes in the average parameters that are significant for shielding. The burden of representing fluctuations in the size of the dilute cross section is taken over entirely by File 3.

4. The same representation can be used by codes requiring probability tables. For this application, the average parameters in File 2 can be used to generate random ladders of resonances, and the resulting cross sections can be used to calculate probability tables in the usual way. However, instead of using the tables directly, they are normalized by dividing the various cross section bands by the average cross section in the interval. These normalized probabilities are then converted back to cross sections by multiplying them into the File 3 values. The rationale is the same as for the shielding-factors - the dilute cross section is represented in "poor-resolution" format in File 3, while the real fine-structure is established in File 2.

The following caution should be noted by evaluators in choosing this option:
Because File 3 is energy varying, it inherently has the possibility to energy-self-shield itself. If File 2 also shields it, one may actually "double-shield". The problem will probably be most acute just above the boundary between the resolved and unresolved regions, since the experimental resolution may still be good enough to see clumps of only a few resonances.

One might consider "correcting" for this in the choice of File 2 parameters, but this would be difficult because the degree of shielding is application dependent. A better procedure would be to insure that each significant structure in File 3 actually represents a statistically meaningful number of resonances, say ten or more. If the raw data do not satisfy this criterion, then additional smoothing should be applied by the evaluator to make it a correct condition on the data. A careful treatment will require the use of statistical level theory to determine the true widths and spacings underlying the File 3 structures.

2.4.18 Procedures for Computing Angular Distributions in the Resolved Resonance Range

2.4.18.1 Background

Quantum mechanical scattering theory, which underlies all of the resonance formalisms in this chapter, describes the angular distribution of exit particles as well as the magnitudes of the various reactions. When the R-matrix formalism is used to parameterize the collision matrix, as in the Reich-Moore format (Section D.1.3) or the RML format (Section D.1.7), then the angular distributions exhibit a resonant behavior, in the sense that they may change substantially in passing through a resonance. An explicit tabulation of this detailed resonance behavior will usually imply a very large data file.

Blatt and Biedenharn [Reference 8] simplified the general expression for the angular distribution, which is an absolute square of an angle-dependent amplitude, so that it became a

single sum over Legendre polynomials. Their expression, particularized to the RML format, is given in Section D.1.7. In the past, Reich-Moore has been a vehicle for low-energy fissionable isotope evaluations, usually s-waves only, so that the angular distribution is isotropic. If it were used for higher energies and higher angular momenta, then the angular distributions would become anisotropic. Of course, since the formulae define a center-of-mass distribution, even the isotropic case generally defines an anisotropic laboratory distribution.

In principle, similar angular distribution formulae underlie the SLBW, MLBW, and Adler-Adler formalisms, but since these are not formulated in terms of collision matrix elements (U_{lsJ}), the Blatt and Biedenharn formulas are not immediately applicable to them.

Although the Blatt and Biedenharn formulas have been around for many years, and have been much used in the physics literature of scattering theory, they have not been widely employed in neutron cross section evaluation. ENDF files most often contain either experimental data or calculated data derived from an optical model. Both of these types represent a "smoothing" or "thinning" of the underlying resonant angular distributions. In the case of experiment, the smoothing is done by the resolution-broadening of the measuring apparatus, combined with the necessarily limited number of energies at which data can be taken. In the optical model case, the smoothing is done in an obscure, highly implicit manner. It seems quite clear that an explicit energy-average over resonant Blatt and Biedenharn Legendre coefficients will differ from both of the above representations.

This raises the question of whether the Blatt and Biedenharn average will be better or worse than the others. That question is dealt with in the following paragraphs, which are somewhat "theoretical", since there is not much hard experience in this area.

2.4.18.2 Further Considerations

Firstly, if in some ideal case, all the resonance spins and parities were precisely known, then the Blatt and Biedenharn values would be exact, and clearly superior to any other representation. The next step down the accuracy ladder would be a case where the major resonances, or antiresonances ("windows") were known, but some minor, narrower ones were uncertain. For this case, one might find that errors in the "minor" resonances canceled each other, again producing a superior result, or one might find an erroneous cooperation, resulting in spurious values.

Finally, there are evaluations that use compiled resonance parameters, with many guessed J and l-values, in which case the cancellations and/or cooperations dominate the angular distributions. In both of the two latter cases, the evaluator either will or will not have compared with experiment and made a decision on the accuracy of the Blatt and Biedenharn representation. The flag LAD allows him to inform the processing code whether or not it is "safe" to calculate from the Blatt and Biedenharn formulas. Such a flag is necessary because File 4 is limited in the number of points to represent the angular distributions (see Appendix G), which is usually not enough for a fully-detailed Blatt and Biedenharn representation. The recommended ENDF procedure is for the evaluator to provide a low energy-resolution representation in File 4, and to signal the user with LAD whether he can independently generate $\sigma(\theta)$ on a finer energy mesh.

For the File 4 representation, the evaluation should smooth the data so as to preserve significant structure in the first Legendre coefficient, *i.e.* the average cosine of scattering in

the laboratory system μ. As always, the word ***significant*** is difficult to define exactly but should be interpreted as accurate enough to meet the target accuracy requirements for most ordinary reactor engineering applications.

In any case, a user who wishes to examine the implications for his own work of a finer mesh is free to use the Blatt and Biedenharn formulas. The flag LAD tells him either that the evaluator has approved this procedure (LAD=1), or that it is either of unknown quality or known to be poor (LAD=0). In the case of LAD=0, the evaluator should tell which of these is the case by putting comments into File 1 and the associated documentation.

2.4.18.3 Summary of Recommendations for Evaluation Procedures

1. Supply a coarse-mesh representation of the elastic scattering angular distribution in File 4 that meets the ENDF-6 limits on the umber of points (see Appendix G). Preserve significant structure in μ.

2. If the Blatt and Biedenharn angular distributions were not examined, or if they were examined and found to be inaccurate, supply LAD=0 in File 2. Tell which of these is the case in File 1 and in the associated documentation.

3. If the Blatt and Biedenharn angular distributions were found, or are believed, to be accurate, supply LAD=1, and describe the evaluation procedures in the documentation.

2.4.19 Completeness and Convergence of Channel Sums

Two possible errors in the calculation of cross sections from a sum over individual channels are:

1. omission of channels because they contain no resonances (such "non-resonant" or "phase-shift-only" channels must still be included because they contribute to the potential scattering cross section), and

2. failure to include enough non-resonant channels to insure convergence of the potential-scattering cross section with respect to l at high energy.

Avoiding the first is the responsibility of the processing codes for the SLBW, MLBW, AA, and RM formalisms, since the formats do not allow the evaluator to specify empty channels explicitly. For the RML formalism, where such specification ***is*** explicit, the responsibility is the evaluator's. Avoiding the second is always the evaluator's responsibility, since it would be awkward for a processing code to decide whether the omission was intentional or not.

In the channel spin representation, the incident spin, i, is coupled to the target spin, I, to form the channel spin, s, which takes on the values:

$$|I - i| \leq s \leq I + i.$$

The channel spin couples to the orbital angular momentum to form the total angular momentum J, with the values:

$$|l - s| \leq J \leq l + s.$$

If $I > 0$ and $l > 0$, the same J-value may occur for each of the two channel spins, $s = I \pm 1/2$, and ***each*** of these J-values must be ***separately*** included. A width Γ_{lJ} is a sum of the two components, Γ_{ls_1J} and Γ_{ls_2J}; and in the SLBW, MLBW, and A-A formalisms, only the sum is used. In the Reich-Moore format, the specification of J is implicit (via the use of a signed AJ value). For the RML format, the evaluator should specify two separate channels (for the two values of s) within the same spin group in this situation.

There is rarely enough information on channel-spin widths to guide the evaluator in apportioning the total width between the two subchannels, but fortunately, most neutron reactions are insensitive to the split, so that putting it all in one and none in the other, or splitting it 50/50 works equally well. Angular distributions are in principle more sensitive, but it is similarly unusual to find measured data of sufficiently high precision to show an effect.

The channel sums are infinite,

$$\sum_{l=0}^{\infty} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \chi_{lsJ} \tag{2.7}$$

so the question of convergence arises. The simplest case is where the summand is an SLBW ***reaction*** term, in which case one sums only over channels in which there are resonances. There are then no convergence considerations.

If one is summing ***scattering*** cross section terms, there is a potential-scattering amplitude in ***every*** channel, independent of whether there are resonances or not. The l=0, or s-wave amplitudes, are finite at zero energy, but the higher l-waves only come in at higher energies. The convergence criterion is therefore that the addition of the next higher l-wave produces a negligible change in the cross section at the highest energy covered by the resonance region. In a conventional R-matrix treatment, the non-resonant channels contain hard-sphere phase shifts whose behavior has to be compared with experiment.

For the RM format, NLS is defined as that value which converges the cross section calculation. This is different from the SLBW/MLBW definition, which is the number of l-channels with resonances. The latter is more liable to cause neglect of higher l non-resonant channels. Such neglect would show up as incorrect between-resonance scattering at high energies, admittedly not the easiest defect to see.

If ***angular distributions*** are to be calculated, besides having more complicated sums, the range of l-values is much greater, the requirement being that the angular distributions converge at the highest energies. Because the high l-amplitudes interfere with the low ones, non-negligible cross terms occur which are absent from the cross section sums. The different convergence criteria, NLS and NLSC, are compatible because only the B_0-moment contributes to the cross sections. All the higher moments integrate to zero. Computer codes which reconstruct such moments should have recursive algorithms for l-dependent quantities up to $l = 20$.

For the R-Matrix Limited format, all terms and only those terms specified by the evaluator (i.e., included in the File 2 information) are to be included in every calculation.

2.4.20 Channel Spin and Other Considerations

For the R-Matrix Limited format, channel spin is explicit and the evaluator must in general provide partial widths that depend on s as well as l and J.

For the Adler-Adler formalism, the usual area of application is to low-energy fissile nuclides, with $l = 0$, so the channel spin is not mentioned in the formulae of Appendix D.

For the Reich-Moore formalism, in those cases where two channel spins are possible, the channel spin is specified by the sign of the AJ parameter. In older evaluations where the channel spin is not specified (i.*e.,* where all AJ are positive), all resonances are assumed to have the same channel spin and the hard-sphere contribution from the second channel spin must be added separately.

For MLBW the absolute square has been expanded out and all imaginary quantities eliminated. This has several consequences.

1. Channel spin is effectively eliminated, because the partial widths occur in "summed" form:

$$\Gamma_{lJ} = \Gamma_{ls_1J} + \Gamma_{ls_2J} \tag{2.8}$$

   Since only the sum is required, the evaluator is spared the necessity of specifying the separate s-values. This converts an (l, s, J) formalism into an (l, J) formalism. The same effect can be achieved by assuming that I=0, a popular assumption often made independently of the truth, as in many optical model calculations.

2. The convergence criterion is more transparent, because the potential-scattering cross section splits off from the resonance and interference terms, as

$$\frac{4\pi}{k^2}(2l+1)\sin^2\phi_l. \tag{2.9}$$

   Despite the simpler nature of this term than its parent amplitudes, one must still carry enough terms to make the results physically correct, and if this cannot be done, then File 3 must be invoked to achieve that goal.

3. The resonance profiles are expressible in terms of symmetric and asymmetric Breit-Wigner shapes, and thus permit $\psi - \chi$ Doppler broadening. The price one pays for these three advantages is increased computing time, when the number of resonances is large.

   Similar remarks apply to the SLBW formalism, which is MLBW without the resonance resonance interference terms. The computing time goes way down, but the scattering cross section is very poor. SLBW has useful applications in certain analytical and semi-analytical procedures, but should never be used for the calculation of explicit pointwise scattering cross sections.

   The omission of an explicit channel-spin quantum number in the SLBW formalism, while convenient in the resolved resonance region, has occasioned some difficulty in the unresolved region. Sections D.2.2 and D.2.3 attempt to clarify the situation with respect to level densities, strength functions, and spin statistics.

References for Chapter 2

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Chapter 3

File 3: REACTION CROSS SECTIONS

3.1 General Description

Reaction cross sections and auxiliary quantities are given in File 3 as functions of E, where E is the incident particle energy in the laboratory system. They are given as energy-cross section (or auxiliary quantity) pairs. An interpolation scheme is given that specifies the energy variation of the data for incident energies between a given energy point and the next higher point. File 3 is divided into sections, each containing the data for a particular reaction, identified by the MT number; see Section 0.4.3 and Appendix B. The sections are ordered by increasing MT number. As usual, each section starts with a HEAD record and ends with a SEND record. The file ends with a FEND record.

3.2 Formats

The following quantities are defined:

ZA,AWR Standard material charge and mass parameters.

QM Mass-difference Q value (eV): defined as the mass of the target and projectile minus the mass of the residual nucleus in the ground state and masses of all other reaction products; that is, for the reaction a+A → b+c+...+B,

$$QM = [(m_a + m_A) - (m_b + m_c + ... + m_B)] \times (eV/amu)$$

where the masses are in amu. (See Section 3.3.2 and Appendix H for the mass conversion constant).

QI Reaction Q value for the (lowest energy) state defined by the given MT value in a simple two-body reaction or a breakup reaction. Defined as QM for the ground state of the residual nucleus (or intermediate system before breakup) minus the energy of the excited level in this system. Use QI=QM for reactions with no intermediate states in the residual nucleus and without complex breakup (LR=0). (See Section 3.3.2)

LR Complex or "breakup" reaction flag, which indicates that additional particles not specified by the MT number will be emitted. See Sections 0.4.3.4 and 3.4.4.

NR,NP,E$_{int}$ Standard TAB1 parameters.

$\sigma(E)$ Cross section (barns) for a particular reaction (or the auxiliary quantity) given as a table of NP energy-cross section pairs.

The structure of a section is:

```
[MAT, 3, MT/  ZA,  AWR,  0,  0,  0,  0] HEAD
[MAT, 3, MT/  QM,   QI,  0, LR, NR, NP/ E_int/ σ(E)]TAB1
[MAT, 3,  0/ 0.0,  0.0,  0,  0,  0,  0] SEND
```

3.3 General Procedures

3.3.1 Cross Sections, Energy Ranges, and Thresholds

For incident neutrons, the cross-section data must extend to the lower energy limit of 10^{-5} eV, except for threshold reactions, for which tabulation should start at the reaction threshold energy (with a value of 0.0 barns); the data should cover the energy range up to the ***common upper energy limit*** EMAX (see Section 1.1) of at least 20 MeV.

In case there is a change in the data representation at a certain energy E_x, duplicate energy points may be entered to allow for the discontinuity. If the tabulated cross section below E_x is zero (*e.g.* in the region where resonance parameter representation is used), the first duplicate point has a cross section value of zero, preceeded by another zero value at 10^{-5} eV. If the tabulated cross section above E_x is zero (*e.g.* in the region where the cross section is included in the lumped reaction MT=5, or otherwise), the second duplicate point has a cross section value of zero, followed by another zero value at energy EMAX. The evaluator should document the change in data representation (if any) in the comments in File 1.

For some charged-particle emission reactions, the cross section might have a low threshold (or no threshold at all), but could be very small ($< 10^{-10}$ barns) due to the Coulomb barrier up to an ***effective threshold***. The evaluator should be careful to enter a zero value at the true threshold (or 10^{-5} eV), as well as at the effective threshold, in order to avoid interpolation problems.

A cross section (or auxiliary quantity) in File 3 may become zero at and above a certain energy (e.g. the cross section may become very small for physical reasons or due to a change in representation). The energy at which the cross section becomes zero and the maximum energy EMAX must be given in the file with zero cross section values.

The limit on the number of energy points (NP) to be used to represent a particular cross section is given in Appendix G. The evaluator should not use more points than are necessary to represent the cross section accurately. When appropriate, resonance parameters can be used to help reduce the number of points needed. The evaluator should avoid sharp features such as triangles or steps (except for the required discontinuities discussed above), because such features my cause unphysical results during processing (*e.g.* Doppler broadening).

3.3.2 Q-Values

Accurate reaction Q-values should be given for all reactions, if possible. If QI is not well defined (as for a range of levels in MT=91, 649, 699, 749, 799, or 849), use the value of QI which corresponds to the threshold of the reaction. Similarly, if the value of QM is not well defined (as in elements or for summation reactions like MT=5), use the value of QM which gives the threshold. If there is no threshold, use the most positive Q value of the component reactions. Note that these ill-defined values of QM cannot be relied on for energy-release calculations.

In general, the masses used in the calculation of QM and QI should correspond the rest masses of the target and residual nuclei. If the target or residual is in the ground state, the rest mass is just the nuclear mass. If the target or residual is an isomer, the rest mass is the nuclear mass plus the excitation energy of the nucleus, which should be specified in the ELIS field in the MF=1 MT=451 file.

As an example to clarify the use of QM and QI, consider the reaction α +^{9}Be $\rightarrow$ n+X. After the neutron has been emitted, the compound system is ^{12}C with QM=5.702 MeV and energy levels (E_x) at 0.0, 4.439, 7.654, and 9.641 MeV. The ground state is stable against particle breakup, the first level decays by photon emission, and the higher levels decay with a high probability of breaking up into three alpha particles (7.275 MeV is required). This pattern can be represented as follows:

Reaction	**QM**	**QI**	EX	**MT**
^{9}Be(α,n$_0$)^{12}C	5.702	5.702	0.000	50
^{9}Be(α,n$_1$)^{12}C	5.702	1.263	4.439	51
^{9}Be(α,n$_2$)^{12}C(3α)	-1.573	-1.952	7.654	52
^{9}Be(α,n$_3$)^{12}C(3α)	-1.573	-3.939	9.641	53
^{9}Be(α,n$_C$)^{12}C(3α)	-1.573	-1.573		91

The emitted gamma photons for the second and higher reactions are not represented explicitly in this notation. The last reaction includes the contributions of all the levels above 9.641 MeV, any missed levels, and any direct four-body breakup; therefore, the threshold for MT=91 may be lower than implied by the fourth level of ^{12}C. Note the value used for QI.

3.3.3 Relationship Between File 3 and File 2

If File 2 (Resonance Parameters) contains resolved and/or unresolved parameters (LRP=1), then the cross sections or self-shielding factors computed from these parameters in the resonance energy range for elastic scattering (MT=2), fission (MT=18), and radiative capture (MT=102) must be combined with the cross sections given in File 3. The resonance contributions must also be included in any summation reactions that involve the three resonance reactions (for example, MT=1, 3, or 5). The resonance energy range is defined in File 2. Double-valued energy points will normally be given in File 3 at the upper and lower limits of the unresolved and resolved resonance regions.

Some material evaluations for incident neutrons will not have resonance parameters but will have a File 2 (LRP=0) that contains only the effective scattering radius. This quantity is sometimes used to calculate the potential scattering cross section in self-shielding codes. For these materials, the potential scattering cross section computed from File 2 *must not* be added to the cross section given in File 3. The File 3 data for such materials comprise the entire scattering cross section.

In certain derived libraries, the resonance cross sections have been reconstructed and stored in File 3. Such files may have LRP=0 as described in the preceding paragraph. Alternatively, they may have LRP=2 and include a full File 2 with complete resonance parameters. In this case, resonance cross sections or self-shielding factors computed from File 2 *are not* to be combined with the cross sections in File 3.

3.4 Procedures for Incident Neutrons

Cross section data for non-threshold reaction types must cover the energy range from a lower limit of 10^{-5} eV to an upper limit of ***at least*** 20 MeV for all materials. For non-threshold reactions, a cross section value must be given at 0.0253 eV. The limit on the number of energy points (NP) to be used to represent a particular cross section is given in Appendix G. The evaluator should not use more points than are necessary to represent the cross section accurately.

The choice of data to be included in an evaluation depends on the intended application. For neutron sublibraries, it is natural to define "transport" evaluations and "reaction" evaluations. The transport category can be further subdivided into "low-energy transport" and "high-energy transport."

A ***reaction evaluation*** will contain File 1, File 2, File 3, and sometimes File 32 and/or File 33. File 2 can contain resonance parameters. If radioactive products must be described, Files 8, 9, 10, 39, and/or 40 may be present. File 3 may tabulate one or more reaction cross sections. The total cross section is usually not well defined in reaction evaluations since they may be incomplete. Examples of this class of evaluations include activation data and dosimetry data.

A ***low-energy transport evaluation*** should be adequate for calculating neutron transport and simple transmutations for energies below about 6-10 MeV. Photon production and covariance data should be included when possible. Typical evaluations will include Files 1, 2, 3, 4, 5, and sometimes Files 8, 9, 10, 12, 13, 14, 15, 31, 32, 33, 34, 35, 39, and/or 40. Resonance parameters will usually be given so that self shielding can be computed. Charged-particle spectra (MT=600-849) and neutron energy-angle correlation (MF=6) will often be omitted. File 3 should include all reactions important in the target energy range, including the total (MT=1) and elastic scattering (MT=2). Other reactions commonly included are inelastic scattering (MT=4,51-91), radiative capture (MT=102), fission (MT=18,19-21,38), absorption (MT=103,104,105, *etc.*), and other neutron emitting reactions such as MT=16,17,22,28, *etc.* Specific procedures for some specific reactions are given below. Examples of this class of evaluations include fission-product data and actinide data.

A ***high-energy transport evaluation*** should be adequate for calculating neutron transport, transmutation, photon production, nuclear heating, radiation damage, gas pro-

duction, radioactivity, and charged-particle source terms for energies up to at least 20 MeV. In some cases, the energy limit needs to be extended to 60 or even 150 MeV. These evaluations use Files 1, 2, 3, 4, 5, 6, 12, 13, 14, 15, and sometimes 8, 9, 10, 31, 32, 33, 34, 35, 39, and/or 40. Once again, File 3 should give cross sections for all reactions important in the target energy range, including MT=1 and 2. This will normally include many of the reactions mentioned above plus the series MT=600-849. At high energies, some reactions may be combined using the "complex reaction" identifier MT=5. File 6 will normally be needed at high energies to represent energy-angle correlation for scattered neutrons and to give particle and recoil energies for heating and damage calculations. Special attention to energy balance is required. High-energy evaluations are important for materials used in fusion reactor designs, in shielding calculations, and in medical radiation-therapy equipment (including the constituents of the human body).

3.4.1 Total Cross Section (MT=1)

The total is often the best-known cross section, and it is generally the most important cross section of a shielding material. Considerable care should be exercised in evaluating this cross section and in deciding how to represent it.

Cross section minima (potential windows) and cross section structure should be carefully examined. Sufficient energy points must be used in describing the structure and minima to reproduce the experimental data to the measured degree of accuracy. However, the maximum number of points should not exceed the limits specified in Appendix G.

The set of points or energy mesh for the total cross section must be a union of all energy meshes used for the partial cross sections. Within the above constraints, every attempt should be made to minimize the number of points used. The total cross section must be the sum of MT=2 (elastic) and MT=3 (nonelastic). If MT=3 is not given explicitly, then the elastic cross section plus all implied components of the nonelastic cross section must sum to the total cross section.

The fact that the total cross section is given at every energy point at which at least one partial cross section is given allows the partial cross sections to be added together and checked against the total for any possible errors. In certain cases, more points may be necessary in the total cross section over a given energy range than are required to specify the corresponding partial cross sections. For example, a constant elastic scattering cross section and a $1/v$ radiative capture cross section could be exactly specified over a given energy range by log-log interpolation (INT=5), but the sum of the two cross sections would not be exactly linear on a log-log scale. As a general rule, the total cross section at any energy should be calculated from the sum of the partial cross sections.

3.4.2 Elastic Scattering Cross Section (MT=2)

The elastic scattering cross section is generally not known to the same accuracy as the total cross section. Frequently, the elastic scattering cross section is evaluated as the difference between the total and the nonelastic cross section. This procedure can cause problems: the resulting elastic scattering cross section shape may contain unreal structure. There may be several causes. First, the nonelastic cross section, or any part thereof, is not generally

measured with the same energy resolution as the total cross section. When the somewhat poorer resolution nonelastic data are subtracted from the total, the resolution effects appear in the elastic cross section. Second, if the evaluated structure in the nonelastic cross section is incorrect or improperly correlated with the structure in the total cross section (energy-scale errors), an unrealistic structure is generated in the elastic scattering cross section.

The experimental elastic cross section is obtained by integrating measured angular distributions. These data may not cover the entire angular range or may contain contributions from nonelastic neutrons. Such contamination is generally due to contributions from inelastic scattering to low-lying levels that were not resolved in the experiment. Care must be taken in evaluating such results to obtain integrated cross sections. Similarly, experimental angular distribution data can also cause problems when evaluating File 4.

3.4.3 Nonelastic Cross Section (MT=3)

The nonelastic cross section is not required unless any part of the photon production multiplicities given in File 12 uses MT=3. In this case, MT=3 is required in File 3. If MT=3 is given, then the set of points used to specify this cross section must be a union of the sets used for its partials.

3.4.4 Inelastic Scattering Cross Sections (MT=4,51-91)

The total inelastic scattering cross section (MT=4) must be given if any partials are given; that is, discrete level excitation cross sections (MT=51-90), or continuum inelastic scattering (MT=91). The set of incident energy points used for the total inelastic cross section must be a union of all the sets used for the partials.

Values should be assigned to the level excitation cross sections for as many levels as possible and extended to as high an energy as possible. Any remaining inelastic scattering should be treated as continuum. In particular, low-lying levels with significant direct interaction contributions (such as deformed nuclei with 0^+ ground states) should be extended to the upper limit of the file (at least 20 MeV) in competition with continuum scattering. The secondary energy distribution for such neutrons resembles elastic scattering more than an evaporation spectrum.

Level excitation cross sections must start with zero cross section at the threshold energy. If the cross section for a particular level does not extend to the upper limit for the file (*e.g.*, 20 MeV), it must be ***double-valued*** at the highest energy point for which the cross section is non-zero. The second cross section value at the point must be zero, and it should be followed by another zero value at the upper limit. This will positively show that the cross section has been truncated.

If LR=0, a section defined by a particular MT represents the (n,n'γ) reaction. The angular distribution for the scattered neutron must be given in the corresponding section of File 4 or 6. The associated photons should be given in a corresponding section of File 6 or 12 and 14, if possible. If the inelastic photons cannot be assigned to particular levels, they can be represented using MT=4 in File 6, 12 or 13 and 14. When inelastic photons cannot be separated from other nonelastic photons, they can be included under MT=3 in Files 13, 14 and 15.

A LR flag greater than zero indicates inelastic scattering to levels that de-excite by breakup, particle emission, or pair production rather than by photon emission (see Section 0.5)[1]. If LR=1, the identities, yields, and distributions for all particles and photons can be given in File 6. If LR > 1, angular distributions for the neutron must be given in File 4, and distributions are not available for the other emitted particles. In this case, photon production is handled as described above for LR=0.

If a particular level decays in more than one way, then File 6 can be used or several sections can be given in File 3 for that level. Consider the case in which an excited state sometimes decays by emitting a proton, and sometimes by emitting an alpha particle. That part of the reaction that represents (n,n' α) would use LR=22, and the other part would be given the next higher section number (MT) and would use LR=28 (n,n'p). The angular distribution for the neutron would have to be given in two different MT numbers in File 4, even though they represent the same neutron. The sections must be ordered by decreasing values of QI (increasing excitation energy).

3.4.5 Fission (MT=18,19-21,38)

The total fission cross section is given in MT=18 for fissionable materials. Every attempt should be made to break this cross section up into its various parts: first-chance fission (n,f), MT=19; second-chance fission (n,n'f), MT=20; third-chance fission (n,2nf), MT=21; and fourth-chance fission (n,3nf), MT=38. The data in MT=18 must be the sum of the data in MT=19, 20, 21, and 38. The energy grid for MT=18 must be the union of the grids for all the partials.

If resolved or unresolved resonance parameters are given in File 2, the fission cross section computed from the parameters must be included in both MT=18 and MT=19.

The Q-value for MT=18, 19, 20, 21, and 38 is the energy released per fission minus the neutrino energy. It should agree with the corresponding value given in MT=458 in File 1.

Secondary neutrons from fission are usually stated to be isotropic in the laboratory system in File 4 and energy distributions are given in File 5. However, higher-chance fission neutrons can have some degree of anisotropy and the data can be coded in File 6. The complex rules associated with the partial fission reactions are described in Section 5.

3.4.6 Charged-Particle Emission to Discrete and Continuum Levels (MT=600-849)

The (n,p) reaction can be represented using a summation cross section (MT=103), or discrete levels, and a continuum (MT=600-648, and 649) in the same way that the (n,n') reaction is represented using MT=4, 51-90, and 91 (see Section 3.4.4). Similarly, (n,d) uses MT=104 and 650-699, and so on for t, ^{3}He, and α emission. Of course, MT=600, 650, 700, *etc.*, represent the ground state and would not have corresponding sections in the photon production files, unless the flag LR > 0 (such as in the ^{10}B(n,t)^{8}Be reaction).

[1] LR=31 is still allowed, to uniquely define the γ-decay when using MF=3, and MF=12 (or 15) and MF=4.

3.5 Procedures for Incident Charged Particles and Photons

See Table 3 for sublibrary numbers for incident charged particles and photons. Procedures for incident charged particles are generally the same as for neutrons, as given in Section 3.4. The exceptions are noted below.

3.5.1 Total Cross Sections

The total cross section is undefined for incident charged particles. MT=1 should be used for the photonuclear total cross section, while MT=501 is used for the total atomic photon interaction cross section.

3.5.2 Elastic Scattering Cross Sections

As discussed in detail in Section 6.2.6, it is not possible to construct an integrated cross section for charged-particle elastic scattering because of the Coulomb term. Therefore, the cross section is either set to 1.0 or to a "nuclear plus interference" value using a cutoff angle. This value may in theory be 0.0, but for the purpose of the evaluation should be chosen as a finite (small) number, *e.g.*, 10^{-38}. The first and the last energy points used for MT=2 in File 3 define the range of applicability of the cross section representation given in File 6. The cross section need not cover the complete range from 10^{-5} eV to 20 MeV. MT=2 is used for the elastic scattering cross section for all incident particles and photons (resonance fluorescence). For photons, MT=502 and 504 are used for coherent and incoherent atomic scattering, respectively.

3.5.3 Inelastic Scattering Cross Sections

The procedure for inelastic cross section for incident charged particles and photons is the same as for neutrons. The following MT combinations should be used.

Incident Particle	MT's for Excited States	MT for Total Inelastic
γ	undefined	102
n	51-91	4
p	601-649	103
d	651-699	104
t	701-749	105
^{3}He	751-799	106
α	801-849	107

3.5.4 Stopping Power

The total charged-particle stopping power in eV·barns is given in MF=3, MT=500. This is basically an atomic property representing the shielding of the nuclear charge by the electrons. The same data should be included in all isotopic evaluations of an element, if applicable. It is a "total" stopping power in that most tabulations implicitly include large-angle coulomb scattering which is also represented here in File 6. In practice, this contribution is probably small enough to keep double counting from being a problem. At low particle energies, mixture effects are sometimes noticeable. They are not accounted for by this representation.

Chapter 4

FILE 4: ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES

4.1 General Description

File 4 is used to describe the angular distribution of emitted particles. It is used for reactions with incident neutrons only, and should not be used for any other incident particle. Angular distributions of emitted neutrons should be given for elastically scattered neutrons, and for the neutrons resulting from discrete level excitation due to inelastic scattering. However, angular distributions may also be given for particles resulting from (n,n'$_{continuum}$), (n,2n), and other neutron emitting reactions. In these cases, the angular distributions will be integrated over all final energies. File 4 may also contain angular distributions of emitted charged particles for a reaction where only a single outgoing charged particle is possible (MT=600 through 849, see Section 3.4.6). Emitted photon angular distributions are given in File 14 when the particle angular distributions are given in File 4.

The use of File 6 to describe all emitted particle angular distributions is preferred when charged particles are emitted, or when the emitted particle's energy and angular distributions are strongly correlated. In these cases, Files 4 and 14 should not be used.

In some cases, it may be possible to compute the angular distributions in the resolved range from resonance parameters (see Section 2.4.18 for further discussion). In such cases, the computed distributions may be preferable to the distributions from File 4 for deep penetration calculations. However, for many practical applications, the smoothed distributions in File 4 are adequate.

Angular distributions for a specific reaction type (MT number) are given for a series of incident energies, in order of increasing energy. The energy range covered should be the same as that for the same reaction type in File 3. Angular distributions for several different reaction types (MT's) may be given in File 4 for each material, in ascending order of MT number.

The angular distributions are expressed as normalized probability distributions, *i.e.*,

$$\int_{-1}^{1} f(\mu, E) d\mu = 1 \tag{4.1}$$

where $f(\mu, E)\ d\mu$ is the probability that a particle of incident energy E will be scattered into the interval $d\mu$ about an angle whose cosine is μ. The units of $f(\mu, E)$ are (unit-cosine)$^{-1}$. Since the angular distribution of scattered neutrons is generally assumed to have azimuthal symmetry, the distribution may be represented as a Legendre polynomial series,

$$f(\mu, E) = \frac{2\pi}{\sigma_s(E)}\ \sigma(\mu, E) = \sum_{l=0}^{\mathrm{NL}} \frac{2l+1}{2}\ a_l(E)\ P_l(\mu) \tag{4.2}$$

where:

- μ cosine of the scattered angle in either the laboratory or the center-of-mass system
- E energy of the incident particle in the laboratory system
- $\sigma_s(E)$ the scattering cross section, *e.g.*, elastic scattering at energy E as given in File 3 for the particular reaction type (MT)
- l order of the Legendre polynomial
- $\sigma(\mu, E)$ differential scattering cross section in units of barns per steradian
- a_l the lth Legendre polynomial coefficient; it is implicitly understood that $a_0 = 1.0$ and is not given in the file.

The angular distributions may be given by one of two forms, and in either the center-of-mass (CM) or laboratory (LAB) coordinate systems. In the first form, the distributions are given by tabulating the normalized probability distribution, $f(\mu, E)$, as a function of incident energy. In the second form, the Legendre polynomial expansion coefficients, $a_l(E)$, are tabulated as a function of incident neutron energy.

Absolute differential cross sections are obtained by combining data from Files 3 and 4. If tabulated distributions are given, the absolute differential cross section (in barns per steradian) is obtained by

$$\sigma(\mu, E) = \frac{\sigma_s(E)}{2\pi}\ f(\mu, E) \tag{4.3}$$

where $\sigma_s(E)$ is given in File 3 (for the same MT number) and $f(\mu, E)$ is given in File 4. If the angular distributions are represented as Legendre polynomial coefficients, the absolute differential cross sections are obtained by

$$\sigma(\mu, E) = \frac{\sigma_s(E)}{2\pi} \sum_{l=0}^{\mathrm{NL}} \frac{2l+1}{2}\ a_l(E)\ P_l(\mu) \tag{4.4}$$

where $\sigma_s(E)$ is given in File 3 (for the same MT number) and the coefficients $a_l(E)$ are given in File 4.

Transformation matrices to convert Legendre coefficients from CM to LAB coordinate system and vice versa are no longer permitted in ENDF-6 formatted files. Expressions defining elements of the transformation matrices can be found in papers by Zweifel and Hurwitz[1] and Amster[2] .

4.2 Formats

File 4 is divided into sections, each containing data for a particular reaction type (MT number) and ordered by increasing MT number. Each section always starts with a HEAD record and ends with a SEND record. The following quantities are defined.

LTT Flag to specify the representation used and it may have the following values:
LTT=0, all angular distributions are isotropic
LTT=l, the data are given as Legendre expansion coefficients, a_l(E)
LTT=2, the data are given as tabulated probability distributions, $f(\mu, E)$
LTT=3, low energy region is represented by as Legendre coefficients; higher region is represented by tabulated data.

LI Flag to specify whether all the angular distributions are isotropic
LI=0, not all isotropic
LI=1, all isotropic

LCT Flag to specify the frame of reference used
LCT=l, the data are given in the LAB system
LCT=2, the data are given in the CM system

NE Number of incident energy points at which angular distributions are given (See Appendix G for the limit on NE).

NL Highest order Legendre polynomial that is given at each energy (NL $\leq$ NM)

NM Maximum order Legendre polynomial that is required to describe the angular distributions in either the center-of-mass or the laboratory system. NM should be an even number. See Appendix G for the limit on NM.

NP Number of angular points (cosines) used to give the tabulated probability distributions for each energy (See Appendix G for the limit on NP).

Other commonly used variables are given in the Glossary (Appendix A).

The structure of a section depends on the values of LTT (*i.e.* the representation used: $a_l(E)$ Legendre polynomial expansion or $f(\mu, E)$ tabulated normalised probability distribution) but it always starts with a HEAD record of the form

[1] P.F. Zweifel and H. Hurwitz, Jr., J. Appl. Phys. 25,1241 (1954).
[2] H. Amster, J. Appl. Phys. 29, 623 (1958).

```
[MAT, 4, MT/ ZA, AWR, 0, LTT, 0, 0]HEAD
```

4.2.1 Legendre Polynomial Coefficients (LTT=1, LI=0)

When LTT=1 (angular distributions given in terms of Legendre polynomial coefficients), the structure of the section is:

```
[MAT, 4, MT/  ZA, AWR,  0, LTT,  0,  0]HEAD     (LTT=1)
[MAT, 4, MT/ 0.0, AWR, LI, LCT,  0,  0]CONT     (LI=0)
[MAT, 4, MT/ 0.0, 0.0,  0,   0, NR, NE/ E_int]TAB2
[MAT, 4, MT/   T,  E_1, LT,   0, NL,  0/ a_l(E_1)]LIST
[MAT, 4, MT/   T,  E_2, LT,   0, NL,  0/ a_l(E_2)]LIST
   ----------------------------------------------
   ----------------------------------------------
[MAT, 4, MT/   T,E_NE, LT,   0, NL,  0/ a_l(E_NE)]LIST
[MAT, 4,  0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

Note that T and LT refer to temperature (in K) and a test for temperature dependence, respectively. These values are normally zero, however.

4.2.2 Tabulated Probability Distributions (LTT=2, LI=0)

If the angular distributions are given as tabulated probability distributions, LTT=2, the structure of a section is:

```
[MAT, 4, MT/  ZA, AWR,   0, LTT,  0,  0]HEAD   (LTT=2)
[MAT, 4, MT/ 0.0, AWR,  LI, LCT,  0,  0]CONT   (LI=0)
[MAT, 4, MT/ 0.0, 0.0,   0,   0, NR, NE/ E_int] TAB2
[MAT, 4, MT/   T,  E_1,  LT,   0, NR, NP/ μ_int/f(μ,E_1)]TAB1
[MAT, 4, MT/   T,  E_2,  LT,   0, NR, NP/ μ_int/f(μ,E_2)]TAB1
   ----------------------------------------------
   ----------------------------------------------
[MAT, 4, MT/   T, E_NE, LT,   0, NR, NP/ μ_int/f(μ,E_NE)]TAB1
[MAT, 4,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

Parameters T and LT are normally zero.

4.2.3 Purely Isotropic Angular Distributions (LTT=0, LI=1)

When *all* angular distributions for a given MT are assumed to be isotropic then the section structure is:

```
[MAT, 4, MT/  ZA, AWR,   0, LTT,  0,  0]HEAD   (LTT=0)
[MAT, 4, MT/ 0.0, AWR,  LI, LCT,  0,  0]CONT   (LI=1)
[MAT, 4,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

4.2.4 Angular Distribution Over Two Energy Ranges (LTT=3, LI=0)

If LTT=3, angular distributions are given as Legendre coefficients over the lower energy range and as Probability Distributions over the higher energy range. The structure of a subsection is:

```
[MAT, 4, MT/  ZA, AWR,   0, LTT,  0,   0]HEAD   (LTT=3)
[MAT, 4, MT/ 0.0, AWR,  LI, LCT,  0,  NM]CONT   (LI=0)
    (Legendre coefficients)
[MAT, 4, MT/ 0.0, 0.0,   0,   0, NR, NE1/ E_int]TAB2
[MAT, 4, MT/   T,  E_1,  LT,   0, NL,   0/ a_l(E_1)]LIST
    ----------------------------------------------
    ----------------------------------------------
[MAT, 4, MT/   T,E_NE1,  LT,   0,  NL,   0/ a_l(E_NE1)]LIST
    (Tabulated data)
[MAT, 4, MT/ 0.0, 0.0,   0,   0,  NR, NE2/ E_int]TAB2
[MAT, 4, MT/   T,E_NE1, LT,   0,  NR,  NP/  μ_int / f(μ,E_NE1) ]TAB1
    ----------------------------------------------
    ----------------------------------------------
[MAT, 4, MT/   T,E_NET, LT,   0,  NR,  NP/ μ_int / f(μ,E_NET) ]TAB1
   (NET = NE1+NE2-1)
[MAT, 4,  0/ 0.0, 0.0,   0,   0,   0,   0]SEND
```

Note that there is a double energy point at the boundary E_{NE1}, which appears as the last point in the Legendre expansion tables and the first point in the tabulated distribution tables.

4.3 Procedures

The angular distributions for two-body reactions should be given in the CM system (LCT=2). It is recommended that other reactions (such as continuum inelastic, fission, *etc.*) should be given in the *LAB system*. All angular distribution data should be given at the minimum number of incident energy points that will accurately describe the energy variation of the distributions. Legendre coefficients are preferred unless they cannot give an adequate representation of the data.

When the data are represented as *Legendre polynomial coefficients*, certain procedures should be followed. Enough Legendre coefficients should be used to accurately represent the recommended angular distribution at a particular energy point, and to ensure that the interpolated distribution is everywhere positive. The number of coefficients (NL) may vary from energy point to energy point; in general, NL will increase with increasing incident energy. A linear-linear interpolation scheme (INT=2) must be used to obtain coefficients at intermediate energies. This is required to ensure that the interpolated distribution is positive over the cosine interval from -1.0 to +1.0; it is also required because some coefficients may be negative. In no case should NL exceed the limit NM, defined in Appendix G. If more coefficients appear to be required to obtain a non-negative distribution, either a constrained

Legendre polynomial fit to the data should be given, or the evaluator should switch to tabular distributions at some energy (LTT=2 or LTT=3 representation). NL=1 is allowed at low energies to specify an isotropic angular distribution.

When angular distributions are represented as tabular data, certain procedures should be followed. Sufficient angular points (cosine values) should be given to accurately represent the recommended distribution. The number of angular points may vary from distribution to distribution. The cosine interval must be from -1.0 to +1.0. The log-linear interpolation scheme (INT=4) for $f(\mu, E)$ vs. μ is recommended; the linear-linear (INT=2) interpolation scheme for $f(\mu, E)$ vs. E is recommended.

Accurate angular distributions for the thermal energy range must be obtained using File 7 or a detailed free-gas calculation. File 4 can only give distributions for stationary free targets.

The ENDF-6 format rules do not allow transformation matrices for conversion between CM and LAB coordinate systems. If needed, the conversion has to be done at the level of the processing codes.

4.4 Procedures for Specific Reactions

4.4.1 Elastic Scattering (MT=2)

1. Legendre polynomial representation in the CM coordinate system is preferred for angular distributions of the elastic scattering reaction channel. However, if the number of Legendre coefficients needed to adequately describe the distribution (making sure it is non-negative at all angles) would exceed the NM limit (see Appendix G), the evaluator should switch to tabular representation at some energy.

2. Care must be exercised in selecting an incident energy mesh for certain light-to-medium mass materials. Here it is important to relate any known structure in the elastic scattering cross section to the energy dependent variations in the angular distributions. These two features of the cross sections cannot be analyzed independently of one another. Remember, processing codes operate on MT=2 data that are given in Files 3 and 4. (Structure of the total cross section is not considered when generating energy transfer arrays). It is better to maintain consistency in any structure effects between File 3 and File 4 data than to introduce structure in one File and ignore it in the other.

3. Consistency must be maintained between angular distribution data given for elastic and inelastic scattering. This applies not only to structural effects, but also to how the distributions were obtained.

   Frequently, the evaluated elastic scattering angular distributions are based on experimental results that, at times, contain contributions from inelastic scattering to low-lying levels (which in turn may contain direct interaction effects). If inelastic contributions have been subtracted from the experimental angular distributions, the same have to be subtracted for the angle-integrated elastic scattering cross sections and added to the inelastic cross sections in File 3 for consistency. This is particularly

important when the inelastic contributions are due to direct interaction, since the angular distributions are not isotropic or symmetric about 90°, but they are generally forward peaked.

4. Do not use an excessive number of incident energy points for the angular distributions. The number used should be determined by the amount of variation in the angular distributions but should not exceed the NE limit defined in Appendix G.

5. The energy range for which the angular distributions are given must correspond exactly with the range given in File 3 for the same reaction channel (*i.e.* the same MT number).

6. In the case of neutrons, a relationship exists between the total cross section and the differential cross section at forward angles (Wick's limit or optical theorem):

$$\begin{aligned} \sigma(0^\circ) \geq \sigma_W &= \left(\frac{k\sigma_T}{4\pi}\right)^2 \\ \sigma_W &= 10^{-28}\,\frac{m}{2h^2}\frac{u}{c^2}\left(\frac{\text{AWR}}{1+\text{AWR}}\right)^2 E\,\sigma_T^2 \end{aligned}$$

where:

k $= 2\pi\sqrt{2m^*E_0}/h$; the wave number

h is Planck's constant in units eV.s (see Appendix H),

m mass in atomic mass units,

m^* $= mu/c^2$; mass in absolute units,

u atomic mass unit (amu) in eV.s/c^2 (see Appendix H),

c speed of light in vacuum in m.s^{-1} (see Appendix H),

E incident energy in the lab system in eV,

E_0 incident energy in the center-of-mass system in eV,

$$E_0 = \left(\frac{\text{AWR}}{1+\text{AWR}}\right)^2 E$$

AWR atomic mass ratio to the neutron,

σ_T total cross section.

4.4.2 Discrete Channel Two-Body Reactions

1. Do not give angular distribution data for cumulative reactions (MT=4, 103, 104, 105, 106, 107) if discrete level data are present.

2. Always give angular distribution data for single-particle emission (two-body) discrete level reactions, if they are given in File 3; namely MT = 50 through 91, 600 through 649, 650 through 699, 700 through 749, 750 through 799 and 800 through 849.

3. Discrete channel (two body) angular distributions (*e.g.*, MT = 2, 50 through 91, 600 through 649, 650 through 699, 700 through 749, 750 through 799 and 800 through 849) should be given as Legendre coefficients in the CM system, if possible.

4. The continuum reactions (MT=91, 649, 699, 749, 799, 849) should normally be given in the LAB system.

5. Isotropic angular distributions should be used unless the degree of the isotropy exceeds 5%. If any level excitation cross sections contain significant direct interaction contributions, angular distributions are very important.

6. Use the precautions outlined above when dealing with the level excitation cross sections that contain a large amount of structure.

7. Do not overcomplicate the data files. Restrict the number of distributions to the minimum required to accurately represent the data.

4.4.3 Other Particle-Producing Reactions

Neutron angular distribution data must be given for all other neutron producing reactions, such as fission, (n,n′α), or (n,2n) in File 4 or File 6. File 4 is only appropriate if the distributions are fairly isotropic without strong pre-equilibrium components. The LAB system should be used.

If angular data is needed for other more complex reactions, File 6 is usually more appropriate.

Chapter 5

File 5: ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES

5.1 General Description

File 5 describes the energy distributions of secondary particles expressed as normalized probability distributions. It is designed for incident neutron reactions and spontaneous fission only, and should not be used for any other incident particle. Data are given in File 5 for all reaction types that produce secondary neutrons, unless the secondary neutron energy distributions can be implicitly determined from the data given in File 3 and/or File 4. For example, no data will be given in File 5 for elastic scattering (MT=2), since the secondary energy distributions can be obtained from the angular distributions in File 4 and the kinematic equations for a two-body interaction (see Appendix E). Similarly, no data will be given for neutrons that result from the excitation of discrete inelastic levels (MT=51, 52, ..., 90).

Data should be given in File 5 for MT=91 (inelastic scattering to a continuum of levels), MT=18 (prompt neutrons from fission), MT=16 (n,2n), MT=17 (n,3n), MT=455 (delayed neutrons from fission), and certain other nonelastic reactions that produce secondary neutrons, unless they are given in File 6. The energy distribution for spontaneous fission is given in File 5 (in sub-library 4).

Despite its important application in equilibrium reactor calculations, the "total" fission spectrum (prompt plus delayed) corresponding to the total number of neutrons per fission tabulated in File 1 under MT 452, is not specified in ENDF, but must be reconstituted by the processing code.

File 5 may also contain energy distributions of secondary charged particles for continuum reactions where only a single outgoing charged particle is possible (MT=649, 699, *etc.*). Continuum photon distributions should be described in File 15.

The use of File 6 to describe all particle energy distributions is preferred when several charged particles are emitted or the particle energy and angular distribution are strongly correlated. In these cases Files 5 and 15 should not be used.

Each section of the file gives the data for a particular reaction type (MT number). The sections are then ordered by increasing MT number. The energy distributions $p(E \rightarrow E')$

are normalized so that

$$\int_0^{E'_{\max}} p(E \rightarrow E')dE' = 1 \tag{5.1}$$

where E'_{max} is the maximum possible secondary particle energy and its value depends on the incoming particle energy E and the analytic representation of $p(E \rightarrow E')$. The secondary particle energy E' is always expressed in the *laboratory system*.

The differential cross section is obtained from

$$\frac{d\sigma(E \rightarrow E')}{dE'} = y\ \sigma(E)\ p(E \rightarrow E') \tag{5.2}$$

where $\sigma(E)$ is the cross section as given in File 3 for the same reaction type number (MT) and y is the neutron multiplicity for this reaction (for some reactions y is implicit; *e.g.*, $y = 2$ for the (n,2n) reaction, *etc.*).

The energy distributions $p(E \rightarrow E')$ can be broken down into partial energy distributions $f_k(E \rightarrow E')$, where each of the partial distributions can be described by a different analytic representation;

$$p(E \rightarrow E') = \sum_{k=1}^{\mathrm{NK}} p_k(E) f_k(E \rightarrow E') \tag{5.3}$$

and at a particular incident neutron energy E,

$$\sum_{k=1}^{\mathrm{NK}} p_k(E) = 1 \tag{5.4}$$

where $p_k(E)$ is the fractional probability that the distribution $f_k(E \rightarrow E')$ can be used at energy E.

The partial energy distributions $f_k(E \rightarrow E')$ are represented by various analytical formulations. Each formulation is called an energy distribution law and has an identification number associated with it (LF number). The allowed energy distribution laws are given below. [1]

5.1.1 Secondary Energy Distribution Laws

The data are given in each section by specifying the number of partial energy distributions that will be used. The same energy mesh should be used for each one. The partial energy distributions may all use the same energy distribution law (LF number) or they may use different laws.

[1] Distribution laws for LF=2, 3, 4, 6, 8, and 10 are not presented because these laws are no longer supported in ENDF-6 formats.

5.1.1.1 Arbitrary Tabulated Function (LF=1)

$$f(E \to E') = g(E \to E')$$

For a set of incident energy points E, the distribution $g(E \to E')$ is tabulated as a function of outgoing particle energy E'.

5.1.1.2 General Evaporation Spectrum (LF=5)

$$f(E \to E') = g\left(E'/\theta(E)\right)$$

where:

$\theta(E)$ is tabulated as a function of incident neutron energy E,

$g(x)$ is tabulated as a function of x, and $x = E'/\theta(E)$.

5.1.1.3 Simple Maxwellian Fission Spectrum (LF=7)

$$f(E \to E') = \frac{\sqrt{E'}}{I} e^{-E'/\theta(E)}$$

where

I is the normalization constant, defined by

$$I = \theta^{3/2}\left[\frac{\sqrt{\pi}}{2}\mathrm{erf}\left(\sqrt{(E-U)/\theta}\right) - \sqrt{(E-U)/\theta}\ \ e^{-(E-U)/\theta}\right]$$

θ is tabulated as a function of energy, E;

U is a constant introduced to define the proper upper limit for the final particle energy such that $0 \le E' \le (E-U)$.

5.1.1.4 Evaporation Spectrum (LF=9)

$$f(E \to E') = \frac{E'}{I} e^{-E'/\theta(E)}$$

where

I is the normalization constant:

$$I = \theta^2\left[1 - e^{-(E-U)/\theta}\left(1 + \frac{E-U}{\theta}\right)\right]$$

θ is tabulated as a function of incident neutron energy, E;

U is a constant introduced to define the proper upper limit for the final particle energy such that $0 \le E' \le (E-U)$.

5.1.1.5 Energy-Dependent Watt Spectrum (LF=11)

$$f(E \to E') = \frac{e^{-E'/a}}{I} \sinh\left(\sqrt{bE'}\right)$$

where

I is the normalization constant:

$$\begin{aligned} I &= \frac{1}{2}\sqrt{\frac{\pi a^3 b}{4}} \exp\left(\frac{ab}{4}\right) \left[\mathrm{erf}\left(\sqrt{\frac{E-U}{a}} - \sqrt{\frac{ab}{4}}\right) + \mathrm{erf}\left(\sqrt{\frac{E-U}{a}} + \sqrt{\frac{ab}{4}}\right)\right] \\ &- a \exp\left[-\left(\frac{E-U}{a}\right)\right] \sinh\sqrt{b(E-U)} \end{aligned}$$

a and b are tabulated energy-dependent parameters;

U is a constant introduced to define the proper upper limit for the final particle energy such that $0 \le E' \le (E-U)$.

5.1.1.6 Energy-Dependent Fission Neutron Spectrum (Madland and Nix) (LF=12)

$$\begin{aligned} f(E \to E') &= \frac{1}{2}\left[g(E', E_F(L)) + g(E', E_F(H))\right] \\ g(E', E_F) &= \frac{1}{3\sqrt{(E_F\, T_M)}} \left[u_2^{3/2}\mathrm{E}_1(u_2) - u_1^{3/2}\mathrm{E}_1(u_1) + \gamma\left(\frac{3}{2}, u_2\right) - \gamma\left(\frac{3}{2}, u_1\right)\right] \\ u_1 &= \left(\sqrt{E'} - \sqrt{E_F}\right)^2 / T_M \\ u_2 &= \left(\sqrt{E'} + \sqrt{E_F}\right)^2 / T_M \end{aligned}$$

where:

$E_F(X)$ are constant, which represent the average kinetic energy per nucleon of the fission fragment; arguments L and H refer to the average light fragment (given by the parameter EFL in the file) and the average heavy fragment (given by the parameter EFH in the file), respectively.

T_M parameter tabulated as a function of incident neutron energy,

$\mathrm{E}_1(x)$ is the exponential integral,

$\gamma(a, x)$ is the incomplete gamma function. The integral of this spectrum between zero and infinity is one. The value of the integral for a finite integration range is given in Section 5.4.10.

5.2 Formats

Each section of File 5 contains the data for a particular reaction type (MT number), starts with a HEAD record, and ends with a SEND record. Each subsection contains the data for one partial energy distribution. The structure of a subsection depends on the value of LF (the energy distribution law). The following quantities are defined.

NK Number of partial energy distributions. There will be one subsection for each partial distribution.

U Constant that defines the upper energy limit for the secondary particle so that $0 \leq$ E′ $\leq$ E - U (given in the LAB coordinate system).

θ Effective temperature used to describe the secondary energy distribution for LF = 5, 7, or 9.

LF Flag specifying the energy distribution law used for a particular subsection (partial energy distribution). (The definitions for LF are given in Section 5.1).

$p_k(E_i)$ Fractional part of the particular cross section which can be described by the kth partial energy distribution at the i-th incident energy point, subject to the condition

$$\sum_{k=1}^{NK} p_k(E_i) = 1.0$$

$f_k(E \rightarrow E')$ k^{th} partial energy distribution. The definition depends on the value of LF.

NR Number of interpolation ranges.

NP Number of incident energy points at which $p_k(E)$ is given.

a,b Parameters used in the energy dependent Watt spectrum, LF = 11.

EFL,EFH Constants $E_F(L)$ and $E_F(H)$ used in the energy-dependent fission neutron spectrum (Madland and Nix), LF = 12.

TM Maximum temperature parameter, $T_M(E)$, of the energy-dependent fission neutron spectrum (Madland and Nix), LF =12.

NE Number of incident energy points at which a tabulated distribution is given; For the maximum limit on NE see Appendix G.

NF Number of secondary energy points in a tabulation; For the maximum limit on NF see Appendix G.

The structure of a section has the following form:

```
[MAT, 5, MT/  ZA,  AWR,  0,  0, NK,  0]HEAD
      <subsection for k = 1 >
      <subsection for k = 2 >
      -----------------------
      -----------------------
      <subsection for k = NK>
[MAT, 5, MT/ 0.0,  0.0,  0,  0,  0,  0]SEND
```

The structure of a subsection depends on the value of LF. The formats for the various values of LF are given below.

5.2.1 Arbitrary Tabulated Function (LF=1)

The structure of a section has the following form:

[MAT, 5, MT/ 0.0, 0.0, 0, LF, NR, NP/ E_{int} /$p(E)$]TAB1 LF=1
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ E_{int}]TAB2
[MAT, 5, MT/ 0.0, E_1, 0, 0, NR, NF/ E'_{int} /
E'_1 0.0, E'_2, $g(E_1 \to E'_2)$, E'_3, $g(E_1 \to E'_3)$

--- E'_{NF-1}, $g(E_1 \to E'_{NF-1})$, E'_{NF}, 0.0]TAB1
[MAT, 5, MT/ 0.0, E_2, 0, 0, NR, NF/ E'_{int} /
E'_1 0.0, E'_2, $g(E_2 \to E'_2)$, E'_3, $g(E_2 \to E'_3)$

--- E'_{NF-1}, $g(E_2 \to E'_{NF-1})$, E'_{NF}, 0.0]TAB1
[MAT, 5, MT/ 0.0,E_{NE}, 0, 0, NR, NF/ E'_{int} /
E'_1 0.0, E'_2, $g(E_{NE} \to E'_2)$, E'_3, $g(E_{NE} \to E'_3)$

--- E'_{NF-1}, $g(E_2 \to E'_{NF-1})$, E'_{NF}, 0.0]TAB1

Note that the incident energy mesh for $p_k(E)$ does not have to be the same as the E mesh used to specify the energy distributions. The interpolation scheme used between incident energy points E, and between secondary energy points E', should be linear-linear.

5.2.2 General Evaporation Spectrum (LF=5)

The structure of a section has the following form:

[MAT, 5, MT/ U, 0.0, 0, LF, NR, NP/ E_{int} / $p(E)$]TAB1 (LF=5)
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ E_{int} / $\theta(E)$]TAB1
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NF/ x_{int} / $g(x)$]TAB1 $x = E'/\theta(E)$

5.2.3 Simple Maxwellian Fission Spectrum (LF=7)

The structure of a section has the following form:

```
[MAT, 5, MT/   U, 0.0,  0, LF, NR, NP/ E_int / p(E)]TAB1 (LF=7)
[MAT, 5, MT/ 0.0, 0.0,  0,  0, NR, NE/ E_int / θ(E)]TAB1
```

5.2.4 Evaporation Spectrum (LF=9)

The structure of a section has the following form:

```
[MAT, 5, MT/   U, 0.0,  0, LF, NR, NP/ E_int / p(E)]TAB1 (LF=9)
[MAT, 5, MT/ 0.0, 0.0,  0,  0, NR, NE/ E_int / θ(E)]TAB1
```

5.2.5 Energy-Dependent Watt Spectrum (LF=11)

The structure of a section has the following form:

```
[MAT, 5, MT/   U, 0.0,  0, LF, NR, NP / E_int / p(E)]TAB1 (LF=11)
[MAT, 5, MT/ 0.0, 0.0,  0,  0, NR, NE / E_int / a(E)]TAB1
[MAT, 5, MT/ 0.0, 0.0,  0,  0, NR, NE / E_int / b(E)]TAB1
```

5.2.6 Energy-Dependent Fission Neutron Spectrum (Madland and Nix) (LF=12)

The structure of a section has the following form:

```
[MAT, 5, MT/ 0.0, 0.0,  0, LF, NR, NP/ E_int / p(E)  ]TAB1 (LF=12)
[MAT, 5, MT/ EFL, EFH,  0,  0, NR, NE/ E_int / T_M(E)]TAB1
```

5.3 Procedures

As many as three different energy meshes may be required to describe the data in a subsection (one partial distribution). These are the incident energy mesh for $p_k(E)$, the incident energy mesh at which the secondary neutrons are given, $f_k(E \rightarrow E')$, and the secondary energy mesh for $f_k(E \rightarrow E')$. It is recommended that a linear-linear or a linear-log interpolation scheme be used for the first two energy meshes, and a linear-linear interpolation for the last energy mesh.

Double energy points must be given in the incident energy mesh whenever there is a discontinuity in any of the $p_k(E)$'s (this situation occurs fairly frequently). This energy mesh must also include threshold energy values for all reactions being described by the $p_k(E)$'s. Zero values for p_k must be given for energies below the threshold (if applicable).

Two nuclear temperatures may be given for the (n,2n) reaction. Each temperature θ may be given as a function of incident neutron energy. In this case $p_1(E) = p_2(E) = 0.5$. A similar procedure may be followed for the (n,3n) and other reactions.

A constant, U, is given for certain distribution laws (LF=5, 7, 9, or 11). The constant, U, is provided to define the proper upper limit for the secondary energy distribution so that

$0 \leq E' \leq E - U$. The value of U depends on how the data are represented for a particular reaction type. Consider U for inelastic scattering.

Case A: The total inelastic scattering cross section is described as a continuum. U is the threshold energy for exciting the lowest level in the residual nucleus.

Case B: For the energy range considered, the first three levels are described explicitly (either in File 3, MT = 51, 52, and 53, or in File 5), and the rest of the inelastic cross section is treated as a continuum. U is the threshold energy (known or estimated) for the fourth level in the residual nucleus.

If the reaction being described is fission, then U should be a large negative value ($U = -20.0 \times 10^6$ eV to -30×10^6 eV). In this case neutrons can be born with energies much larger than the incident neutron energy. It is common practice to describe the inelastic cross section as the sum of excitation cross sections (for discrete levels) for neutron energies up to the point where level positions are no longer known. At this energy point, the total inelastic cross section is treated as a continuum. This practice can lead to erroneous secondary energy distributions for incident neutron energies just above the cutoff energy. It is recommended that the level excitation cross sections for the first several levels (*e.g.*, 4 or 5 levels) be estimated for several MeV above the cutoff energy. The continuum portion of the inelastic cross section will be zero at the cutoff energy, and it will not become the total inelastic cross section until several MeV above the cutoff energy.

It is recommended that the cross sections for excitation of discrete inelastic levels be described in File 3 (MT=51, 52, ..., *etc.*). The angular distributions for the neutrons resulting from these levels should be given in File 4 (the same MT numbers). The secondary energy distributions for these neutrons can be obtained analytically from the data in Files 3 and 4. This procedure is the only way in which the energy distributions can be given for these neutrons. For inelastic scattering, the only data required in Files 5 are for MT=91 (continuum part).

5.4 Additional Procedures

5.4.1 General Comments

1. Do not give File 5 data for the discrete level excitation given in File 3 as MT=51, 52, ..., 90. If MT=91 is given in File 3, a section for MT=91 must be given in File 5 or File 6. A section must also be given in File 5 or File 6 for all other neutron-producing reactions. Continuum energy distributions for emitted protons, deuterons *etc.*, may be given in MT=649 *etc.*, and for photons, in File 6 or File 15. When more than one particle type is emitted, File 6 should be used to assure energy conservation.

2. Care must be used in selecting the distribution law number (LF) to represent the data. As a rule, use the simplest law that will accurately represent the data.

3. A section in File 5 must cover the same incident energy range as was used for the same MT number in File 3. The sum of the probabilities for all laws used must be equal to unity for all incident energy points.

4. If the incident neutron energy exceeds several MeV, pre-equilibrium neutron emission can be important, as illustrated from high-resolution neutron and proton spectra measurements and analysis of pulsed sphere experiments. In these cases either tabulated spectra or "mocked-up" levels can be constructed to supplement or replace simple evaporation spectra.

5. Prompt-neutron fission spectra are given under MT=18, 19, 20, 21, and 38. Delayed-neutron fission spectra are given under MT=455.

6. The energy distribution of prompt-neutrons from spontaneous fission is given in File 5 for MT=18, but in the decay data sublibrary (NSUB=4). It is used with ν_p from File 1 (MT=456) to determine the prompt-neutron spontaneous-fission spectrum. The delayed-neutron spontaneous-fission spectrum is determined from ν_d from File 1 (MT=455) and the delayed-neutron energy-distribution in File 5 MT=455. Note that for the specification of spontaneous-fission spectra no cross sections in File 3 are given.

5.4.2 Tabulated Distributions (LF=1)

Use only tabulated distributions to represent complicated energy distributions. Use the minimum number of incident energy points and secondary neutron energy points to accurately represent the data. The integral over secondary neutron energies for each incident energy point must be unity to within four significant figures. All interpolation schemes must be with linear-linear or linear-log (INT=1,2, or 3) to preserve probabilities upon interpolation. All secondary energy distributions must start and end with zero values for the distribution function $g(E \rightarrow E')$.

5.4.3 Maxwellian Spectrum (LF=7)

A linear-linear interpolation scheme is preferred for specifying the nuclear temperature as a function of energy.

5.4.4 Evaporation Spectrum (LF=9)

An evaporation spectrum is preferred for most reactions. Care must be taken in describing the nuclear temperature near the threshold of a reaction. Nuclear temperatures that are too large can violate conservation of energy.

5.4.5 Watt Spectrum (LF=11)

A linear-linear interpolation scheme is preferred for specifying the parameters a and b as a function of energy.

5.4.6 Madland-Nix Spectrum (LF=12)

A log-log interpolation scheme may be used for specifying the parameter T_M as a function of incident neutron energy.

5.4.7 Selection of the Integration Constant, U

1. When LF = 5, 7, 9, or 11 is used, an integration constant U is required. This constant is used in defining the upper energy limit of secondary neutrons; *i.e.*, $E'_{max} = E_n - U$, where E_n is the incident neutron energy. U is a constant for the complete energy range covered by a subsection in File 5 and is given in the LAB system.

2. U is negative for fission reactions. The preferred value is -20 MeV.

3. In practice, U can be taken to be the absolute value of Q for the lowest level (known or estimated) that can be excited by the particular reaction within the incident energy range covered by the subsection. U is actually a function of the incident neutron energy, but it can be shown that it is always greater than the absolute value of Q and less than the threshold energy of the reaction. At large AWR, since E_{th} and $|Q|$ are approximately equal, either could be used but the absolute value of Q is preferred. At small AWR, using $|Q|$ for U is the best approximation and must be used.

4. The following four cases commonly occur in data files; procedures are given for obtaining U values.

Case A: The complete reaction is treated as a continuum.
$U = -Q$, where Q is the reaction Q-value.

Case B: The reaction is described by excitation of three levels (in File 3 as MT = 51, 52, 53) and a continuum part where Q_4 is the known or estimated Q-value for the fourth level:
$U = -Q_4$.

Case C: The reaction is described by excitation of three levels (in File 3 as MT=51, 52, and 53) and a continuum part which extends below the threshold for MT=51. If, for example, the reaction is a 3-body breakup reaction, use
$U = -Q$,
where Q is the energy required for 3-body breakup.

Case D: The reaction is described by excitation of the first three levels (in File 3 as MT=51, 52, 53) for neutron energies from the level thresholds up to 20 MeV, excitation of the next five levels (in File 3 as MT=54, ..., 58) from their thresholds up to 8 MeV, and by a continuum part that starts at 5 MeV.

In this case two subsections should be used, one to describe the energy range from 5 to 8 MeV and another to describe the energy region from 8 to 20 MeV. In the first subsection (5 - 8 MeV),

$U = -Q_9$,

and the second (8 - 20 MeV),

$U = -Q_4$.

5.4.8 Multiple Nuclear Temperatures

Certain reactions, such as (n,2n), may require specification of more than one nuclear temperature. $\theta(E)$ should be given for each neutron in the exit channels; this is done by using more than one subsection for a reaction. The U value is the same for all subsections. The upper energy limit is determined by the threshold energy and not by level densities in the residual nuclei.

5.4.9 Average Energy for a Distribution

The average energy of a secondary neutron distribution must be less than the available energy for the reaction:

$$E_{\text{avail}} = E + \frac{1 + \text{AWR}}{\text{AWR}}\, Q,$$

where E_{avail} is greater than the neutron multiplicity times the average energy of all the emitted neutrons, $\nu\overline{E'}$, where ν is the multiplicity. The mean energy $\overline{E'}$ should be calculated from the distribution at each value of E. This mean is analytic in the four cases given below:

LF=7 $\quad \overline{E'} = \frac{3}{2}\theta - \frac{\theta^{5/2}}{I}\left(\frac{E-U}{\theta}\right)^{3/2} e^{-(E-U)/\theta}$

LF=9 $\quad \overline{E'} = 2\theta - \frac{\theta^3}{I}\left(\frac{E-U}{\theta}\right)^{2} e^{-(E-U)/\theta}$

L=11
$$\begin{aligned}\overline{E'} &= \frac{1}{2I}\Bigg\{a\exp\left(\frac{ab}{4}\right)\sqrt{\pi\frac{a^3b}{4}}\left(\frac{3}{2}+\frac{ab}{4}\right)\left[\operatorname{erf}\left(\sqrt{\frac{E_r}{a}}-\sqrt{\frac{ab}{4}}\right)+\operatorname{erf}\left(\sqrt{\frac{E_r}{4}}+\sqrt{\frac{ab}{4}}\right)\right]\\ &- 3a^2\sqrt{ab}\exp\left(-\frac{E_r}{a}\right)\left[\sqrt{\frac{E_r}{a}}\cosh\sqrt{bE_r}-\sqrt{\frac{ab}{4}}\sinh\sqrt{bE_r}\right]\\ &- 2a^2\exp\left(-\frac{E_r}{a}\right)\left[\left(\frac{E_r}{a}+\frac{ab}{4}\right)\sinh\sqrt{bE_r}-\sqrt{bE_r}\cosh\sqrt{bE_r}\right]\Bigg\}\end{aligned}$$
where $E_r = E - U$

LF=12 $\quad \overline{E'} = \frac{1}{2}\left[E_F(L) + E_F(H)\right] + \frac{4}{3}T_M$

Parameter U is described in Section 5.3. The analytic functions for I are given in Section 5.1 for LF=7, 9, 11. For LF=12, Section 5.4.10 gives the method for obtaining the integral of the distribution function.

5.4.10 Additional Procedures for Energy-Dependent Fission Neutron Spectrum (Madland and Nix)

To define the integral over a finite energy range $[a, b]$, set:

$\alpha = \sqrt{T_M}$
$\beta = \sqrt{E_F}$
$A = \left(\sqrt{a} + \beta\right)^2 / \alpha^2$
$B = \left(\sqrt{b} + \beta\right)^2 / \alpha^2$
$A' = \left(\sqrt{a} - \beta\right)^2 / \alpha^2$
$B' = \left(\sqrt{b} - \beta\right)^2 / \alpha^2$

The integral is given by one of the following three expressions depending on the region of integration in which a and b lie.

5.4.10.1 Region I ($a > E_F, b > E_F$)

$$
\begin{aligned}
3\sqrt{E_T T_M} \quad & \int_a^b g(E', E_F) dE' \; = \\
& = \left[\left(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2\right) \mathrm{E}_1(B) - \left(\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2\right) \mathrm{E}_1(A)\right] \\
& - \left[\left(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2\right) \mathrm{E}_1(B') - \left(\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2\right) \mathrm{E}_1(A')\right] \\
& + \left[\left(\alpha^2 B - 2\alpha\beta\sqrt{B}\right) \gamma\left(\frac{3}{2}, B\right) - \left(\alpha^2 A - 2\alpha\beta\sqrt{A}\right) \gamma\left(\frac{3}{2}, A\right)\right] \\
& - \left[\left(\alpha^2 B' + 2\alpha\beta\sqrt{B'}\right) \gamma\left(\frac{3}{2}, B'\right) - \left(\alpha^2 A' + 2\alpha\beta\sqrt{A'}\right) \gamma\left(\frac{3}{2}, A'\right)\right] \\
& - \frac{3}{5}\alpha^2 \left[\gamma\left(\frac{5}{2}, B\right) - \gamma\left(\frac{5}{2}, A\right) - \gamma\left(\frac{5}{2}, B'\right) - \gamma\left(\frac{5}{2}, A'\right)\right] \\
& - \frac{3}{5}\alpha\beta \left[e^{-B}(1 + B) - e^{-A}(1 + A) + e^{-B'}(1 + B') - e^{-A'}(1 + A')\right]
\end{aligned}
$$

5.4.10.2 Region II ($a < E_F, b < E_F$)

$$
\begin{aligned}
3\sqrt{E_T T_M} \quad & \int_a^b g(E', E_F) dE' = \\
& = \left[\left(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2\right) \mathrm{E}_1(B) - \left(\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2\right) \mathrm{E}_1(A)\right] \\
& - \left[\left(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2\right) \mathrm{E}_1(B') - \left(\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2\right) \mathrm{E}_1(A')\right] \\
& + \left[\left(\alpha^2 B - 2\alpha\beta\sqrt{B}\right) \gamma\left(\frac{3}{2}, B\right) - \left(\alpha^2 A - 2\alpha\beta\sqrt{A}\right) \gamma\left(\frac{3}{2}, A\right)\right] \\
& - \left[\left(\alpha^2 B' - 2\alpha\beta\sqrt{B'}\right) \gamma\left(\frac{3}{2}, B'\right) - \left(\alpha^2 A' - 2\alpha\beta\sqrt{A'}\right) \gamma\left(\frac{3}{2}, A'\right)\right] \\
& - \frac{3}{5}\alpha^2 \left[\gamma\left(\frac{5}{2}, B\right) - \gamma\left(\frac{5}{2}, A\right) - \gamma\left(\frac{5}{2}, B'\right) - \gamma\left(\frac{5}{2}, A'\right)\right] \\
& - \frac{3}{5}\alpha\beta \left[e^{-B}(1+B) - e^{-A}(1+A) + e^{-B'}(1+B') + e^{-A'}(1+A')\right]
\end{aligned}
$$

5.4.10.3 Region III ($a < E_F, b > E_F$)

$$
\begin{aligned}
3\sqrt{E_T T_M} \quad & \int_a^b g(E', E_F) dE' = \\
& = \left[\left(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2\right) \mathrm{E}_1(B) - \left(\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2\right) \mathrm{E}_1(A)\right] \\
& - \left[\left(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2\right) \mathrm{E}_1(B') - \left(\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2\right) \mathrm{E}_1(A')\right] \\
& + \left[\left(\alpha^2 B - 2\alpha\beta\sqrt{B}\right) \gamma\left(\frac{3}{2}, B\right) - \left(\alpha^2 A - 2\alpha\beta\sqrt{A}\right) \gamma\left(\frac{3}{2}, A\right)\right] \\
& - \left[\left(\alpha^2 B' + 2\alpha\beta\sqrt{B'}\right) \gamma\left(\frac{3}{2}, B'\right) - \left(\alpha^2 A' + 2\alpha\beta\sqrt{A'}\right) \gamma\left(\frac{3}{2}, A'\right)\right] \\
& - \frac{3}{5}\alpha^2 \left[\gamma\left(\frac{5}{2}, B\right) - \gamma\left(\frac{5}{2}, A\right) - \gamma\left(\frac{5}{2}, B'\right) + \gamma\left(\frac{5}{2}, A'\right)\right] \\
& - \frac{3}{5}\alpha\beta \left[e^{-B}(1+B) - e^{-A}(1+A) + e^{-B'}(1+B') + e^{-A'}(1+A') - 2\right]
\end{aligned}
$$

The expression for Region III would be used to calculate a normalization integral I for the finite integration constant U, if a physical basis existed by which U could be well determined.

Chapter 6

File 6: PRODUCT ENERGY-ANGLE DISTRIBUTIONS

6.1 General Description

This file is provided to represent the distribution of reaction products (*i.e.*, neutrons, photons, charged particles, and residual nuclei) in energy and angle. It works together with File 3, which contains the reaction cross sections, and replaces the combination of Files 4 and 5. Radioactive products are identified in File 8. The use of File 6 is recommended when the energy and angular distributions of the emitted particles must be coupled, when it is important to give a concurrent description of neutron scattering and particle emission, when so many reaction channels are open that it is difficult to provide separate reactions, or when accurate charged-particle or residual-nucleus distributions are required for particle transport, heat deposition, or radiation damage calculations.

For the purposes of this file, any reaction is defined by giving the production cross section for each reaction product in barns/steradian assuming azimuthal symmetry:

$$\sigma_i(\mu, E, E') = \sigma(E)\ y_i(E)\ f_i(\mu, E, E')/2\pi \tag{6.1}$$

where:

i denotes one particular product,

E is the incident energy,

E' is the energy of the product emitted with cosine μ,

$\sigma(E)$ is the interaction cross section (File 3),

y_i is the product yield or multiplicity, and

f_i is the normalized distribution with units (eV.unit-cosine)$^{-1}$ where

$$\int dE' \int d\mu\ f_i(\mu, E, E') = 1 \tag{6.2}$$

This representation ignores most correlations between products and most sequential reactions; that is, the distributions given here are those, which would be seen by an observer outside of a "black box" looking at one particle at a time. The process being described may be a combination of several different reactions, and the product distributions may be described using several different representations.

6.2 Formats

The following quantities are defined for all representations:

ZA, AWR Standard material charge and mass parameters.

LCT Reference system for secondary energy and angle (incident energy is always given in the LAB system).
LCT=1, laboratory (LAB) coordinates used for both;
LCT=2, center-of-mass (CM) system used for both;
LCT=3, center-of-mass system for both angle and energy of light particles (A$\leq$ 4), laboratory system for heavy recoils (A>4).

NK Number of subsections in this section (MT). Each subsection describes one reaction product. There can be more than one subsection for a given particle or residual nucleus (see LIP). For the limit on NK see Appendix G.

ZAP Product identifier $1000 * Z + A$ with $Z = 0$ for photons and $A = 0$ for electrons and positrons. A section with $A = 0$ can also be used to represent the average recoil energy or spectrum for an elemental target (see text).

AWP Product mass in neutron units. When ZAP=0, this field can contain the energy of a primary photon. In that case, this section will contain an angular distribution (LAW=2) for the primary photon.

LIP Product modifier flag. Its main use is to identify the isomeric state of a product nucleus. In this case, LIP=0 for the ground state, LIP=1 for the first isomeric state, *etc.* These values should be consistent with LISO in File 8, MT=457.

In some cases, it may be useful to use LIP to, distinguish between different subsections with the same value of ZAP for light particles. For example, LIP=0 could be the first neutron out for a sequential reaction, LIP=1 could be the second neutron, and so on. Other possible uses might be to indicate which compound system emitted the particles, or to distinguish between the neutron from the (n,np) channel and that from the (n,pn) channel. The exact meaning assigned to LIP should be explained in the File 1, MT=451 comments.

LAW Flag to distinguish between different representations of the distribution function, f_i:

LAW=0, unknown distribution;
LAW=1, continuum energy-angle distribution;
LAW=2, two-body reaction angular distribution;
LAW=3, isotropic two-body distribution;
LAW=4, recoil distribution of a two-body reaction;
LAW=5, charged-particle elastic scattering;
LAW=6, n-body phase-space distribution; and
LAW=7, laboratory angle-energy law.

NR, NP, $\mathbf{E}_{int}$ Standard TAB1 interpolation parameters.

A section in File 6 has the following form:

```
[MAT, 6, MT/  ZA, AWR,   0, LCT,  NK,   0]HEAD
[MAT, 6, MT/ ZAP, AWP, LIP, LAW,  NR,  NP/ E_int  / y_i(E)]TAB1
           <LAW-dependent structure for product 1>
                ----------------------------
           <repeat TAB1 and LAW-dependent structures>
           <for the rest of the NK subsections      >
                ----------------------------
[MAT, 6, MT/ 0.0, 0.0,   0,   0,   0,   0]SEND
```

File 6 should have a subsection for every product of the reaction or sum of reactions being described except for MT = 3, 4, 103-107 when they are being used to represent lumped photons. An exception to this ordering is made when capture primary photons are being described. Then the ordering is (1) angular distribution of primary photon to ground state (LAW=2), (2) corresponding recoil (LAW=4), (3) angular distribuiton of primary photon to first excited state, (4) corresponding recoil, (5) energy distribution of cascade photons from first excited state (LAW=1 delta function), and so on, until all primary photons have been described. The subsections are arranged in the following order:

1. particles (n, p, d, *etc.*) in order of ZAP and LIP,
2. residual nuclei and isomers in order of ZAP and LIP,
3. photons, and
4. electrons.

The contents of the subsection for each LAW are described below.

6.2.1 Unknown Distribution (LAW=0)

This law simply identifies a product without specifying a distribution. It can be used to give production yields for particles, isomers, radioactive nuclei, or other interesting nuclei in materials that are not important for particle transport, heating, or radiation damage calculations. No law-dependent structure is given.

6.2.2 Continuum Energy-Angle Distributions (LAW=1)

This law is used to describe particles emitted in multi-body reactions or combinations of several reactions, such as scattering through a range of levels or reactions at high energies where many channels are normally open. For isotropic reactions, it is very similar to File 5, LF=1 except for a special option to represent sharp peaks as "delta functions" and the use of LIST instead of TAB1 record. The following quantities are defined for LAW=1:

LANG Indicator which selects the angular representation to be used; if
LANG=1, Legendre coefficients are used,
LANG=2, Kalbach-Mann systematics are used,
LANG=11-15, a tabulated angular distribution is given using NA/2 cosines and the interpolation scheme specified by LANG-10 (for example, LANG=12 selects linear-linear interpolation).

LEP Interpolation scheme for secondary energy;
LEP=1 for histogram,
LEP=2 for linear-linear, *etc.*

NR, NE, E_{int} Standard TAB2 interpolation parameters.
INT=1 is allowed (the upper limit is implied by File 3),
INT=12-15 is allowed for corresponding-point interpolation,
INT=21-25 is allowed for unit base interpolation.

NW Total number of words in the LIST record; NW = NEP (NA+2).

NEP Number of secondary energy points in the distribution.

ND Number of discrete energies given.

The first ND≥0 entries in the list of NEP energies are discrete, and the remaining (NEP-ND)≥ 0 entries are to be used with LEP to describe a continuous distribution. Discrete primary photons should be flagged with negative energies.

NA Number of angular parameters.

Use NA=0 for isotropic distributions (note that all options are identical if NA=0).

Use NA=1 or 2 with LANG=2 (Kalbach-Mann).

The structure of a subsection is:

```
[MAT, 6, MT/  0.0,   0.0,  LANG,  LEP,   NR,   NE/ E_int]TAB2
[MAT, 6, MT/  0.0,    E1,    ND,   NA,   NW,  NEP/
    E'_1,    b_0(E_1,E'_1),     b_1(E_1,E'_1), --------  b_NA(E_1,E'_1),
    E'_2,    b_0(E_1,E'_2),     b_1(E_1,E'_2), --------  b_NA(E_1,E'_2),
   ---------------------------------------------
    E'_NEP, b_0(E_1,E'_NEP),  b_1(E_1,E'_NEP), ----  b_NA(E_1,E'_NEP)]LIST
   <repeat the LIST structure for all the NE incident energies>
```

where the contents of the b_i depend on LANG.

The angular part of f_i can be represented in several different ways (denoted by LANG).

6.2.2.1 Legendre Coefficients Representation (LANG=1)

Legendre coefficients are used as follows:

$$f_l(\mu, E, E') = \sum_{l=0}^{NA} \frac{2l+1}{2} \; f_l(E, E') \; P_l(\mu) \tag{6.3}$$

where NA is the number of angular parameters, and the other parameters have their previous meanings. Note that these coefficients are not normalized like those for discrete two-body scattering (LAW=2); by definition, $f_0(E, E')$ gives the total probability of scattering from E to E' integrated over all angles. This is equivalent to the function $g(E, E')$ that would normally be given in File 5. The Legendre coefficients are stored with f_0 in b_0, f_1 in b_1, *etc.*

6.2.2.2 Kalbach-Mann Systematics Representation (LANG=2)

The angular distributions are represented by using the Kalbach-Mann systematics [Ref.1] in the extended form developed by Kalbach [Ref.2], hereinafter referred to as KA88. The distribution is given in terms of the parameters r and a, which are described below. If NA=1, the parameter r is given and a is calculated. If NA=2, then both parameters r and a are given explicitly.

The formulation addresses reactions of the form

A + a → C → B + b,

where:

A is the target,

a is the incident projectile,

C is the compound nucleus,

b is the emitted particle,

B is the residual nucleus.

The following quantities are defined:

E_a energy of the incident projectile a in the *laboratory system*

ϵ_a entrance channel energy, the kinetic energy of the incident projectile a and the target particle A in the *center-of-mass system*, defined by:

$$\varepsilon_a = E_a \times \frac{\mathrm{AWR}_A}{\mathrm{AWR}_A + \mathrm{AWR}_a}$$

E_b energy of the emitted particle in the *laboratory system*

ϵ_b emission channel energy, the kinetic energy of the emission particle b and the residual nucleus B in the *center-of-mass system*, defined by:

$$\varepsilon_b = E_b \times \frac{\mathrm{AWR}_B}{\mathrm{AWR}_B + \mathrm{AWR}_b}$$

μ_b cosine of the scattering angle of the emitted particle b in the *center-of-mass system*

It is ***required*** that LCT=2 with LANG=2.

The KA88 distribution is represented by:

$$f(\mu_b, E_a, E_b) = \frac{a(E_a, E_b) f_0(E_a, E_b)}{2\sinh\left(a(E_a, E_b)\right)} \left[\cosh\left(a(E_a, E_b)\mu_b\right) + r(E_a, E_b)\sinh\left(a(E_a, E_b)\mu_b\right)\right] \tag{6.4}$$

where $r(E_a, E_b)$ is the pre-compound fraction as given by the evaluator and $a(E_a, E_b)$ is a simple parameterized function that depends mostly on the center-of-mass emission energy E_b, but also depends slightly on particle type and the incident energy at higher values of E_a.

The center-of-mass energies and angles E_b and μ_b are transformed into the laboratory system using the expressions:

$$\begin{aligned} E_{b,\mathrm{lab}} &= E_{b,\mathrm{cm}} + \frac{\mathrm{AWR}_a \mathrm{AWR}_b}{(\mathrm{AWR}_A + \mathrm{AWR}_a)^2} E_{a,\mathrm{lab}} + 2\frac{\sqrt{\mathrm{AWR}_a}\sqrt{\mathrm{AWR}_b}}{\mathrm{AWR}_A + \mathrm{AWR}_a}\sqrt{E_{a,\mathrm{lab}} E_{b,\mathrm{cm}}}\,\mu_{b,\mathrm{cm}} \\ \mu_{b,\mathrm{lab}} &= \sqrt{\frac{E_{b,\mathrm{cm}}}{E_{b,\mathrm{lab}}}}\,\mu_{b,\mathrm{cm}} + \frac{\sqrt{\mathrm{AWR}_a}\sqrt{\mathrm{AWR}_b}}{\mathrm{AWR}_A + \mathrm{AWR}_a}\sqrt{\frac{E_{a,\mathrm{lab}}}{E_{b,\mathrm{lab}}}} \end{aligned} \tag{6.5}$$

The pre-compound fraction r, where r ranges from 0.0 to 1.0, is usually computed by a model code, although it can be chosen to fit experimental data.

The formula[1] for calculating the slope value $a(E_a, E_b)$ is:

$$a(E_a, E_b) = C_1 X_1 + C_2 X_1^3 + C_3 M_a m_b X_3^4$$

where:

$e_a = \epsilon_a + S_a$	$e_b = \epsilon_b + S_b$
$R_1 = \mathrm{minimum}(e_a, E_{t1})$	$R_3 = \mathrm{minimum}(e_a, E_{t3})$
$X_1 = R_1 e_b / e_a$	$X_3 = R_3 e_b / e_a$

The parameter values for light particle induced reactions as given in KA88[2] are:

[1] Equation 10 of Ref. 2.
[2] Table V of ref. 2.

$C_1 = 0.04/\text{MeV}$	$C_2 = 1.8\times10^{-6}/(\text{MeV})^3$
$C_3 = 6.7\times10^{-7}/(\text{MeV})^4$	
$E_{t1} = 130$ MeV	$E_{t3} = 41$ MeV
$M_n = 1$	$M_p = 1$
$M_d = 1$	$M_\alpha = 0$
$m_n = 1/2$	$m_p = 1$
$m_d = 1$	$m_t = 1$
$m_{3He} = 1$	$m_\alpha = 2$

S_a and S_b are the separation energies for the incident and emitted particles, respectively, neglecting pairing and other effects for the reaction A + a → C → B + b. The formulae for the separation energies[3] in MeV are:

$$\begin{aligned} S_a &= 15.68\,[A_C - A_A] - 28.07\left[\frac{(N_C-Z_C)^2}{A_C} - \frac{(N_A-Z_A)^2}{A_A}\right] \\ &- 18.56\left[A_C^{2/3} - A_A^{2/3}\right] + 33.22\left[\frac{(N_C-Z_C)^2}{A_C^{4/3}} - \frac{(N_A-Z_A)^2}{A_A^{4/3}}\right] \\ &- 0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_A^2}{A_A^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_A^2}{A_A}\right] - I_a \end{aligned}$$

and

$$\begin{aligned} S_b &= 15.68\,[A_C - A_B] - 28.07\left[\frac{(N_C-Z_C)^2}{A_C} - \frac{(N_B-Z_B)^2}{A_B}\right] \\ &- 18.56\left[A_C^{2/3} - A_B^{2/3}\right] + 33.22\left[\frac{(N_C-Z_C)^2}{A_C^{4/3}} - \frac{(N_B-Z_B)^2}{A_B^{4/3}}\right] \\ &- 0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_B^2}{A_B^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_B^2}{A_B}\right] - I_b \end{aligned}$$

where:

A, B, C — subscripts refer to the target nucleus, the residual nucleus, and the compound nucleus, as before,

N, Z, A — are the neutron, proton, and mass numbers of the nuclei,

I_a, I_b — are the energies required to separate the incident and emitted particles into their constituent nucleons (see Appendix H for values used for given particles).

[3] Equation 4 of Ref. 2.

The parameter $f_0(E_a, E_b)$ has the same meaning as f_0 in equation (6.3); that is, the total emission probability for this E_a and E_b. The *number of angular parameters* (NA) for LANG=2 can be:

NA=1 in which case f_0 and r are stored in the positions b_0 and b_1, respectively, or

NA=2 where f_0, r and a are stored in the positions of b_0, b_1 and b_2, respectively.

This formulation uses a single-particle-emission concept; it is assumed that each and every secondary particle is emitted from the original compound nucleus C. When the incident projectile a, and the emitted particle b, are the same, $S_a = S_b$, regardless of the reaction. For incident projectile z, if neutrons emitted from the compound nucleus C are detected, there will be one and only one S_b appropriate for all reactions, for example, (z,nα), (z,n3α), (z,2nα), (z,np), (z,2n2α), and (z,nt2α). Furthermore, if the incident projectile is a neutron (z=n in previous examples), then $S_a = S_b$ in all cases; even for neutrons emitted in neutron-induced reactions, Sa and S_b will be identical.

6.2.2.3 Tabulated Function Representation (LANG=11-15)

For LANG=11-15, a tabulated function is given for $f(\mu)$ using the interpolation scheme defined by (LANG - 10). For example, if LANG=12, use linear-linear interpolation (do not use log interpolation with the cosine). The cosine grid of NA/2 values, μ_i, must span the entire angular range open to the particle for E and E', and the integral of $f(\mu)$ over all angles must give the total emission probability for this E and E' (that is, it must equal f_0, as defined above). The value of f below μ_1 or above $\mu_{\mathrm{NA}/2}$ is zero.

The tabulation is stored in the angular parameters as follows:

$b_0 = f_0,$

$b_1 = \mu_1,$

$b_2 = 0.5\ f_1(\mu_1)/f_0,$

$b_3 = \mu_2,$

...

...

$b_{\mathrm{NA}} = 0.5\ f_{\mathrm{NA}/2}(\mu_{\mathrm{NA}/2})/f_0.$

The preferred values for NA are 4, 10, 16, 22, *etc.*

In order to provide a good representation of sharp peaks, LAW=1 allows for a superposition of a continuum and a set of delta functions. These discrete lines could be used to represent particle excitations in the CM frame because the method of corresponding points can be used to supply the correct energy dependence. However, the use of LAW=2 together with MT=50-90, 600-650, *etc.*, is preferred. This option is also useful when photon production is given in File 6.

6.2.3 Discrete Two-Body Scattering (LAW=2)

This law is used to describe the distribution in energy and angle of particles described by two-body kinematics. It is very similar to File 4, except its use in File 6 allows the concurrent description of the emission of positrons, electrons, photons, neutrons, charged particles, residual nuclei, and isomers. Since the energy of a particle emitted with a particular scattering cosine μ is determined by kinematics, it is only necessary to give:

$$\begin{aligned} p_i(\mu, E) &= \int dE' \; f_i(\mu, E, E') \\ &= \frac{1}{2} + \sum_{l+1}^{\mathrm{NL}} \frac{2l+1}{2} \; a_l(E) \; P_l(\mu) \end{aligned} \tag{6.6}$$

,
where the P_l are the Legendre polynomials with the maximum order NL. Note that the angular distribution p_i is normalized. The following quantities are defined for LAW=2:

LANG flag that indicates the representation:
LANG=0, Legendre expansion;
LANG=12, tabulation with $p_i(\mu)$ linear in μ;
LANG=14, tabulation with $\log(p_i)$ linear in μ.

NR, NE, E$_{int}$ standard TAB2 interpolation parameters.

NL for LANG=0, NL is the highest Legendre order used;
for LANG>0, NL is the number of cosines tabulated.

NW number of parameters given in the LIST record:
for LANG=0, NW=NL;
for LANG>0, NW=2*NL.

A$_l$ for LANG=0, the Legendre coefficients,
for LANG>0, the, (μ, p_i) pairs for the tabulated angular distribution

The format for a subsection with LAW=2 is:

```
[MAT, 6, MT/ 0.0, 0.0,   0,  0,  NR,  NE/ E_int ]TAB2
[MAT, 6, MT/ 0.0,  E_1,LANG,  0,  NW,  NL/ A_l(E)]LIST
            ----------------------------
            <repeat the LIST records for all the incident energies>
            ----------------------------
```

Note that the Legendre expansion option LANG=0 is very similar to File 4, LTT=1. The tabulated option LANG¿0 is similar to File 4, LTT=2, except that a LIST record is used instead of TAB1. The kinematical equations require AWR and AWP from File 6 and QI from File 3.

LAW=2 can be used in sections with MT=50-90, 600-648, 650-698, *etc.*, only, and the center-of-mass system must be used (LCT=2). In addition, LAW=2 can be used to give the angular distributions for primary photons in sections with MT=102.

6.2.4 Isotropic Discrete Emission (LAW=3)

This law serves the same purpose as LAW=2, but the angular distribution is assumed to be isotropic in the CM system for all incident energies. No LAW-dependent structure is given. This option is similar to LI=1 in File 4. The energy of the emitted particle is completely determined by AWR and AWP in this section and QI from File 3.

6.2.5 Discrete Two-Body Recoils (LAW=4)

If the recoil nucleus of a two-body reaction (*e.g.*, (n,n'), (p,n), *etc.*) described using LAW=2 or 3 does not break up, its energy and angular distribution can be determined from the kinematics. No LAW-dependent structure is given. If isomer production is possible, multiple subsections with LAW=4 can be given to define the energy-dependent branching ratio for the production of each excited nucleus. Finally, LAW=4 may be used to describe the recoil nucleus after radiative capture (MT=102), with the understanding that photon momentum at low energies must be treated approximately, or when detailed angular distributions are given for primary photons.

6.2.6 Charged-Particle Elastic Scattering (LAW=5)

Elastic scattering of charged particles includes components from Coulomb scattering, nuclear scattering, and the interference between them. The Coulomb scattering is represented by the Rutherford formula and electronic screening is ignored. The following parameters are defined.

$\sigma_{cd}(\mu, E)$	differential Coulomb scattering cross section the *center-of-mass system* for distinguishable particles (barns/sr)
$\sigma_{ci}(\mu, E)$	cross section the *center-of-mass system* for identical particles (barns/sr)
E	energy of the incident particle in the *laboratory system* (eV)
μ	cosine of the scattering angle in the *center-of-mass system*
m_1	incident particle mass (amu)
Z_1, Z_2	charge numbers of the incident particle and target, respectively
s	spin (identical particles only, $s = 0, \frac{1}{2}, 1, \frac{3}{2},$ *etc.*)
A	target/projectile mass ratio
k	particle wave number (barns$^{-1/2}$)

η dimensionless Coulomb parameter

$u, c, \hbar, \alpha$ fundamental constants (see Appendix H).

The cross sections can then be written:

$$\sigma_{cd}(\mu, E) = \frac{\eta^2}{k^2(1-\mu)^2} \tag{6.7}$$

$$\sigma_{ci}(\mu, E) = \frac{2\eta^2}{k^2(1-\mu^2)}\left[\frac{1+\mu^2}{1-\mu^2} + \frac{(-1)^{2s}}{2s+1}\cos\left(\eta\ \ln\frac{1+\mu}{1-\mu}\right)\right] \tag{6.8}$$

$$\text{where} \quad k = \frac{A}{1+A}\sqrt{\frac{2}{\hbar^2}\frac{u}{c^2}\ m_1 E}\ \times 10^{-14} \tag{6.9}$$

$$\eta = Z_1 Z_2 \sqrt{\frac{\alpha^2 u}{2}\ \frac{m_1}{E}} \tag{6.10}$$

Note that $A = 1$ and $Z_1 = Z_2$ for identical particles.

The net elastic scattering cross section for distinguishable particles may be written as:

$$\begin{aligned}\sigma_{ed}(\mu, E) = \sigma_{cd}(\mu, E) \quad &- \quad \frac{2\eta}{1-\mu}\mathrm{Re}\left\{\exp\left(i\eta\ln\frac{1-\mu}{2}\right)\sum_{l=0}^{\mathrm{NL}}\frac{2l+1}{2}a_l(E)P_l(\mu)\right\} \\ &+ \quad \sum_{l=0}^{2\mathrm{NL}}\frac{2l+1}{2}b_l(E)P_l(\mu)\end{aligned} \tag{6.11}$$

and the cross section for identical particles is:

$$\begin{aligned}\sigma_{ei}(\mu, E) &= \sigma_{ci}(\mu, E) \\ &- \frac{2\eta}{1-\mu^2}\ \mathrm{Re}\left\{\sum_{l=0}^{\mathrm{NL}}\left[\begin{array}{r}(1+\mu)\exp\left(i\eta\ln\frac{1-\mu}{2}\right)\\ +(-1)^l(1-\mu)\exp\left(i\eta\ln\frac{1+\mu}{2}\right)\end{array}\right]\frac{2l+1}{2}a_l(E)P_l(\mu)\right\} \\ &+ \sum_{l=0}^{\mathrm{NL}}\frac{4l+1}{2}\ b_l(E)P_{2l}(\mu)\end{aligned} \tag{6.12}$$

where the a_l are complex coefficients for expanding the trace of the nuclear scattering amplitude matrix and the b_l are real coefficients for expanding the nuclear scattering cross section. The value of NL represents the highest partial wave contributing to nuclear scattering. Note that $\sigma_{ei}(-\mu, E) = \sigma_{ei}(\mu, E)$.

The three terms in Equations (6.11) and (6.12) are Coulomb, interference, and nuclear scattering, respectively. Since an integrated cross section is not defined for this representation, a value of 1.0 is used in File 3.

When only experimental data are available, it is convenient to remove the infinity due to σ_C by subtraction and to remove the remaining infinity in the interference term by multiplication, thereby obtaining the residual cross sections:

$$\sigma_{Rd}(\mu, E) = (1-\mu)\left[\sigma_{ed}(\mu, E) - \sigma_{cd}(\mu, E)\right] \tag{6.13}$$

and

$$\sigma_{Ri}(\mu, E) = (1-\mu^2)\left[\sigma_{ei}(\mu, E) - \sigma_{ci}(\mu, E)\right] \tag{6.14}$$

Then σ_R can be given as a Legendre polynomial expansion in the forms:

$$\sigma_{Rd}(\mu, E) = \sum_{l=0}^{\mathrm{NL}} \frac{2l+1}{2} c_{ld}(E) P_l(\mu) \tag{6.15}$$

and

$$\sigma_{Ri}(\mu, E) = \sum_{l=0}^{\mathrm{NL}} \frac{4l+1}{2} c_{li}(E) P_{2l}(\mu) \tag{6.16}$$

A cross section value of 1.0 is used in File 3.

Because the interference term oscillates as μ goes to 1, the limit of the Legendre representation of the residual cross section at small angles may not be well defined. However, if the coefficients are chosen properly, the effect of this region will be small because the Coulomb term is large.

It is also possible to represent experimental data using the "nuclear plus interference" cross section and angular distribution in the CM system defined by:

$$\sigma_{NI}(\mu, E) = \int_{\mu_{\min}}^{\mu_{\max}} \left[\sigma_e(\mu, E) - \sigma_c(\mu, E)\right] d\mu \tag{6.17}$$

and

$$P_{NI}(\mu, E) = \begin{cases} \dfrac{\sigma_e(\mu, E) - \sigma_c(\mu, E)}{\sigma_{NI}(E)}, & \mu_{\min} \le \mu \le \mu_{\max} \\ 0 & \text{otherwise,} \end{cases} \tag{6.18}$$

where $\mu_{min} = -1$ for different particles and 0 for identical particles. The maximum cosine should be as close to 1.0 as possible, especially at high energies where Coulomb scattering is less important. The Coulomb cross section $\sigma_c(\mu, E)$ is to be computed using equations (6.7) or (6.8) for different or identical particles, respectively. The angular distribution p_{NI} is given in File 6 as a tabulated function of μ, and $\sigma_{NI}(E)$ in barns is given in File 3. The following quantities are defined for LAW=5:

SPI Spin of the particle. Used for identical particles (SPI=0, 1/2, 1, *etc.*).

LIDP Indicates that the particles are identical when LIDP=1; otherwise, LIDP=0.

LTP Indicates the representation:

LTP=1 nuclear amplitude expansion, equations (6.11) and (6.12);

LTP=2 residual cross section expansion as Legendre coefficients, equations (6.13) through (6.16);

LTP=12 nuclear plus interference distribution with p_{NI} linear in μ, equations (6.17) and (6.18);

LTP=14 tabulation with $\ln(P_{NI})$ linear in μ, equations (6.17) and (6.18).

LTP=15 tabulation with P_{NI} linear in μ, equations (6.17) and (6.18).

NR, NE, $\mathbf{E}_{int}$ Standard TAB2 parameters.

NL For LTP≤2, NL is the highest Legendre order of nuclear partial waves used; For LTP>2, NL is the number of cosines tabulated.

NW Number of parameters given in the LIST record:
for LTP=1 and LIDP=0, NW=4*NL+3;
for LTP=1 and LIDP=1, NW=3*NL+3;
for LTP=2, NW=NL+1; and for LTP>2, NW=2*NL.

$\mathbf{A}_i$(E) Coefficients (a_i, b_i, or c_i as described below) in barns/sr or (μ, p) pairs, where p is dimensionless.

A subsection for LAW=5 has the following form:

```
[MAT, 6, MT/ SPI, 0.0, LIDP, 0,  NR,  NE/ E_int ]TAB2
[MAT, 6, MT/ 0.0, E_1,  LTP,  0,  NW,  NL/ A_1(E_1)]LIST
  -------------------------------
  <repeat the LIST records for all of the NE
   incident energies>
  -------------------------------
```

The coefficients witin the LIST array A_i are organized as follows:
LTP=1 and LIDP=0,

b_0, b_1, ...b_{2NL}, Ra_0, Ia_0, Ra_1, Ia_1, ...Ia_{NL};

LTP=1 and LIDP=1,

b_0, b_1, ...b_{2NL}, Ra_0, Ia_0, Ra_1, Ia_1, ...Ia_{NL};

LTP=2,

c_0, c_1, ... c_{NL}

LTP>2,

μ_1, $p_{NI}(\mu_1)$, ... μ_{NL}, $p_{NI}(\mu_{NL})$.

6.2.7 N-Body Phase-Space Distributions (LAW=6)

In the absence of detailed information, it is often useful to use n-body phase-space distributions for the particles emitted from neutron and charged-particle reactions. These distributions conserve energy and momentum, and they provide reasonable kinematic limits for secondary energy and angle in the LAB system.

The phase-space distribution for particle i in the CM system is

$$P_i^{\mathrm{CM}}(\mu, E, E') = C_n \sqrt{E'}(E_i^{\max} - E')^{(3n/2)-4} \tag{6.19}$$

where

$E_i^{\max}$ is the maximum possible center-of-mass energy for particle i,

μ, E' are cosine of the scattering angle and outgoing particle energy in the CM system, and

C_n are normalization constants:

$$\begin{aligned} C_3 &= \frac{4}{\pi(E_i^{\max})^2} \\ C_4 &= \frac{105}{32(E_i^{\max})^{7/2}} \\ C_5 &= \frac{256}{14\pi(E_i^{\max})^5} \end{aligned}$$

In the laboratory system, the distributions become

$$P_i^{\mathrm{lab}}(\mu, E, E') = C_n \sqrt{E'} \left[E_i^{\max} - \left(E^* + E' - 2\mu\sqrt{E^* E'} \right) \right]^{(3n/2)-4} \tag{6.20}$$

where μ and E' are in the laboratory system and E^* is given by:

$$E^* = E \frac{A^{\mathrm{incident}}}{\mathrm{AWR} + A^{\mathrm{exit}}}$$

and A^{incident} and A^{exit} are the mass ratios to the neutron mass of the incident and exit particles, respectively. In the general case, the range of both E' and μ is limited by the condition that the quantity in square brackets remains non-negative.

The value of E_i^{max} is a fraction of the energy available in CM,

$$E_i^{\max} = \frac{M - m_i}{M} E_a$$

where M is the total mass of the n particles being treated by this law. Note that M may be less than the total mass of the products for reactions such as:

$\alpha + {}^9\mathrm{Be} \rightarrow \mathrm{n} + 3\alpha$

where the neutron can be treated as a two-body event and the alphas by a 3-body phase-space law. The parameter M=APSX is provided so that E_i^{max} can be determined without having to process the other subsections of this section.

The energy available in CM for one-step reactions is

$$E_a = \frac{m_T}{m_p + m_T} E + Q$$

where

m_T is the target mass,

m_p is the projectile mass,

E is the energy in the LAB system, and

Q is the reaction QI value from File 3.

For two-step reactions such as the one discussed above, E_a is just the recoil energy from the first step. The following quantities are defined for LAW=6:

APSX total mass in neutron units of the n particles being treated by the law.

NPSX number of particles distributed according to the phase-space law.

Only a CONT record is given

```
[MAT, 6, MT/ APSX, 0.0,  0,  0,  0, NPSX]CONT
```

6.2.8 Laboratory Angle-Energy Law (LAW=7)

The continuum energy-angle representation (LAW=1) is good for nuclear model code results and for experimental data that have been converted to Legendre coefficients. However, since experiments normally give spectra at various fixed angles, some evaluators may prefer to enter data sorted according to (E, μ, E'), rather than the LAW=1 ordering (E, E', μ). The following quantities are defined for LAW=7:

NR, NE, E$_{int}$ normal TAB2 interpolation parameters for incident energy, E.
NRM, NMU, μ_{int} normal TAB2 interpolation parameters for emission cosine, μ.
NRP, NEP, E'$_{int}$ normal TAB1 interpolation parameters for secondary energy, E'.

The structure of a subsection is:

```
[MAT, 6, MT/ 0.0,    0.0,   0,  0,   NR,  NE/E_int]TAB2
[MAT, 6, MT/ 0.0,     E_1,   0,  0,  NRM, NMU/μ_int]TAB2
[MAT, 6, MT/ 0.0,     μ_1,   0,  0,  NRP, NEP/E'_int/
   E'_1,f(μ_1,E_1,E'_1), E'_2,f(μ_1,E_1,E'_2), -----
   ------------------------- E'_NEP,f(μ_1,E_1,E'_NEP)]TAB1
   -----------------------------------
   <repeat TAB2 structures for all the NMU emission cosines>
   -----------------------------------
   <repeat TAB2/TAB1 structures for all the NE incident energies>
   -----------------------------------
```

The distribution f(μ, E, E') is defined by equation (6.1). Emission cosine and secondary energy must be given in the laboratory system for LAW=7. Also, both variables must cover the entire angle-energy range open to the emitted particle.

6.3 Procedures

File 6 and incident charged particles are new for ENDF-6, and it will take time for detailed procedures to evolve. The following comments are intended to clarify some features of the format.

6.3.1 Elastic Scattering

According to ENDF-6 format the neutron elastic scattering is represented by giving a cross section in File 3, MT=2 (with resonance contributions in File 2) and angular distributions in File 4, MT=2. This representation is compatible with previous versions of the ENDF format.

Charged-particle elastic cross section is infinite due to the Coulomb contribution. For formal reasons MT=2 in File 3 must be present. With LPT=1 and LPT=2 representations the elastic cross section in File 3 is arbitrarily set to 1.0 at all energies. With LPT=12 and LPT=14 representation, MT=2 in File 3 contains $\sigma_{NI}(E)$ in barns. The elastic angular distributions in File 6 use LAW=5.

Whenever possible, the nuclear amplitude expansion should be used with LAW=5. Note that the a_i and b_i coefficients are not independent, being related by their mutual dependence on the nuclear scattering amplitudes, which are themselves constrained by unitarity and various conservation conditions. Thus, any attempt to fit data directly with expressions (6.13) or (6.14) would under-determine the a_i's and b_i's, giving spurious values for them. The only feasible procedure is to fit the experimental data in terms of a direct parametrization of the nuclear scattering amplitudes (phase shifts, *etc.*) and extract the a_i and b_i coefficients from them.

The second representation (LTP=2) can be used when an approximate direct fit to the experimental data is desired. The simple pole approximation for the Coulomb amplitude implied by this representation becomes increasingly poor at lower energies and smaller angles. Since the deficiencies of the approximation are masked by the dominance of the Rutherford cross section in the same region, however, one could expect a reasonable representation of the net scattering cross section at all energies and angles, provided that the coefficients C_1 are determined by fitting data *excluding* the angular region where the Rutherford cross section is dominant.

Tabulated distributions (LTP=12 or 14) are also useful for direct fits to experimental data. In this case, the choice of the cutoff cosine is used to indicate the angular region where Rutherford scattering is dominant.

Figures 6.1 and 6.2 illustrate a typical cross section computed with amplitudes and the corresponding residual cross-section representation.

6.3.2 Photons

Emitted photons are described using a subsection with ZAP=0. The spectrum is obtained as a sum of discrete photons (delta functions) and a continuum distribution packed into one LIST record. The discrete photons (if any) are given first. They are tabulated in order of decreasing energy, and their energy range may overlap the continuum. The continuum (if

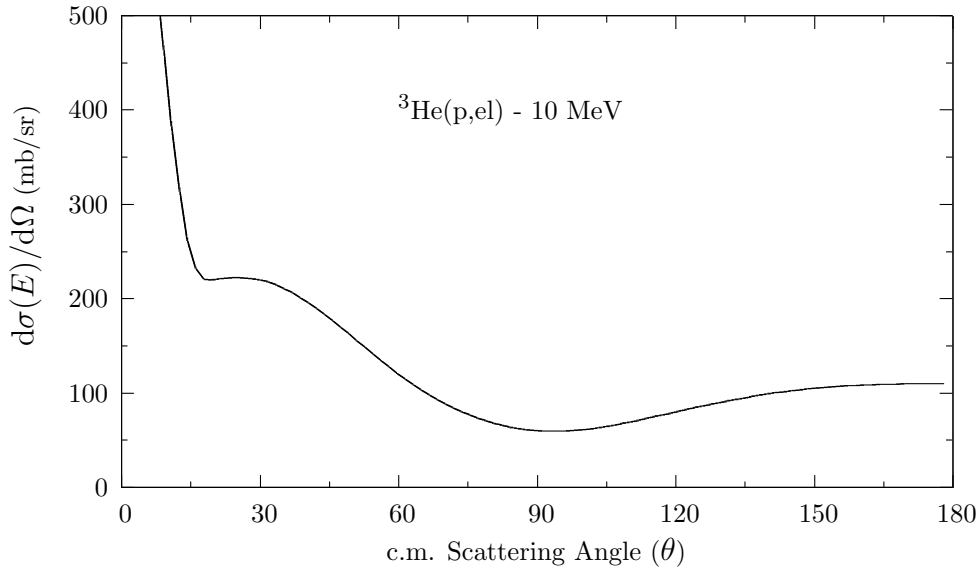

Figure 6.1: Example of Charged-Particle Elastic Scattering Cross Section

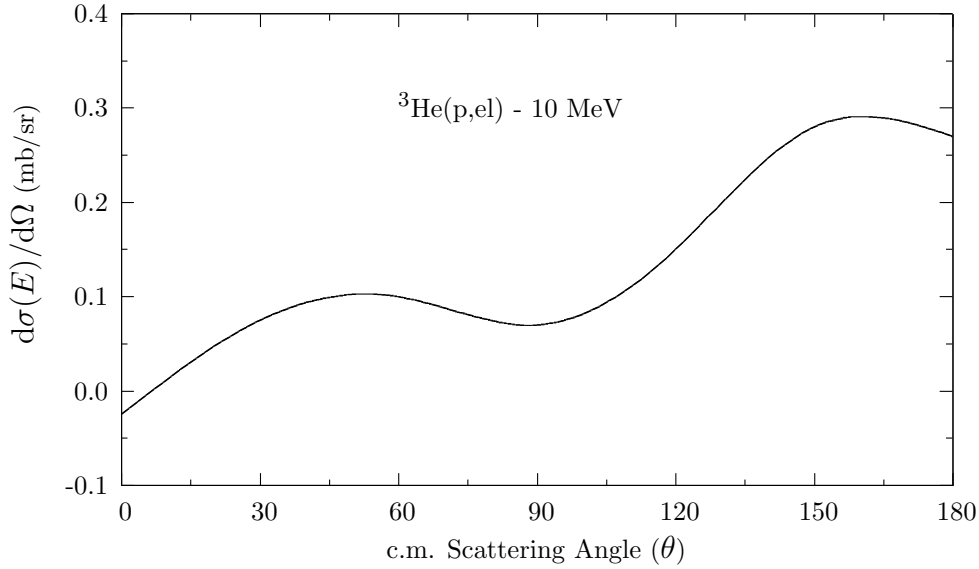

Figure 6.2: Example of Residual Cross Section for Elastic Scattering

any) is given next, and the energies must be in increasing order. Corresponding-point or unit-base interpolation is applied separately to the discrete and continuum segments of the record. A separate angular distribution can be attached to each discrete photon or to each energy of a distribution, but the isotropic form (NA=0) is usually adequate.

For a two-body discrete-level reaction, all the discrete photons produced by cascades from the given level should be included under the same reaction (MT) so that the reaction explicitly conserves energy. This scheme also gives simple energy-independent yields and simple spectra. If the level structure is not known well enough to separate the contributions to the intensity of a particular photon by reaction, the photons can be lumped together in a summation MT with the restriction that energy be conserved for the sum of all reactions.

As an example, consider the typical level structure for the reaction A(i,p)R shown in Figure 6.3. Assume that the secondary protons are described by discrete levels in MT=600-603 and a continuum in MT=649. As many discrete photons as possible should be given with their associated direct level. Thus, the production of photons arising from direct excitation of the first level should be given in MT=601 (the yield will be 1.0 in the absence of internal conversion).

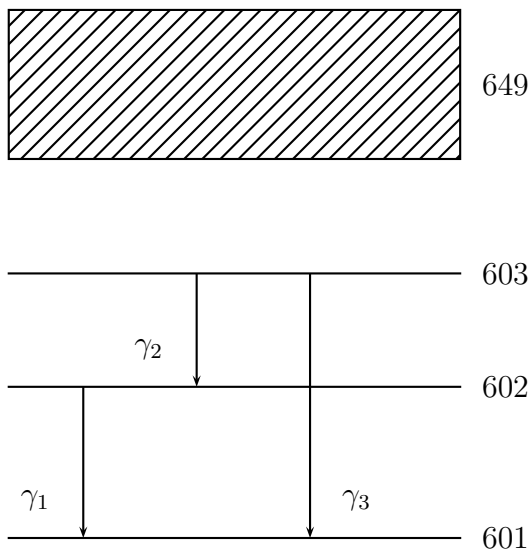

Figure 6.3: Typical Level Structure for Proton-Induced Photon Production

Photons (γ_1, γ_2, and γ_3) should be given in MT=602 using the simple constant yields computed from the branching factors and conversion ratios. This process should be continued until the knowledge of the cascades begins to get fuzzy. All the remaining production of γ_1, γ_2, γ_3, and all photons associated with higher levels (603 and 649 in this case), are then given in the redundant MT=103 using energy-dependent yields and a combination of discrete bins and a continuous distribution.

Photons produced during multi-body reactions should also be tabulated under the reaction MT number so that each reaction independently conserves energy when possible. If necessary, the photons can be lumped together under the redundant MT=3 as long as energy

is conserved for the sum of all reactions.

A special represention of primary capture photons for light isotopes is allowed using MT=102. The first subsection gives the angular distribution in the center of mass for the primary photon to the ground state using LAW=2. The next subsection gives the two-body recoil for this event using LAW=4. This is followed by a subsection giving the angular distribution for the primary photon to the first excited state and a subsection giving the corresponding recoil. The next subsection gives the energy spectrum of the gamma cascade from de-exciting this level using LAW=1, NA=0, and ND=NEP discrete photon lines. This pattern is continued until all the primary photons have been described. In each section with LAW=2, ZA=0 and the AWP field contains the energy of the primary photon. The laboratory energies and cosines for the primary gamma and its corresponding recoil particle must be computed using relativistic kinematics as described in Appendix E.

6.3.3 Particles

Isotropic or low-order distributions are often sufficient for the charged particles emitted in continuum reactions because of their short ranges. The angular distributions of emitted neutrons may be needed in more detail because of their importance in shielding calculations.

Note that the angular distributions of identical particles must be symmetric in the CM system. This is true whether the identical particles are in the entrance channel or the exit channel. Symmetry is enforced by setting all odd Legendre components to zero, or by making $p_i(\mu) = p_i(-\mu)$.

6.3.4 Neutron Emission

It is important to represent the spectrum of emitted neutrons as realistically as possible due to their importance for shielding, activation, and fission. Small emission probabilities for low-energy neutrons may acquire increased importance due to the large cross sections at low energies. However, many modern evaluations are done with nuclear model codes that represent emission in energy bins (that is, histograms). Direct use of such calculations would severely distort the effects of emitted neutrons (although the representation would be reasonable for emitted charged particles). In such cases, the evaluator should fit a realistic evaporation shape to his low-energy neutron emission and use this shape to generate additional points for the energy distribution.

6.3.5 Recoil Distributions

The energy distribution of the recoil nucleus is needed to compute radiation damage and should be provided for structural materials whenever possible. Nuclear heating depends on the average recoil energy, and an average or full distribution should be provided for all isotopes that are used in reasonable concentrations in the common applications. All recoil information can be omitted for minor isotopes that only affect activation. Recoil angular distributions are rarely needed. Particle, photon, and recoil distributions taken together should conserve energy.

To enter only recoil average energy, use NEP=1 and ND=1; the recoil spectrum becomes a delta function at the average energy. Average energy must be entered even though it can be computed from the other distributions.

At high energies, it becomes difficult to represent the recoil distribution in the center-of-mass frame, even when that frame remains appropriate for the distribution of light particles (A$\leq$ 4). In such cases, use the LCT=3 option[4], giving the light particles in the CM frame (normally with Kalbach systematics), and the heavy recoil energy spectrum as isotropic in the laboratory frame. Such isotropic distributions are normally adequate for representing energy deposition and damage.

6.3.6 Elements as Targets

Targets which are elements can be represented by using a ZA with A=0 as usual. An attempt should be made to tabulate every product of a reaction on that element.

As an example, ^{nat}Fe(n,2n) will produce ^{53}Fe and ^{54}Fe in addition to more ^{56}Fe and ^{57}Fe. The product yields in File 6 can be converted to production or activation cross sections for each of these species without having recourse to isotopic evaluations. However, it would be difficult to give a recoil spectrum for each of these nuclei in full detail. Therefore, the evaluator is allowed to give a single total recoil spectrum with ZAP=ZA, where A=0. The yield should be 1.0 and AWP should be an appropriate average recoil mass.

6.3.7 CM versus LAB Coordinate System

Some energy-angle distributions show relatively sharp features (from levels) superimposed on a smoother continuum (see Figure 6.4). If such a distribution is given in the CM system, the position of these peaks in E' is independent of the scattering angle as shown in Equation (C.5). This helps assure that the angular distribution given for each E and E' will be fairly simple. Furthermore, the E' for a given sharp peak is a linear function of incident energy E, thus the corresponding-point or unit-base interpolation schemes can be set up to follow the peak exactly. Sharp lines can be represented as delta functions as described for photons, or a more realistic width and shape can be given in tabulated form.

Therefore, the CM system should be used for representing secondary energy and scattering angle whenever relatively sharp features are found, even for reactions with three or more particles in the final state. The transformation to LAB coordinates is made by doing vector sums of the emitted particle CM velocities and the LAB velocity of the center of mass of the initial colliding system.

Experimental data are usually provided at fixed angles in the LAB system. It may often be difficult to convert the data to constant energies in the CM system as recommended by this format. However, transport calculations require data for the full range of angles and energies, and full ranges are required to get accurate values of the integrated cross sections from the experimental distributions. The most accurate way to do this process of interpolation and extrapolation is probably to model the distribution in the CM and adjust

[4] LCT=3 is only appropriate for LAW=1 .

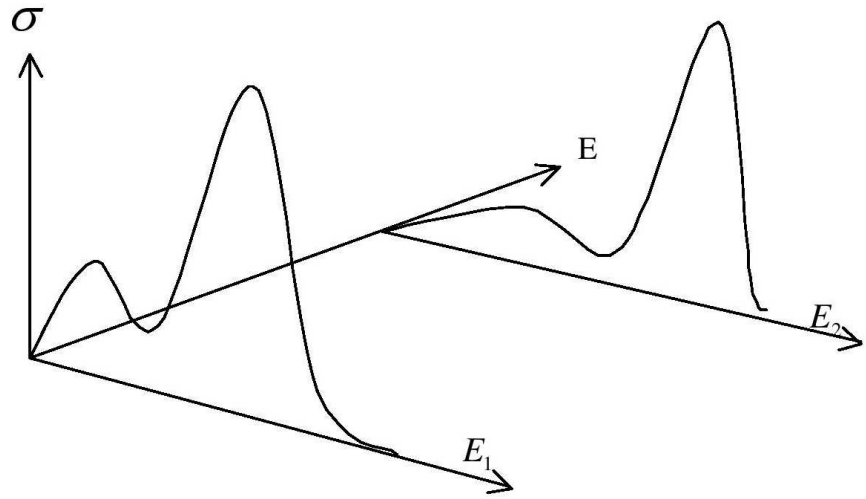

Figure 6.4: Typical Energy Spectrum Showing Levels on a Continuum

it to represent the LAB data. The numbers recommended for this format automatically arise from this process.

6.3.8 Phase Space

Comparison of experimental data with a phase-space prediction will often show overall qualitative agreement except for several broad or narrow peaks. It is desirable to represent those peaks using LAW=2 or 3. The remainder may be small enough to represent reasonably well with one of the phase-space laws.

In the absence of complete experimental data, it is recommended that the evaluator supply a phase-space distribution. This assures that energy will be conserved and gives reasonable kinematic limits on energy and angle in the laboratory system. Later comparisons between the evaluation and data may indicate possible improvements in the evaluation.

References for Chapter 6

1. C. Kalbach and F. M. Mann, *Phenomenology of continuous angular distributions. I. Systematics and parametrization*, ***Phys. Rev.***C **23** (1981) 112

2. C. Kalbach, *Systematics of Continuum Angular Distributions: Extensions to Higher Energies*, ***Phys. Rev. C*** **37** (1988) 2350

Chapter 7

File 7: THERMAL NEUTRON SCATTERING LAW DATA

7.1 General Description

File 7 contains neutron scattering data for the thermal neutron energy range ($E < 5$ eV) for moderating materials. Sections are provided for elastic (MT=2) and inelastic (MT=4) scattering. In the ENDF-6 formats, File 7 is complete in itself, and Files 3 and 4 are no longer required to obtain the total scattering cross section in the thermal energy range.

7.2 Coherent Elastic Scattering

The coherent elastic scattering from a powdered crystalline material may be represented as follows:

$$\frac{d^2\sigma}{dE'\,d\Omega}(E \rightarrow E', \mu, T) = \frac{1}{E} \sum_{i=1}^{E_i<E} s_i(T)\ \delta(\mu - \mu_i)\ \delta(E - E')/2\pi \tag{7.1}$$

where:

$$\mu_i = 1 - \frac{2E_i}{E} \tag{7.2}$$

In these formulas:

E incident neutron energy (eV),

E' secondary neutron energy (eV),

μ cosine of the scattering angle,

T moderator temperature (K),

E_i energies of the Bragg edges (eV),

s_i proportional to the structure factors (eV.barns),

μ_i characteristic scattering cosines for each set of lattice planes.

The Bragg edges and structure factors can be calculated from the properties of the crystal lattice and the scattering amplitudes for the various atoms in the unit cell.[1]

The quantity actually given in the file is:

$$S(E,T) = \sum_{i=1}^{E_i<E} S_i(T) \tag{7.3}$$

which is conveniently represented as a stairstep function with breaks at the Bragg edges using histogram interpolation.

7.2.1 Formats for Coherent Elastic Scattering

The parameters to be used to calculate coherent elastic scattering are given in a section of File 7 with MT=2. The following quantities are defined:

ZA, AWR Standard charge and mass parameters.

LTHR Flag indicating which type of thermal data is being represented. LTHR=1 for coherent elastic scattering.

T_i Temperature (K).

LT Flag for temperature dependence. The data for the first temperature are given in a TAB1 record. The data for subsequent LT temperatures are given in LIST records using the same independent variable grid as the TAB1 record.

LI Flag indicating how to interpolate between the previous temperature and current temperature. The values are the same as for INT in standard TAB1 records.

NR, $\mathbf{E}_{int}$ Standard TAB1 interpolation parameters. Use INT=1 (histogram).

NP Number of Bragg edges given.

The structure of a section is

```
[MAT, 7, 2/ ZA, AWR, LTHR, 0,  0,  0] HEAD   LTHR=1
[MAT, 7, 2/ T0, 0.0,   LT, 0, NR, NP/ Eint / S(E,T0) ] TAB1
[MAT, 7, 2/ T1, 0.0,   LI, 0, NP,  0/ S(Ei,T1) ] LIST
  ----------------------------
  <repeat LIST for T2, T3, ...TLT>
  --------------------------
[MAT, 7, 0/0.0, 0.0,    0, 0,  0,  0] SEND
```

[1] As an example, the HEXSCAT code [Ref. 1] can be used for hexagonal crystal lattices.

7.2.2 Procedures for Coherent Elastic Scattering

The coherent elastic scattering cross section is easily computed from $S(E,T)$ by reconstructing an appropriate energy grid and dividing S by E at each point on the grid. A discontinuity should be supplied at each E_i, and log-log interpolation should be used between Bragg edges. The cross section is zero below the first Bragg edge.

The function $S(E,T)$ should be defined up to 5 eV. When the Bragg edges get very close to each other (above 1 eV), the "stair steps" are small. It is permissible to group edges together in this region in order to reduce the number of steps given while still preserving the average value of the cross section. Either discrete angle or Legendre representations of the angular dependence of coherent elastic scattering can be constructed. It is necessary to recover the values of $s_i(T)$ from $S(E,T)$ by subtraction.

7.3 Incoherent Elastic Scattering

Elastic scattering can be treated in the incoherent approximation for partially ordered systems such as ZrH_x and polyethylene. The differential cross section is given by:

$$\frac{d^2\sigma}{dE'\,d\Omega}(E \to E', \mu, T) = \frac{\sigma_b}{4\pi}\, e^{-2EW'(T)(1-\mu)}\ \delta(E - E') \tag{7.4}$$

where:

σ_b is the characteristic bound cross section (barns),

W' is the DebyeWaller integral divided by the atomic mass (eV^{-1}),

and all the other symbols have their previous meanings. The integrated cross section is easily obtained:

$$\sigma(E) = \frac{\sigma_b}{2}\left(\frac{1 - e^{-4EW'}}{2EW'}\right) \tag{7.5}$$

Note that the limit of σ for small E is σ_b.

7.3.1 Format for Incoherent Elastic Scattering

The parameters for incoherent elastic scattering are also given in a section of File 7 with MT=2, because coherent and incoherent representations never occur together for a material. The following quantities are defined:

ZA, AWR Standard charge and mass parameters.

LTHR Flag indicating which type of thermal data is being represented. LTHR=2 for incoherent elastic scattering.

NP Number of temperatures.

SB characteristic bound cross section (barns)

$W'(T)$ Debye-Waller integral divided by the atomic mass (eV^{-1}) as a function of temperature (K).

The structure of a section is

```
[MAT, 7, 2/  ZA, AWR, LTHR, 0,  0,  0]HEAD   (LTHR=2)
[MAT, 7, 2/  SB, 0.0,    0, 0, NR, NP/ T_int / W'(T) ]TAB1
[MAT, 7, 0/ 0.0, 0.0,    0, 0,  0,  0] SEND
```

7.3.2 Procedures for Incoherent Elastic Scattering

This formalism can be used for energies up to 5 eV.

For some moderator materials containing more than one kind of atom, the incoherent elastic cross section is computed as the sum of contributions from two different materials. As an example, H in ZrH_x is given in MAT 0007, and Zr in ZrH_x is given in MAT 0058.

7.4 Incoherent Inelastic Scattering

Inelastic scattering is represented by the thermal neutron scattering law, $S(\alpha, \beta, T)$, and is defined for a moderating molecule or crystal by:

$$\frac{d^2\sigma}{d\Omega\, dE'}(E \to E', \mu, T) = \sum_{n=0}^{\mathrm{NS}} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S_n(\alpha, \beta, T) \tag{7.6}$$

where (NS+1) types of atoms occur in the molecule or unit cell (*i.e.*, for H_2O, NS=1) and

M_n Number of atoms of n-type in the molecule or unit cell

T Moderator temperature (K)

E Incident neutron energy (eV)

E' Secondary neutron energy (eV)

β Energy transfer, $\beta = (E' - E)/kT$

α Momentum transfer, $\alpha = \left[E' + E - 2\mu\sqrt{EE'}\right] / A_0 kT$

A_n Mass of the nth type atom

A_0 Mass of the principal scattering atom in the molecule

σ_{fn} Free atom scattering cross section of the nth type atom

$$\sigma_{bn} = \sigma_{fn} \left(\frac{A_n + 1}{A_n}\right)^2 \tag{7.7}$$

k Boltzmann's constant (see Appendix H)

μ Cosine of the scattering angle (in the lab system)

The data in File 7 for any particular material contain only the scattering law for the principal scatterer, $S(\alpha, \beta, T)$, *i.e.*, the 0th atom in the molecule. These data are given as an arbitrary tabulated function. The scattering properties for the ***other atom types*** (n=1,2,...,NS) are represented by ***analytical functions***. Note that the scattering properties of all atoms in the molecule may be represented by analytical functions. In this case there is no principal scattering atom.

In some cases, the scattering properties of other atom types in a molecule or crystal may be described by giving $S_0(\alpha, \beta, T)$ in another material. As an example, H in ZrH_x and Zr in ZrH_x are given in separate MATs.

For high incident energies, α and/or β values may be required that are outside the ranges tabulated for $S(\alpha, \beta)$. In these cases, the short-collision-time (SCT) approximation should be used as follows:

$$S^{\mathrm{SCT}}(\alpha, \beta, T) = \frac{\exp\left[-\frac{(\alpha-|\beta|)^2 T}{4\alpha T_{\mathrm{eff}}(T)} - \frac{|\beta|}{2}\right]}{\sqrt{4\pi\alpha\frac{T_{\mathrm{eff}}(T)}{T}}} \tag{7.8}$$

where $T_{eff}(T)$ is the effective temperature, and the other symbols have their previous meanings.

The constants required for the scattering law data and the analytic representations for the non-principal scattering atoms are given in an array, B(N), N=1,2,...,NI, where NI=6(NS+1). Six constants are required for each atom type (one 80-character record). The first six elements pertain to the principal scattering atom, n=0.

The elements of the array B(N) are defined as:

B(1) $M_0 f_0$, the total free atom cross section for the principal scattering atom. If B(1) = 0.0, there is no principal scattering atom and the scattering properties for this material are completely described by the analytic functions for each atom type in this material.

B(2) ϵ, the value of E/kT above which the static model of elastic scattering is adequate (total scattering properties may be obtained from MT=2 as given in File 2 or 3 and File 4 of the appropriate materials).

B(3) A_0, the ratio of the mass of the atom to that of the neutron that was used to compute α.

$$\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{A_0 kT}$$

B(4) E_{max}, the upper energy limit for the constant σ_{f0} (upper energy limit in which $S_0(\alpha, \beta, T)$ may be used).

B(5) not used.

B(6) M_0, the number of principal scattering atoms in the material. (For example, M = 2 for H in H_2O).

The next six constants specify the analytic functions that describe the scattering properties of the first non-principal scattering atom, (n=1); *i.e.*, for H_20, this atom would be oxygen if the principal atom were hydrogen.

B(7) a_1, a test indicating the type of analytic function used for this atom type.
$a_1 = 0.0$, use the atom in SCT approximation only (see below).
$a_1 = 1.0$, use a free gas scattering law.
$a_1 = 2.0$, use a diffusive motion scattering law.

B(8) $M_1\sigma_{f1}$, the total free atom cross section for this atom type.

B(9) A_1, effective mass for this atom type.

B(10) not used.

B(11) not used.

B(12) M_1, the number of atoms of this type in the molecule or unit cell.

The next six constants, B(13) through B(18), are used to describe the second non-principal scattering atom (n=2), if required. The constants are defined in the same way as for n=1; *e.g.*, B(13) is the same type of constant as B(7).

A mixed $S(\alpha, \beta)$ method has sometimes been used. Using BeO as an example, the $S(\alpha, \beta)$ for Be in BeO is combined with that for O in BeO and adjusted to the Be free atom cross section and mass as a reference. The mixed $S(\alpha, \beta)$ is used for the principal atom in equation (7.6) as if NS were zero. However, ***all*** of the NS+1 atoms are used in the SCT contribution to the cross section.

The scattering law is given by $S(\alpha, \beta, T)$ for a series of β values. For each β value, the function versus β is given for a series of temperatures. Thus, the looping order is actually first β, then T, then α. $S(\alpha, \beta)$ is normally a symmetric function of β and only positive values are given. For ortho and parahydrogen and deuterium, this is no longer true. Both negative and positive values must be given in increasing value of β and the flag LASYM is set to one.

In certain cases, a more accurate temperature representation may be obtained by replacing the value of the actual temperature, T, that is used in the definition of α and β with a constant, T_0 ($T_0 = 0.0253$ eV or the equivalent depending on the units of Boltzmann's constant). A flag (LAT) is given for each material to indicate which temperature has been used in generating the $S(\alpha, \beta)$ data.

For down-scattering events with large energy losses and for low temperatures, β can be large and negative. The main contribution to the cross section comes from the region near $\alpha + \beta = 0$. Computer precision can become a real problem in these cases. As an example, for water at room temperature, calculations using equation (7.6) for incident neutrons at 4 eV

require working with products like $e^{80} \times 10^{-34}$. For liquid hydrogen at 20 Kelvin and for 1 eV transfers, the products can be $e^{300} \times 10^{-130}$. These very large and small numbers are difficult to handle on most computers, especially 32-bit machines. The LLN flag is provided for such cases: the evaluator simply stores $\ln S$ instead of S and changes the interpolation scheme accordingly (that is, the normal log-log law changes to log-lin). Values of $S = 0.0$ like those found in the existing ENDF/B-III thermal files really stand for some very small number less than 10^{-32} and should be changed to some large negative value, such as -999.

7.4.1 Formats for Incoherent Inelastic Scattering

The parameters for incoherent inelastic scattering are given in a section of File 7 with MT=4. The following quantities are defined:

LAT Flag indicating which temperature has been used to compute α and β
LAT=0, the actual temperature has been used.
LAT=1, the constant $T_0 = 0.0253$ eV has been used.

LASYM Flag indicating whether an asymmetric $S(\alpha, \beta)$ is given
LASYM=0, S is symmetric.
LASYM=1, S is asymmetric

LLN Flag indicating the form of $S(\alpha, \beta)$ stored in the file
LLN=0, S is stored directly.
LLN=1, $\ln(S)$ is stored.

NS Number of non-principal scattering atom types. For most moderating materials there will be (NS+1) types of atoms in the molecule (NS$\leq$ 3).

NI Total number of items in the $B(N)$ list. NI=6(NS+1).

$B(N)$ List of constants. Definitions are given above (Section 7.4).

NR Number of interpolation ranges for a particular parameter, either β or α .

LT Temperature dependence flag. The data for the first temperature are given in a TAB1 record, and the data for the LT subsequent temperatures are given in LIST records using the same α grid as for the first temperature.

LI Interpolation law to be used between this and the previous temperature. Values of LI are the same as those specified for INT in a standard TAB1 interpolation table.

NT Total number of temperatures given. Note that NT = LT+1.

T_{eff0} Table of effective temperatures (K) for the shortcollision-time approximation given as a function of moderator temperature T(K) for the principal atom.

T_{eff1},T_{eff2}, T_{eff3} Table for effective temperatures for the first, second, and third non-principal atom. Given if $a_1 = 0.0$ only.

NB Total number of β values given.

NP Number of α values given for each value of β for the first temperature described, NP is the number of pairs, α and $S(\alpha, \beta)$, given.

$\beta_{int}, \alpha_{int}$ Interpolation schemes used.

The structure of a section is

```
[MAT, 7, 4 /  ZA, AWR,   0, LAT, LASYM,  0]HEAD
[MAT, 7, 4 / 0.0, 0.0, LLN,   0,    NI, NS/B(N) ] LIST
[MAT, 7, 4 / 0.0, 0.0,   0,   0,    NR, NB/β_int] TAB2
[MAT, 7, 4 /  T_0,  β_1,  LT,   0,    NR, NP/ α_int / S(α,β_1,T_0) ] TAB1
[MAT, 7, 4 /  T_1,  β_1,  LI,   0,    NP,  0/ S(α,β_1,T_1) ] LIST
   ------------------------------
<continue with LIST records for T_2,T_3,...T_LT+1>
------------------------------
[MAT, 7, 4 / T_0, β_2, LT, 0, NR, NP/ α_int / S(α,β_2,T_0) ] TAB1
------------------------------
<continue with TAB1 and LIST records for remaining values of β and
T >
------------------------------
[MAT, 7, 4 / 0.0, 0.0, 0, 0, NR, NT/ T_int / T_eff0(T) ] TAB1
   ------------------------------
<continue with TAB1 records for T_eff1, T_eff2 and/ or T_eff3 if the
corresponding value of a_1, a_2, or a_3 in B(7), B(13), or B(19) is zero>
   ------------------------------
[MAT, 7, 0 / 0.0, 0.0, 0, 0, 0, 0] SEND
```

If the scattering law data are completely specified by analytic functions (no principal scattering atom type, as indicated by B(1)=0), tabulated values of $S(\alpha, \beta)$ are omitted and the TAB2 and TAB1 records are not given.

7.4.2 Procedures for Incoherent Inelastic Scattering

The data in MF=7, MT=4 should be sufficient to describe incoherent inelastic scattering for incident neutron energies up to 5 eV. The tabulated $S(\alpha, \beta)$ function should be useful to energies as high as possible in order to minimize the discontinuities that occur when changing to the short-collisiontime approximation. The β mesh for $S(\alpha, \beta)$ should be selected in such a manner as to accurately represent the scattering properties of the material with a minimum of β points. The α mesh at which $S(\alpha, \beta)$ is given should be the same for each β value and for each temperature.

Experience has shown that temperature interpolation of $S(\alpha, \beta)$ is unreliable. It is recommended that cross sections be computed for the given moderator temperatures only. Data for other temperatures should be obtained by interpolation between the ***cross sections***.

References for Chapter 7

1. Y.D. Naliboff and J.V. Koppel, *HEXSCAT:Coherent Scattering of Neutrons by Hexagonal Lattices*, General Atomic report **GA6026** (1964).

Chapter 8

File 8: RADIOACTIVE DECAY AND FISSION PRODUCT YIELD DATA

8.1 General Description

Information concerning the decay of the reaction products (any MT) is given in this file. In addition, fission product yield data (MT=454 and 459) for fissionable materials (see Section 8.3) and spontaneous radioactive decay data (MT=457) for the nucleus (see Section 8.4) are included. See descriptions of File 9 and File 10 for information on isomeric state production from the various reactions. Since a reaction may result in more than one unstable end product, data for the most important product should be entered, while others are allowed.

8.2 Radioactive Nuclide Production

For any isotope, sections for reactions defined by the MT number may be given, which specify that the end product from the interaction of any incident particle or photon is radioactive. The end-products of the reaction are identified by the ZAP (ZA for the product), and noting how these end products decay. A section will contain only minimal information about the chain that follows each reaction. One or more isomeric states of the target or the radioactive end product isotope will be described.

The following quantities are defined:

ZA Designation of the original nuclide (ZA = $1000Z + A$).

ZAP Designation of the nuclide produced in the reaction (ZAP = $1000Z + A$).

NS Total number of states (LFS) of the radioactive reaction product for which decay data are given.

LMF File number (3, 6, 9, or 10) in which the multiplicity or cross section for this MT number will be found.

LIS State number (including ground and all levels) of the target (ZA).

LISO Isomeric state number of the target.

LFS Level number (including ground and all levels) of the state of ZAP formed by the neutron interaction (to be given in ascending order).

ELFS Excitation energy of the state of ZAP produced in the interaction (in eV above ground state).

NO Flag denoting where the decay information is to be given for an important radioactive end product.
NO = 0, complete decay chain given under this MT.
NO = 1, decay chain given in MT = 457 in the decay data file.

ND Number of branches into which the nuclide ZAP decays.

HL half-life of the nuclide ZAP in seconds.

ZAN Z and mass identifier of the next nuclide produced along the chain.

BR Branching ratio for the production of that particular ZAN and level.

END Endpoint energy of the particle or quantum emitted (this does not include the gamma energy, following beta decay, for example).

CT Chain terminator that gives minimal information about the formation and decay of ZAN. The hundredths digit of CT designates the excited level in which ZAN is formed.

- $1.0 \leq$ CT < 2.0 indicates that the chain terminates with ZAN, possibly after one or more gamma decays.
- CT $\geq$ 2.0 indicates that ZAN is unstable and decays further to other nuclides. For example, consider the nuclide (ZAP) formed via a neutron reaction (MT number) in a final state (LFS number); ZAP then decays to a level in ZAN; the level number is part of the CT indicator and includes non-isomeric states in the count.

The following examples may help explain the use of CT:

CT = 1.00, ZAN was formed in the ground state which is stable.

CT = 1.06, ZAN was formed in the sixth excited state; the sixth state decayed to the ground state which is stable.

CT = 2.00, ZAN was formed in the ground state which is unstable. (No delayed gammas are associated with the formation and decay of this particular ZAN). The next decay in the chain is specified under the RTYP.

CT = 2.11, ZAN was formed in the 11th excited state but the chain does not terminate with that ZAN. The next decay in the chain is specified under the RTYP.

It is readily apparent from the above that CT = "1." indicates that the chain terminates with that particular ZAN and CT = "2." means that one or more decays are involved before stability is reached. Note, however, that stability can be reached ***instantaneously*** upon occasion with the emission of one or more light particles.

RTYP Mode of decay using the same definitions specified in MT=457 (see Section 8.4).
As an example, consider MT=102. Then RTYP = 1.44 would be interpreted as follows:
The first two columns of the RTYP (1.) indicates β^- decay of ZAP; the third and fourth columns (44) indicate that the nucleus ZAN (formed in the β^- decay) then immediately emits two α particles.
This example is represented by the following reaction:

$$\begin{array}{l} \mathrm{n} + {}^{7}\mathrm{Li} \rightarrow \gamma + {}^{8}\mathrm{Li}\ (\text{ground state}) \\ \qquad\qquad\qquad\qquad \beta^- \qquad\qquad\qquad\qquad (\mathrm{MT}{=}102) \\ \qquad\qquad\qquad\qquad\quad \searrow \\ \qquad\qquad\qquad\qquad\quad \underline{2.94\ 2^+{,}0} \\ \qquad\qquad\qquad\qquad\quad {}^{8}\mathrm{Be} \\ \qquad\qquad\qquad\qquad\qquad\quad \searrow \\ \qquad\qquad\qquad\qquad\qquad\quad 2\alpha \end{array}$$

For this example:

ZA(^{7}Li)	= 3007	LIS(^{7}Li)	= 0	LISO(^{7}Li)	= 0
ZAP(^{8}Li)	= 3008	LFS(^{8}Li)	= 0		
ZAN(^{8}Be)	= 4008	CT(^{8}Be)	= 2.01		

Since Be has a half-life of the order of compound-nucleus formation times, decay data for MT=457 are not required, and the complete chain can easily be represented and read from the information given here.

8.2.1 Formats

The structure of each section always starts with a HEAD record and ends with a SEND record. Subsections contain data for a particular final state of the reaction product (LFS).

The number of subsections NS is given on the HEAD record for the section. The subsections are ordered by increasing value of LFS. The structure of a section is:

```
[MAT, 8, MT/ ZA, AWR, LIS, LISO, NS, NO] HEAD
   <subsection for LFS1>
   <subsection for LFS2>
   ---------------------------------
   <subsection for LFSNS >
[MAT, 8, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

For NO=0 the structure of the subsection is:

```
[MAT, 8, MT/ ZAP, ELFS, LMF, LFS, 6*ND, 0/
   HL1, RTYP1, ZAN1, BR1, END1, CT1,
   HL2, RTYP2, ZAN2, BR2, END2, CT2,
   --------------------------------
   HLND,RTYPND,ZANND,BRND, ENDND, CTND] LIST
```

If NO=1, then the reaction gives rise to a significant product which is radioactive, and the evaluator wishes only to identify the radioactive product. The evaluator must supply MF=8, MT=457 data elsewhere to describe the decay of the product. It is understood that the cross section for producing this radioactive product can be determined from the data in File 3, 6, 9, or 10 depending upon the value of LMF.

For NO=1, the structure of the subsection is:

```
[MAT, 8, MT/ ZAP, ELFS, LMF, LFS, 0, 0] CONT
```

8.2.2 Procedures

1. Data should be given for all ***unstable*** states of the reaction product nucleus for which cross sections are given in File 3 or File 10 or multiplicities in File 6 or File 9. No information of this type is allowed in evaluations for mixtures of elements, molecules, or elements with more than one naturally occurring isotope.

2. In order to provide more general usefulness as these files are being constructed, the following procedures are mandatory. For each reaction type (MT), File 6 yields, File 9 multiplicities, or File 10 cross sections must be provided, except when LMF=3.

3. If the ENDF file also contains a complete evaluation of the neutron cross sections for the reaction product nucleus (ZAP, LIS), then the radioactive decay data for the evaluation of (ZAP, LIS) found in MF=8, MT=457 must be consistent with the decay data in this section.

4. The method for calculating the nuclide production cross section is determined by the choice of LMF:

   LMF=3 implies that the production cross section is taken directly from the corresponding sections in File 3.

   LMF=6 implies that the production cross section is the product of the cross section in File 3 and the yield in File 6.

LMF=9 implies that the production cross section is the product of the cross section in File 3 and the multiplicity in File 9.

LMF=10 implies that the production cross section is given explicitly in File 10 (in barns).

8.3 Fission Product Yield Data (MT=454, MT=459)

MT numbers 454 and 459 specify the energy-dependent fission product yield data for each incident particle or photon. These MT numbers can also be used to identify yields for spontaneous fission. A complete set of fission product yield data is given for a particular incident particle energy. Data sets should be given at sufficient incident energies to completely specify yield data for the energy range given for the fission cross section (as determined from Files 2 or 3). These data are given by specifying fission product identifiers and fission product yields.

MT=454 is used for independent yields (YI), and MT=459 is used for cumulative yields (YC). The formats for MT=454 and MT=459 are identical. Independent yields (YI) are direct yields per fission prior to delayed neutron, beta, *etc.*, decay. The sum of all independent yields is 2.0 for any particular incident particle energy, when light charged particles are ignored (*e.g.* ^{1}H, ^{2}H, ^{3}H, ^{3}He and ^{4}He). Cumulative yields (YC) are specified for the same set of fission products. These account for all decay branches, including delayed neutrons.

The fission products are specified by giving an excited state designation (FPS) and a (charge, mass) identifier (ZAFP). Thus, fission product nuclides are given, not mass chains. More than one (Z,A) may be used to represent the yields for a particular mass chain.

The following quantities are defined

NFP Number of fission product nuclide states to be specified at each incident energy point (this is actually the number of sets of fission product identifiers fission product yields). (NFP$\leq$ 2500).

ZAFP (Z,A) identifier for a particular fission product. (ZAFP = $(1000Z + A)$).

FPS State designator (floating-point number) for the fission product nuclide (FPS = 0.0 means the ground state, FPS=1.0 means the first excited state, *etc.*)

YI (MT=454), independent yield for a particular fission product prior to particle decay.

DYI (MT=454) 1σ uncertainty in YI.

YC (MT=459) cumulative yield.

DYC (MT=459) 1σ uncertainty in YC.

$C_n(E_i)$ Array of yield data for the ith energy point. This array contains NFP sets of four parameters in the order ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT=459.

NN Number of items in the $C_n(E_i)$ array, equal to 4*NFP.

E_i Incident particle energy of the ith point (eV).

LE Test to determine whether energy-dependent fission product yields given:

- LE=0 implies no energy-dependence (only one set of fission product yield data given);
- LE>0 indicates that (LE+1) sets of fission product yield data are given at (LE+1) incident particle energies.

I_i Interpolation scheme (see paragraph on Two-dimensional Interpolation Schemes in Section 0.5.2) to be used between the E_{i-1} and E_i energy points.

8.3.1 Formats

The structure of a section always starts with a HEAD record and ends with a SEND record. Sets of fission product yield data are given for one or more incident energies. The sets are ordered by increasing incident energy. For a particular energy the data are presented by giving four parameters (ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT 459) for each fission product state. The data are first ordered by increasing values of ZAFP. If more than one yield is given for the same (Z,A) the data are ordered by increasing value of the state designator (FPS). The structure for a section is:

```
[MAT, 8, MT/ ZA, AWR, LE+1, 0,  0,   0]HEAD
[MAT, 8, MT/ E1, 0.0,   LE, 0, NN, NFP/ Cn(E1) ]LIST
[MAT, 8, MT/ E2, 0.0,    I, 0, NN, NFP/ Cn(E2) ]LIST
[MAT, 8, MT/ E3, 0.0,    I, 0, NN, NFP/ Cn(E3) ]LIST
  -------------------------
[MAT, 8, 0 /0.0, 0.0,    0, 0,  0,   0]SEND
```

where MT=454 for independent yield data, and MT=459 for cumulative yield data. There are (LE+1) LIST records.

8.3.2 Procedures

The data sets for fission product yields should be given over the same energy range as that used in Files 2 and/or File 3 for the fission cross section. The yields are given as a fractional value at each energy, and the independent yields (ignoring light charged particle yields) will sum to 2.0.

This format provides for the yields (YI or YC) to each excited state (FPS) of the nuclide designated by ZAFP, and hence accommodates the many metastable fission products having direct fission yields. Data may be given for one or more fission product nuclide states to represent the yield for a particular mass chain. If independent yield data are given for more than one nuclide, the yield for the lowest Z (charge) nuclide state for a particular mass chain should be the same as the cumulative yield in MT=459, and all other independent yields for this same chain should be direct yields.

The direct fission product yields are those prior to delayed neutron emission; for this reason, the summation of independent yields over the nuclides in each mass chain does ***not*** necessarily equal the isobaric chain yield.

The cumulative yields in MT=459 for each nuclide (ZAFP, FPS) should be consistent with the decay branching fractions in MT=457 and the independent yields in MT=454. It should be noted that the main use of cumulative yields is to carry out calculations without solving the full decay equations. Several extremely long-lived fission products exist that have non-isobaric decay modes (*e.g.* alpha decay). If these are included in the calculation of their daughter products cumulative yields, the yields will be larger that seen in practice. Some evaluators omit nuclides with long half-lives from the cumulative yield of their daughter-products[1] The users should be careful about the interpretation of cumulative yield data.

Yields for the same fission product nuclides should be given at each energy point. This will facilitate interpolation of yield data between incident energy points. Also, a linear-linear interpolation scheme should be used.

8.4 Radioactive Decay Data (MT=457)

The spontaneous radioactive decay data are given in Section 457. This section is restricted to single nuclides in their ground state or an isomeric state. (An isomeric state is a "long-lived" excited state of the nucleus.) The main purpose of MT=457 is to describe the energy spectra resulting from radioactive decay and give average parameters useful for applications such as decay heat, waste disposal, depletion and buildup studies, shielding, and fuel integrity. The information in this section can be divided into three parts:

a.) General information about the material

ZA Designation of the original (radioactive) nuclide (ZA=$1000Z + A$).

AWR Ratio of the LIS state nuclide mass to that of neutron.

LIS State of the original nuclide (LIS=0, ground state, LIS=1, first excited state, *etc.*)

LISO Isomeric state number for the original nuclide (LISO=0, ground state; LISO=1, first isomeric state; *etc.*)

NST Nucleus stability flag (NST=0, radioactive; NST=1, stable)

[1] The JEFF-3.1 evaluator oxcluded nuclides with half-lives greater than 10^{13} seconds (0.32 million years).

$T_{1/2}$ half-life of the original nuclide (seconds).

NC Total number of decay energies (eV) given (NC = 3 or 17).

$\overline{E}_x$ Average decay energy (eV) of radiation x, *e.g.*, for decay heat applications. The average energies must be given in an order specified in Section 8.4.2 Unknown average radiation energies are indicated by a value of -1.0.

SPI Spin of the nuclide in its LIS state.
(SPI=-77.777 implies spin unknown)

PAR Parity of the nuclide in its LIS state (±1.0).

b.) Decay mode information for each mode of decay

NDK Total number of decay modes given.

RTYP Mode of decay of the nuclide in its LIS state.

Decay modes are defined as follows:

RTYP		**Decay Mode**
0.	γ	γ-ray (not used in MT457)
1.	β	Beta decay
2.	e.c., β^+	Electron capture and/or positron emission
3.	IT	Isomeric transition (will in general be present only when the state being considered is an isomeric state)
4.	α	Alpha decay
5.	n	Neutron emission (***not*** *delayed neutron decay*, see below)
6.	SF	Spontaneous fission
7.	p	Proton emission
10.		Unknown origin

Multiple particle decay is also allowed using any combination of the above RTYP variables as illustrated in the following examples:

RTYP		**Decay Mode**
1.5	β^-,n	Beta decay followed by neutron emission (*delayed neutron decay*)
1.4	β^-,α	Beta decay followed by alpha emission (*e.g.* ^{16}N decay)
2.4	β^+,α	Positron decay followed by alpha emission.

RFS Isomeric state flag for daughter nuclide.
RFS=0.0, ground state;
RFS=1.0, first isomeric state, *etc.*

Q Total decay energy (eV) available in the corresponding decay process. This is not necessarily the same as the maximum energy of the emitted radiation. In the case of an isomeric transition Q will be the energy of the isomeric state. For both β^+ and β^-, Q equals the energy corresponding to the mass difference between the initial and final atoms).

BR Fraction of the decay of the nuclide in its LIS state which proceeds by the corresponding decay mode, *e.g.*, if only β^- occurs and no isomeric states in the daughter nucleus are excited then BR=1.0 for β^- decay.

c.) Resulting radiation spectra

NSP Total number of radiation types (STYP) for which spectral information is given (NSP may be zero).

STYP Decay radiation type

Decay radiations are defined as follows:

STYP		Radiation type
0.	γ	Gamma rays
1.	β^-	Beta rays
2.	e.c. β^+	Electron capture and/or positron emission
4.	α	Alpha particles
5.	n	Neutrons
6.	SF	Spontaneous fission fragments
7.	p	Protons
8.	e^-	"Discrete electrons"
9.	x	X-rays and annihilation radiation (photons not arising as transitions between nuclear states)

ER discrete energy (eV) of radiation produced($E_\gamma, E_\beta, E_{e.c.}$, *etc.*)

RI intensity of discrete radiation produced (relative units).

RP spectrum of the continuum component of the radiation in units of probability/eV such that $\int \mathrm{RP}(E)dE = 1$.

TYPE Type of transition for beta and electron capture.

Types Defined:

TYPE	Spectrum Definition
0.0	Not required for STYP
1.0	Allowed, non-unique
2.0	First-forbidden unique
3.0	Second-forbidden unique

RICC Total internal conversion coefficient (STYP=0.0 only)

RICK K-shell internal conversion coefficient (STYP=0.0 only)

RICL L-shell internal conversion coefficient (STYP=0.0 only)

RIS Internal pair formation coefficient (STYP=0.0)
STYP=2.0, positron intensity,
STYP=0.0 otherwise.

LCON [2] Continuum spectrum flag
LCON=0, no continuous spectrum given
LCON=1, only continuous spectrum given
LCON=2, both discrete and continuum spectra.

NT Number of entries given for each discrete energy (ER).

FC Continuum spectrum normalization factor (absolute intensity/relative intensity).

FD Discrete spectrum normalization factor (absolute intensity/relative intensity).

NER Total number of tabulated discrete energies for a given spectral type (STYP).

ER$_{AV}$ [3] Average decay energy of radiation produced.

NR Number of interpolation ranges for the continuum spectrum.

NP Number of points at which the distribution is given.

E$_{int}$ Interpolation scheme for the continuum spectrum.

NK Number of partial energy distributions when LCON = 5 is used.

Δ Uncertainty in any quantity.

[2] RTYP=6.0 , STYP=5.0, spontaneous fission neutron spectra: FC=$\overline{\nu}$ total for LCON=1; FC=$\overline{\nu_p}$, FD=$\overline{\nu_d}$ for LCON=2.

[3] For STYP=2, this is the average positron energy; for STYP=4, this includes energy of recoil nucleus.

LCOV Flag indicating whether covariance data are given for continuum spectrum data. (LCON=1 or 2).
LCOV=0, no covariance data given.
LCOV=1, covariance data given.

LB Flag indicating the meaning of the numbers given in the array {E_k,F_k}. (Only LB=2 presently allowed, See chapter 33).

NPP Number of pairs of numbers in the {E_k,F_k} array.

The array {E_k,F_k} contains pairs of numbers, referred to as an E_k table. In each E_k table the first member of a pair is an energy, E_k, the second member of the pair, F_k, is a number associated with the energy interval between the two entries E_k and E_{k+1}.

The E_k table must cover the complete range of secondary particle energies. Some of the F_k's may be zero, as must be the case below threshold for a threshold reaction, and the last value of F_k in an E_k table must be zero or blank since it is not defined.

The F_k values in the E_k table for the allowed LB=2 representation are fractional components of the covariance matrix, fully correlated over all E_k intervals:

$$\mathrm{Cov}(X_i, X_j) = \sum_{k,k'} S_i^k \; S_j^{k'} \; F_k \; F_{k'} \; X_i \; X_j$$

where $S_i^k = 1$ when the energy E_i is in the interval E_k to E_{k+1} of the E_k table,
0 otherwise.

Here X_i is the normalized spectral intensity at decay particle emitted kinetic energy range E_i obtained from the {E,RP} TAB1 record indicated.

8.4.1 Formats

The structure of this section always starts with a HEAD record and ends with a SEND record. For a radioactive nucleus (NST=0), this section is divided into subsections as follows[4]:

```
[MAT, 8,457/  ZA,   AWR, LIS, LISO,   NST, NSP]HEAD    (NST=0)
[MAT, 8,457/ T1/2, ΔT1/2,   0,    0,  2*NC,   0/(Ex,ΔEx) / LIST
[MAT, 8,457/ SPI,   PAR,   0,    0, 6*NDK, NDK/
         RTYP1, RFS1, Q1, ΔQ1, BR1, ΔBR1,
         ---------------------------------
         RTYPNDK, RFSNDK, QNDK, ΔQNDK, BRNDK,ΔBRNDK] LIST
         <Subsection for Spectrum1>
         <Subsection for Spectrum2>
         ---------------------------------
         <Subsection for SpectrumNSP>
[MAT, 8,  0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

[4] Data in each LIST record must be given in order specified in Section 8.4.2

The structure of a subsection is:

```
[MAT, 8,457/ 0.0, STYP, LCON, 0, 6, NER/
         FD, ΔFD, ER_AV, ΔER_AV, FC, ΔFC] LIST
[MAT, 8,457/ ER_1, ΔER_1, 0, 0, NT, 0/
         RTYP_1, TYPE_1, RI_1, ΔRI_1, RIS_1, ΔRIS_1,
         RICC_1,ΔRICC_1, RICK_1,ΔRICK_1, RICL_1,ΔRICL_1] LIST
         -------------------------------------
         ER_NER, ΔER_NER, 0, 0, NT, 0/
         RTYP_NER,TYPE_NER, RI_NER, RI_NER, ------------] LIST
         (omit these LIST records if LCON=1)
[MAT, 8,457/ RTYP, 0.0, 0, LCOV, NR, NP/ E_int / RP(E) ] TAB1
         (omit if LCON=0)
[MAT, 8,457/ 0.0, 0.0, 0, LB, 2*NPP, NPP/ (E_k,F_k) ] LIST
         (omit if LCOV=0 or LCON=0)
```

For a stable nucleus (NST=1), this section is divided into subsections as follows:

```
[MAT, 8,457/  ZA,  AWR,  LIS,  LISO,   NST,    0]HEAD     (NST=1)
[MAT, 8,457/ 0.0,  0.0,    0,     0,     6,    0/
             0.0,  0.0,  0.0,   0.0,   0.0,  0.0] LIST
[MAT, 8,457/ SPI,  PAR,    0,     0,     6,    0]
             0.0,  0.0,  0.0,   0.0,   0.0,  0.0] LIST
```

8.4.2 Procedures

1. The initial state of the parent nucleus is designated by LISO, which equals 0 for the ground state and equals n for the nth isomeric state. Only isomeric states are included in the count of LISO. (In other files isomeric and nonisomeric states may be included in the count of levels.)

2. The average decay energy $\overline{E}_x$ for decay heat application is given for three general radiation types, $\overline{E}_{LP}$ (for light particles), $\overline{E}_{EM}$ (for electromagnetic radiation), and $\overline{E}_{HP}$ (for heavy particles), followed by the individual components. The sum of these three general quantities is the total average (neutrino energies excluded) energy available per decay to the decay heat problem. The three quantities are more precisely defined as:

$$\begin{aligned}
\overline{E}_{LP} &= \overline{E}_{\beta^-} + \overline{E}_{\beta^+} + \overline{E}_{e^-} + \ldots \\
\overline{E}_{EM} &= \overline{E}_{\gamma} + \overline{E}_{x-ray} + \overline{E}_{annih.rad.} + \ldots \\
\overline{E}_{HP} &= \overline{E}_{\alpha} + \overline{E}_{SF} + \overline{E}_{p} + \overline{E}_{n} + \ldots
\end{aligned}$$

where $\overline{E}_{LP}$ means the average energy of ***all*** "electron-related" radiation such as β^-, β^+ conversion-electrons, Auger, *etc.* The quantity $\overline{E}_{EM}$ means the average energy of all "electromagnetic" radiations such as gamma-rays, x-rays, and annihilation radiation. The quantity $\overline{E}_{HP}$ is the average energy of ***all*** heavy charged particles and neutrons, and also includes the recoil energy; but the alpha energy alone can be separated out

by the usual $M_R/(M_R + M_\alpha)$ factor, where M_R and M_α are the recoil nucleus and alpha masses, respectively.

The average decay energies $\overline{E}_x$ must be given in the following order:

$\overline{E}_{LP}$	Average energy of all light particles.
$\overline{E}_{EM}$	Average energy of all electromagnetic radiation.
$\overline{E}_{HP}$	Average energy of all heavy particles.
$\overline{E}_{\beta^-}$	Average β^- energy.
$\overline{E}_{\beta^+}$	Average β^+ energy.
$\overline{E}_{Ae^-}$	Average Auger-electron energy.
$\overline{E}_{ce^-}$	Average conversion-electron energy.
$\overline{E}_{\gamma}$	Average gamma-ray energy.
$\overline{E}_{x-ray}$	Average X-ray energy.
$\overline{E}_{InB}$	Average internal Bremsstrahlung energy.
$\overline{E}_{annih.rad.}$	Average annihilation energy.
$\overline{E}_{\alpha}$	Average α energy.
$\overline{E}_{recoil}$	Average recoil energy.
$\overline{E}_{SF}$	Average SF energy.
$\overline{E}_{n}$	Average prompt and/or delayed neutron energy.
$\overline{E}_{p}$	Average proton energy.
$\overline{E}_{\nu}$	Average neutrino or antineutrino energy.

3. The symbol RTYP indicates the mode of decay as determined by the initial event. A nucleus undergoing beta decay to an excited state of the daughter nucleus, which subsequently decays by gamma emission, is in the beta decay mode. RTYP = 0.0 is not allowed in MT = 457 (although used under Section 8.2).

   An isomeric state of the daughter nuclide resulting from the decay of parent nuclides is designated by RFS following the procedures used for LISO. Q represents the total energy available in the decay process and is equal to the energy difference available between the initial and final states (both of which may be isomeric). The branching ratio BR for each decay mode is given as a fraction and the sum over all decay modes must equal unity.

   Multiple particle emission is also allowed by using any combination of the RTYP variables. This will account for particle emission from nuclear states excited in the decay of the parent ("delayed-particle" emission) whose half-lives are too short to warrant separate entry in the file. It also allows users and processing codes to identify the various intermediate states, without having to examine all the spectrum listings to determine radiation types. The multiple-particle RTYP should be constructed in the order in which the particles are emitted. (*e.g.*, RTYP = 1.5 indicates decay followed by neutron emission).

4. The source of radiation should be specified for each spectral line or continuous spectra. The source of radiation is a floating-point integer corresponding to the RTYP definitions. If the source of radiation is not known RTYP = 10. should be used.

5. The energy spectra should be specified if they are known and identified by STYP. Gamma spectra are described using STYP = 0.0. Relative intensities and errors in the relative intensity should be specified. Absolute normalization is made through multiplication by FC and FD. If absolute discrete spectra are given, FD must equal unity. The radiation intensity should total the contributions from all decays leading to radiation within a particular decay type, STYP, having energy $E_r \pm \Delta E_r$.

   (a) For gamma ray emission (STYP=0.0), no other information is required if X-ray, Auger electron, conversion electron, and pair formation intensities have not been calculated for these transitions. In this case NT=6.

   The amount of additional information depends upon the detail in which quantities were obtained for inclusion in STYP=8. or 9. spectra, and the number of decay modes. (This detail will also be reflected in the uncertainties assigned in STYP=8. or 9. spectra.) If only the total conversion electron emission is calculated, RICC and ΔRICC should be included and NT is specified as 8. If contributors from the individual K, L, and M shells are calculated, the K and L shell conversion coefficients should be included and NT = 12. In the rare case (*i.e.*, $^{16}_{7}$N), where internal pair formation is needed, the internal pair formation coefficient should be included as the quantities RIS and ΔRIS.

   (b) For electron capture (STYP=2.), the quantity RIS is 0.0 provided $E_{e.c.} \leq 1.022$ MeV. If positron emission is energetically possible, RIS and ΔRIS must be specified (as $I_{\beta+}$ and $\Delta I_{\beta+}$).

   (c) The spectra should be ordered in increasing values of STYP, and discrete spectral data should be specified before continuous spectra.

   (d) For STYP=5. (spontaneous fission neutrons), LCON=0, NER=0, and EAV and ΔEAV should be given.

   (e) For STYP=6. (spontaneous fission fragments) LCON=0, NER=0, and $\overline{E}_{SF}$ and $\overline{\Delta E}_{SF}$ should be given.

6. The specification of data uncertainties is an important quantity which is difficult to represent in a simple way. Although a one sigma variance is desired, a number should be entered that at least indicates qualitatively how well the parameter is known.

   For STYP=8. and 9., ΔE will reflect the detail in which these values were derived. For example, if only the total conversion electron emission has been calculated, ΔE would be the spread between K-conversion and M-conversion electron energies. If a very detailed calculation has been made, ΔE would reflect the uncertainties in the electron binding energy and the transition energy.

7. The spontaneous fission spectrum is specified in File 5 of sub-library 4 (no incoming projectile).

8. Every effort should be made to determine the spin and parity of the original nucleus, either by experimental evidence or by strong theoretical arguments. If the spin cannot be determined, it should be reported as 77.777; if the parity cannot be determined it should be reported as zero.

9. Because the continuum spectrum is normalized, the absolute covariance matrix of a multi-component normalized spectrum processed from this file must have zero for the sum of each row and column. (Processing codes should perform this check).

   Since the covariance form for radioactive product spectra is confined to LB=2, meeting this test is equivalent to the following condition on the F_k of the E_k covariance table:

$$\sum_k F_k\, y_k = 0, \tag{8.1}$$

$$\text{where} \quad y_k = \int_{E_k}^{E_{k+1}} \mathrm{RP}(E) dE \tag{8.2}$$

   and y_k is the energy spectrum on the uncertainty evaluation grid, subject to the condition $\sum y_k = 1$. If the initial F_k do not meet this condition, the corrected values F'_k are given by:

$$F'_k = F_k - \sum_k F_k\, y_k$$

   Note that unlike the case for File 33, some of the F'_k must be negative. Also, the processed multigroup correlation matrix will show some off-diagonal components that are -1 as well as others that are +1.

   When a processing code constructs the absolute covariance V_{mn} on the user's energy grid E_m, the simplest relations to use are

$$V_{mn} = \sigma_m \sigma_n$$

$$\text{where} \quad \sigma_n = \int_{E_n}^{E_{n+1}} F(E)\, \mathrm{RP}(E)\, dE$$

   and the integral is easy because $F(E)$ is piece-wise continuous on the E_k grid. By this construction we are assured that the null sum condition will be retained for the covariance matrix of the processed multigroup spectrum.

Chapter 9

File 9: MULTIPLICITIES FOR PRODUCTION OF RADIOACTIVE NUCLIDES

9.1 General Description

Neutron cross sections for the excitation of metastable states (*i.e.* the activation cross sections) can be reconstructed from the cross sections in File 3 and the multiplicities in File 9. The multiplicity represents that fraction of the cross section in File 3 that produces the LFS state in the daughter nucleus. The multiplicities are given as a function of energy, E, where E is the incident neutron energy (in eV) in the laboratory system. They are given as energy-multiplicity pairs. An interpolation scheme must be given to specify the energy variation of the data for incident energies between a given energy point and the next higher energy point. File 9 is divided into sections, each section containing data for a particular reaction type (MT number). The sections are ordered by increasing MT number. Within a section for a given MT are subsections for different final states of the daughter product (LFS). File 9 is only allowed for evaluations that represent data for single nuclides.

9.2 Formats

File 9 is made up of sections where each section gives the multiplicity for a particular reaction type (MT number). Each section always starts with a HEAD record and ends with a SEND record. For File 9, the following quantities are defined:

LIS Indicator to specify the level number of the target.

LFS Indicator to specify the level number of the nuclide (ZAP) (as defined in File 8) produced in the reaction (MT number).

LFS = 0: the final state is the ground state.

LFS = 1: the final state is the first excited state.

LFS = 2: the final state is the second excited state.

———-

———-

LFS = 98: an unspecified range of final states.

QM Mass-difference Q value (eV); see Section 3.3.2.

QI Reaction Q value (eV) for the state described by the subsection.

For isomeric, states QI is defined as QM minus the residual excitation energy of the isomer.

For the ground state, QI=QM for reactions with no intermediate states in the residual nucleus.

(See Section 3.3.2)

IZAP $1000 \times Z + A$ for the product nucleus

NS Number of final states for each MT for which multiplicities are given.

NR Number of energy ranges. A different interpolation scheme may be given for each range. For the limit on the maximum value of NR see Appendix G.

NP Total number of energy points used to specify the data. For the limit on the maximum value of NP see Appendix G.

E$_{int}$ Interpolation scheme for each energy range. (For details, see Section 0.5.2)

$Y(E)$ Multiplicity for a particular reaction type at incident energy E (eV). Data are given for energy-multiplicity pairs.

The structure of a section is:

```
[MAT, 9, MT/  ZA, AWR, LIS, 0, NS, 0]HEAD
     <NS subsections, one for each value of LFS>
[MAT, 9,  0/ 0.0, 0.0,   0, 0,  0, 0]SEND
```

The structure of a subsection is:

[MAT, 9, MT/ QM, QI, IZAP, LFS, NR, NP/ E$_{int}$ / $Y(E)$]TAB1

9.3 Procedures

Multiplicities must be given in File 9 for those reactions described in File 8 which have LMF=9 in the LIST record of the subsection for that particular MT number and value of LFS. The multiplicities in File 9 describe the fraction of the cross section that produces the LFS state in the daughter nucleus. For a reaction represented by resonance parameters in File 2, File 10 cannot be used; only multiplicities in File 9 are allowed.

The data in File 9 must cover the entire energy range for each reaction in File 3 from threshold to at least 20 MeV. That is, multiplicities cannot be used over a portion of the incident neutron energy range with cross sections covering another portion. For reactions with negative Q-values , the first energy point should be at the threshold given in File 3. If a subsection QI is not equal to the QI in File 3, the multiplicity should be given as zero up to the energy point corresponding to the threshold of the subsection.

The set of points or energy mesh used for the total cross section in File 3 must include the union of all energy meshes in File 9 for each MT number. Although a large number of incident energy points are allowed for the total cross section (see Appendix G), every attempt should be made to minimize the number of points in File 9.

The multiplicities in File 9 should be equal to or less than unity since the cross sections to be generated must be equal to or less than the cross sections in File 3 for each MT number.

In summary, the proper procedure would be to defer entering data into File 8 for a given MT ***until*** the File 9 multiplicities (or File l0 cross sections) are added to the evaluations. That is, every MT number (except MT=454, 457, or 459) in File 8 with LMF=9 as an indicator in the LIST record of the subsection for that particular MT and LFS value must have the corresponding multiplicities in File 9.

Chapter 10

File 10: CROSS SECTIONS FOR PRODUCTION OF RADIOACTIVE NUCLIDES

10.1 General Description

Neutron activation cross sections [such as the (n,p) and (n,2n) cross sections] and cross sections for a particular state of a radioactive target are given in File 10. These cross sections are given as a function of energy E, where E is the incident particle or photon energy (in eV) in the laboratory system. They are given as energy-cross-section pairs. An interpolation scheme must specify the energy variation of the data for energies between a given energy point and the next higher energy point.

File 10 is divided into sections, each section containing the data for a particular reaction type (MT number). The sections are ordered by increasing MT number. Within a section for a given MT are subsections for different final states (LFS) of the daughter product nucleus. File 10 is allowed only for evaluations that represent the data for single isotopes.

10.2 Formats

File 10 is made up of sections where each section gives the cross section for a particular reaction type (MT number). Each section always starts with a HEAD record and ends with a SEND record. For File 10, the following quantities are defined:

LIS Indicator to specify the level number of the target.

LFS Indicator to specify the level number of the nuclide (IZAP) produced in the reaction (MT) number.

LFS=0 the final state is the ground state.

LFS=1 the final state is the first excited state.

LFS=2 the final state is the second excited state.

—-

—-

LFS=98 an unspecified range of final states.

QM Mass-difference Q value (eV); see Section 3.3.2.

QI Reaction Q value (eV) for the state described by the subsection.

For isomeric, states QI is defined as QM minus the residual excitation energy of the isomer.

For the ground state, QI=QM for reactions with no intermediate states in the residual nucleus.

(See Section 3.3.2)

IZAP $1000 \times Z + A$ for the product nucleus

NS Number of final states for each MT for which cross sections are given.

NR Number of energy ranges. A different interpolation scheme may be given for each range. For the limit on the maximum value of NR see Appendix G.

NP Total number of energy points used to specify the data. For the limit on the maximum value of NP see Appendix G.

$\mathbf{E}_{int}$ Interpolation scheme for each energy range. (For details, see Section 0.5.2)

$\sigma(E)$ Cross section in barns for a particular reaction type at incident energy E (eV). Data are given for energy, cross-section pairs.

The structure of a section is:

```
[MAT, 10, MT/  ZA, AWR, LIS, 0, NS, 0]HEAD
  <NS subsections, one for each value of LFS>
[MAT, 10,  0/ 0.0, 0.0,   0, 0,  0, 0]SEND
```

The structure of a subsection is:

[MAT, 10, MT/ QM, QI, IZAP, LFS, NR, NP/ E_{int} / $\sigma(E)$]TAB1

10.3 Procedures

Isomer production cross sections must be given in File 10 for those reactions described in File 8 which have LMF=10 in the LIST record of the subsection for that particular MT number and value of LFS. The data in File 10 are the cross sections for the production of a final state (LFS) of the daughter product nucleus. For a reaction represented by resonance parameters in File 2, File 10 ***cannot*** be used; only multiplicities in File 6 or File 9 are allowed.

The data in File 10 must cover the entire energy range for each reaction from the threshold of the subsection in File 10 up to at least 20 MeV. That is, cross sections cannot be used over a portion of the incident neutron energy range with multiplicities covering another portion. For reactions with negative Q-values, the first energy point should be at the threshold of the subsection in File 10 and the cross section at this point must be zero.

The set of points or energy mesh used for the total cross section in File 3 must be the union of all energy meshes in File 10 for each MT number. The maximum number of points NT for the total cross section is given in Appendix G. However, every attempt should be made to minimize the number of points in File 10.

Using the ^{93}Nb(n,2n)^{92}Nb cross section as an example, only the cross section for the production of the 10.16-day isomer in ^{92}Nb would appear under MT=16 with LIS=0 and LFS=1 in File 10. The sum of all partial cross sections for the (n,2n) reaction would still be found in File 3 under MT=16 [note that this is the only (n,2n) cross section required for neutron transport calculations]. It should be noted, however, in this particular case, that the evaluator would have the choice of using energy-dependent multiplicities in File 9 instead of cross sections in File 10.

The cross sections that appear in File 10 are redundant; that is, they should not be included in the check sum for the total cross section. The cross sections in File 10 must be equal to or less than the cross sections for that MT number that appears in File 3.

In summary, the proper procedure is to defer entering data into File 8 for a given MT ***until*** the File 10 cross sections (or File 9 multiplicities) are added to the evaluations. That is, every MT number (except MT=454, 457, or 459) with LMF=10 as an indicator in the LIST record of the subsection for that particular MT and LFS value must have the corresponding cross sections in File 10.

Chapter 11

File 11: GENERAL COMMENTS ON PHOTON PRODUCTION

11.1 General Description

Photon production data not represented in File 6 may be presented in four distinct files as follows:

File	Description
12	Multiplicities and transition probability arrays
13	Photon production cross sections
14	Photon angular distributions
15	Continuous photon energy spectra

With the exception of File 12, all the files are closely analogous to the corresponding neutron data files with the same number (modulo 10). The purpose of File 12 is to provide additional methods for representing the energy dependence of photon production cross sections. The allowed reaction type (MT) numbers are the same as those assigned for neutron reactions, Files 1 through 7. However, they may have somewhat different meanings for photon production that require additional explanation in some cases:

1. MT=3 should be used in File 12 through 15 to represent composite cross sections, that is, photon production cross sections from more than one reaction type that have been lumped together.

2. There is no apparent reason to have redundant or derived data for the photon production files, as is the case for the neutron files, *i.e.*, MT=3, 4, etc. Therefore, to avoid confusion, the join of all sections of Files 6, 12 and 13 should represent the photon production, with each section being disjoint from all others.

3. Using Figure 11.1 as a guide, let us consider how one might represent inelastic γ-ray production. The differential cross section for producing γ ray of energy E_γ resulting from the excitation of the m_0^{th} level of the residual nucleus and the subsequent transition between two definite levels ($j \rightarrow i$), which need not be adjacent, including the

effects of cascading from the $m_0 - j$ levels higher than j, is given by:

$$\frac{d\sigma}{dE_\gamma}(E_\gamma, E, m_0, i, j) = \delta\left\{E_\gamma - (\varepsilon_j - \varepsilon_i)\right\} A_{j,i}\sigma_{m0}(E) \sum_{\alpha=1}^{m_0-j} R_{m_0 j\alpha} \ , \tag{11.1}$$

where:

σ_{m0} Cross section for exciting the m_0^{th} level with incident particle of energy E, taken from File 3 for the MT corresponding to the m_0^{th} level,

$\delta\left\{E_\gamma - (\varepsilon_j - \varepsilon_i)\right\}$ Delta function defining the discrete gamma-ray of energy E_γ that results from the transition from level j to level i,

A_{ij} Probability that a gamma ray of energy of E_γ is emitted in the transition from level j to i, taken as the gamma-ray branching ratio,

$R_{m_0 j\alpha}$ Probability that the nucleus initially excited at level m_0 will de-excite to level j in α transitions, where α ranges from 1 to $m_0 - j$,

$$R_{m_0 j\alpha} = \sum_{m_1=\alpha+(j-1)}^{m_0-1} \sum_{m_2=\alpha+(j-2)}^{m_1-1} \cdots \sum_{m_{\alpha-1}=j+1}^{m_{\alpha-2}-1} \sum_{m_\alpha}^{j} \prod_{l=1}^{\alpha} T_{m_{l-1}m_l}$$

T_{kj} probability of the residual nucleus having a transition to the lth level given that it was in the excited state corresponding to the kth level, *i.e.*, the branching ratio for a gamma ray transition from the $k \rightarrow l$ level.

In general, $R_{m_0 ja}$ is the sum of the products of a transition probabilities (branching ratios) leading from level m_0 through intermediate levels to level j. In the example shown for initial excitation of level $m_0 = 5$ and interest being in the resulting γ-ray due to transition between levels 2 and 1:

$$\begin{aligned} R_{m_0 j} &= T_{m_0 j} = T_{52} \\ R_{m_0 j2} &= T_{m_0 m_1} T m_1 j + T_{m_0 m_2} T_{m_2 j} = T_{52}.T_{42} + T_{53}.T_{32} = 0 + 0 = 0 \end{aligned}$$

The relevant quantities for this example are $[E_\gamma = E_{\gamma 2} = (\varepsilon_2 - \varepsilon_1)]$, and

$$R_{m_0 j3} = T_{m_0 m_1} T_{m_1 m_2} T_{m_2 j} = T_{54}.T_{43}.T_{32}$$

If m_0 and j are separated by many levels, the scheme becomes very involved.

We are at once beset by the problem that no clear choice of ENDF representation in terms of section number is possible. The data may naturally be identified with both the m_0^{th} level and the jth level. To avoid this problem, we can sum equation (11.1) over m_0:

$$\frac{d\sigma_1}{dE_\gamma}(E_\gamma, E, i, j) = \sum_{m_0=j}^{N} \frac{d\sigma}{dE_\gamma}(E_\gamma, E, m_0, i, j) \tag{11.2}$$

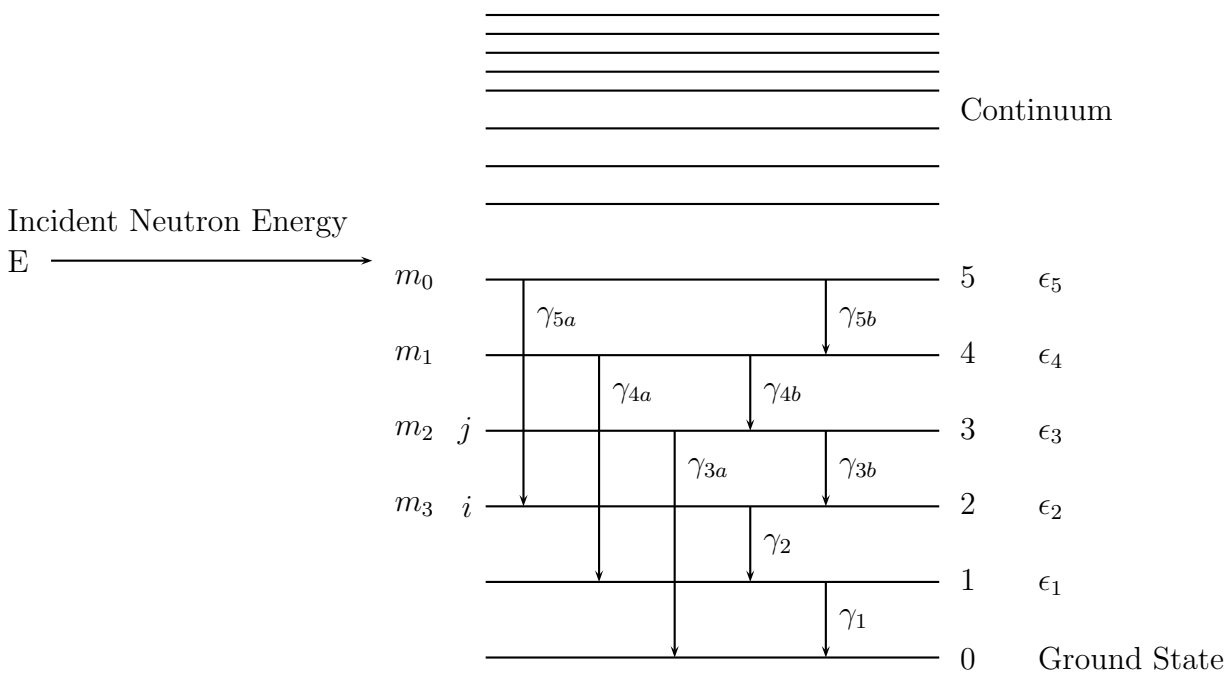

Figure 11.1: Schematic diagram of a level scheme to illustrate gamma production.

where N is the highest level that can be excited by a neutron of incident energy E [*i.e.*, $\varepsilon_N \leq E.\mathrm{AWR}/(\mathrm{AWR}+1)$]. This gives a *de-excitation* cross section that can single out a definite γ-ray transition and has the advantage when experimental data are to be represented. The de-excitation cross section is identified with the jth level.

Alternatively, we can sum equation (11.1) over i and j:

$$\frac{d\sigma_2}{dE_\gamma}(E_\gamma, E, m_0) = \sum_{j=1}^{m_0}\sum_{i=0}^{j-1}\frac{d\sigma}{dE_\gamma}(E_\gamma, E, m_0, i, j) \ . \tag{11.3}$$

This gives an excitation cross section that can single out a definite excited state and has the advantage when calculated data are to be represented. The excitation cross section is identified with the m_0^{th} level. If equation (11.2) is summed over i and j, or if equation (11.3) is summed over m_0 then:

$$\begin{aligned}\frac{d\sigma}{dE_\gamma}(E_\gamma, E) &= \sum_{m_0=1}^{N}\frac{d\sigma_2}{dE_\gamma}(E_\gamma, E, m_0) \\ &\equiv \sum_{j=1}^{N}\sum_{i=0}^{j=l}\frac{d\sigma_1}{dE_\gamma}(E_\gamma, E, i, j)\end{aligned} \tag{11.4}$$

This gives a cross section for all possible excitations and transitions and thus corresponds to the total inelastic neutron cross section for discrete levels. It is recommended

that MT=4 be used for the data represented by equation (11.4), as well as for the continuum. If, however, it is expedient or useful to use MT=51 through 91, then one must use either the de excitation cross sections of equation (11.2) or the excitation cross sections of equation (11.3), but not both. A restriction is imposed if the transition probability array option is used and if the entire neutron energy range is not covered by the known transition probabilities. Then, for MT=51 through 90 in File 12 to be used for the remaining neutron energy range, a representation by excitation multiplicities must be used. The integrated cross sections of File 13 are obtained by integrating equations (11.1) through (11.4) over E_γ.

4. The remarks in Item 3 apply for discrete rays from (n,pγ), (n,dγ), (n,tγ), (n,^{3}Heγ), (n,$\alpha\gamma$) reactions, and the use of MT=103, 101, 105, 106, and 107 is recommended for these cases.

Chapter 12

File 12: PHOTON PRODUCTION MULTIPLICITIES AND TRANSITION PROBABILITY ARRAYS

12.1 General Description

File 12 can be used to represent the neutron energy dependence of photon production cross sections or delayed photon source functions by means of either multiplicities or transition probability arrays. Both methods rely upon processing codes that use either neutron cross sections from File 2 and/or File 3 to generate absolute photon production cross sections or time constants from File 1 (MT=460) to generate delayed photon source functions.

Multiplicities can be used to represent the cross sections of discrete photons and/or the integrated cross sections of continuous photon spectra. The MT numbers in File 12 designate the particular neutron cross sections (File 2 and/or File 3) to which the multiplicities are referred. The use of multiplicities is the recommended method of presenting (n,γ) capture γ-ray cross sections, provided, of course, that the (n,γ) cross section is adequately represented in File 2 and/or File 3.

For well-established level decay schemes, the use of transition probability arrays offers a concise method for presenting (n,xγ) information. With this method, the actual decay scheme of the residual nucleus for a particular reaction (defined by MT number) is entered in File 12. This information can then be used by a processing code together with discrete level excitation cross sections from File 3 to calculate discrete γ-ray production cross sections. This option cannot be used to represent the integrals of continuous photon spectra.

12.2 Formats

Each section of File 12 gives information for a particular reaction type (MT number), either as multiplicities (LO=1) or as transition probability arrays (LO=2). Each section always starts with a HEAD record and ends with a SEND record.

12.2.1 Option 1: Multiplicities (LO=1)

The neutron energy dependence of photon production cross section is represented by tabulating a set of neutron energy and multiplicity pairs $\{E, y_k(E)\}$ for each discrete photon and for the photon energy continuum[1]. The subscript k designates a particular discrete photon or a photon continuum, and the total number of such sets is represented by NK.

The multiplicity or yield $y_k(E)$ is defined by:

$$y_k(E) = \frac{\sigma_k^\gamma}{\sigma(E)} \qquad \text{(photons)} \tag{12.1}$$

where E designates the neutron energy and $\sigma(E)$ is the neutron cross section in File 2 and/or File 3 to which the multiplicity is referred (by the MT number). For discrete photons, $\sigma_k^\gamma(E)$ is the photon production cross section for the discrete photon designated by k. For photon continua, $\sigma_k^\gamma(E)$ is the cross section for the photon continuum integrated over photon energy.

In the continuum case,

$$\begin{aligned} y_k(E) &= \frac{\sigma_k^\gamma(E)}{\sigma(E)} = \frac{\int \frac{d\sigma_k^\gamma}{dE_\gamma}\,(E_\gamma \leftarrow E)\,dE_\gamma}{\sigma(E)} \\ &= \frac{\int \sigma(E)\; y_k\,(E_\gamma \leftarrow E)\;\; dE_\gamma}{\sigma(E)} = \int_0^{E_\gamma^{\max}} y_k\,(E_\gamma \leftarrow E)\;\; dE_\gamma \end{aligned} \tag{12.2}$$

where E_γ designates photon energy (eV), the term:

$$\frac{d\sigma_k^\gamma}{E_\gamma}(E_\gamma \leftarrow E)$$

is the absolute photon energy distribution in barns/eV, and $y_k(E_\gamma \leftarrow E)$ is the relative energy distribution in photons/eV. The quantity $y_k(E_\gamma \leftarrow E)$ can be broken down further as:

$$y_k(E_\gamma \leftarrow E) = y_k(E) f_k(E_\gamma \leftarrow E),$$

which results in the requirements that

$$\int_0^{E_\gamma^{\max}} f_k(E_\gamma \leftarrow E)\,dE_\gamma = 1.$$

Any time a continuum representation is used for a given MT number in either File 12 or 13, then the normalized energy distribution $f_k(E_\gamma \leftarrow E)$ must be given in File 15 under the same MT number.

As a check quantity, the total yield from the NK contributions:

$$Y(E) = \sum_{k=1}^{\text{NK}} y_k(E) \qquad \text{(photons)}$$

[1]There should be no more than one energy continuum for each MT number used. If the decomposition of a continuum into several parts is desired, this can be accomplished in File 15.

is also tabulated for each MT number if NK>1.

The structure of a section for LO=1 is[2]:

```
[MAT, 12, MT/ ZA, AWR, LO, 0, NK,  0]HEAD     (LO=1)
[MAT, 12, MT/ 0.0, 0.0, 0, 0, NR, NP/E_int / Y(E)] TAB1    (if NK>1)
         <subsection for k =1>
         <subsection for k=2>
         ......
         ......
        <subsection for k=NK>
[MAT, 12, 0/ 0.0, 0.0, 0, 0,  0,  0] SEND
```

and the structure of each subsection is

```
[MAT, 12, MT/ Eg_k, ES_k, LP, LF, NR, NP/ E_int / y_k(E)] TAB1
```

where:

NK number of discrete photons including the continuum.

ES_k energy of the level from which the photon originates. If the level is unknown or if a continuous photon spectrum is produced, then $ES_k \equiv 0.0$ should be used.

EG_k photon energy for LP=0 or 1 or Binding Energy for LP=2. For a continuous photon energy distribution, $EG_k \equiv 0.0$ should be used.

LP indicator of whether or not the particular photon is a primary:

- LP=0 origin of photons is not designated or not known, and the photon energy is EG_k;
- LP=1 for non-primary photons where the photon energy is again simply EG_k;
- LP=2 for primary photons where the photon energy EG'_k is given by

$$EG'_k = EG_k + \frac{AWR}{AWR + 1} E_n.$$

LF the photon energy distribution law number, which presently has only two values defined:
LF=1, a normalized tabulated function (in File 15), and
LF=2, a discrete photon energy.

[2] If the total number of discrete photons and photon continua is one (NK=1), the TAB1 record is omitted.

12.2.2 Option 2: Transition Probability Arrays (LO=2)

With this option, the only data required are the level energies, de-excitation transition probabilities, and (where necessary) conditional photon emission probabilities. Given this information, the photon energies and their multiplicities can readily be calculated. Photon production cross sections can then be computed for any given level from the excitation cross sections in File 3, along with the transition probability array. Similarly, multiplicities and photon production cross sections can be constructed for the total cascade. For any given level, the transition and photon emission probability data given in the section are for photons originating at that level only; any further cascading is determined from the data for the lower levels. The following quantities are defined:

LG LG=1, simple case (all transitions are γ emission).
LG=2, complex case (internal conversion or other competing processes occur).

NS Number of levels below the present one, including the ground state. (The present level is also uniquely defined by the MT number and by its energy level).

NT Number of transitions for which data are given in a list to follow (*i.e.*, number of non-zero transition probabilities), NT$\leq$ NS.

ES$_i$ Energy of the ith level, i=0,1,2... NS.
ES $\equiv$ 0.0 implies the ground state.

TP$_i$ TP$_{NS,i}$, probability of a direct transition from level NS to level i, i=0,1,2... (NS1).

GP$_i$ GP$_{NS,i}$, the probability that, given a transition from level NS to level i, the transition is a photon transition (*i.e.*, the conditional probability of photon emission).

B$_i$ Array of NT doublets or triplets depending on the LG value.

Note that each level can be identified by its NS number. Then the energy of a photon from a transition to level i is given by $E_\gamma = \mathrm{ES}_{NS} - \mathrm{ES}_i$, and its multiplicity is given by $y(E_\gamma \leftarrow E) = (\mathrm{TP}_i)(\mathrm{GP}_i)$. It is implicitly assumed that the transition probability array is independent of incident neutron energy. The structure of a section for LO=2 is:

```
[MAT, 12, MT/   ZA, AWR, LO, LG,        NS,    0]HEAD    (LO=2)
[MAT, 12, MT/ ES_NS, 0.0, LP,  0, (LG+1)*NT, NT/B]LIST
[MAT, 12,  0/  0.0, 0.0,  0,  0,         0,    0]SEND
```

If LG=1, the array B$_i$ consists of NT doublets {ES$_i$,TP$_i$};
if LG=2, it consists of NT triplets {ES$_i$,TP$_i$,GP$_i$}.
Here the subscript i is a running index over the levels below the level for which the transition probability array is being given (*i.e.*, below level NS). The doublets or triplets are given in decreasing magnitude of energy ES$_i$.

12.3 Procedures

1. Under Option 1, the subsections are given in decreasing magnitude of EG_k.

2. Under Option 1, the convention is that the subsection for the continuum photons, if present, is last. In this case, the last value of EG_k (EG_{NK}) is set equal to 0.0, and logical consistency with Procedure 1 is maintained.

3. Under Option 1, the values of EG_k should be consistent to within four significant figures with the corresponding EG_k values for the File 14 photon angular distributions. This allows processing and "physics" checking codes to match photon yields with the corresponding angular distributions.

4. Under Option 1, ES_k is the energy of the level from which the photon originates. If ES_k is unknown or not meaningful (as for the continuous photon spectrum), the value 0.0 should be entered.

5. If capture and fission resonance parameters are given in File 2, photon production for these reactions should be given by using Option 1 of File 12, instead of using photon production cross sections in File 13. This is due to the voluminous data required to represent the resonance structure in File 13 and the difficulty of calculating multigroup photon production matrices from such data.

6. Under Option 1, the total yield table, $Y(E)$, should span exactly the same energy range as the combined energy ranges of all the $y_k(E)$. Within that range,

$$Y(E) = \sum_{k=1}^{\mathrm{NK}} y_k(E)$$

   should hold within four significant figures.

7. The excitation cross sections for all the levels appearing in the transition probability arrays must, of course, be given in File 3.

8. The join of all sections, regardless of the option used, should represent the photon production data, with no redundancy. For example, MT=4 cannot include any photons given elsewhere under MT=51 through 91. Likewise, there can be no redundancy between Files 12 and 13.

9. If only one energy distribution is given under Option 1 (NK=1), the TAB1 record for the Y(E) table is deleted to avoid repetitive entries.

10. Data should not be given in File 12 for reaction types that do not appear in Files 2 and/or 3.

11. Under Option 2, the level energies, ES_i, in the transition probability arrays are given in decreasing magnitude.

12. The MT numbers for which transition probability data are given should be for consecutive levels, beginning at the first level, with no embedded levels omitted.

13. The energies of photons arising from level transitions should be consistent within four significant figures with the corresponding EG_k values in File 14. Therefore, care must be taken to specify level energies to the appropriate number of significant figures.

14. Under Option 2, the sum of the transition probabilities (TP_i) over i should equal 1.0000 (that is, should be unity to within five significant figures).

15. The limit on the number of energy points for the tabulations of $Y(E)$ or $y_k(E)$ is given in Appendix G. This is an upper limit that will rarely be approached in practice because yields are normally smoothly varying functions of incident neutron energy.

16. The limit on the number of interpolation regions is also given in Appendix G.

17. Tabulations of non-threshold data should normally cover at least the energy range 10^{-5} eV $\leq E \leq 2 \times 10^7$ eV, where practical. Threshold data should be given from threshold energy up to at least 2×10^7 eV, where practical.

18. Transition Probability Arrays for (n,n'γ) photons:

    (a) The use of transition probability arrays (File 12, LO=2) is a convenient way to represent a portion of the γ-rays produced by deexcitation of discrete levels populated by (n,n'γ) and other reactions.

    (b) Several conditions must be met before this representation can be used. Level excitation cross sections (*e.g.* given in File 3 for neutrons as MT=51,...) must be given from threshold energies up to the same maximum energy (no exceptions). Decay properties of all levels must be known. The information given in File 12 must be consistent with data given in File 3.

    (c) Usually, not all the conditions can be met. Part of the problem is the recommendation that level excitation cross sections for the first few levels be given for neutron energies up to at least 20 MeV. This might be difficult to achieve, unless one relies on nuclear model calculations.

Chapter 13

File 13: PHOTON PRODUCTION CROSS SECTIONS

13.1 General Description

The purpose of File 13 is the same as that of File 12, namely, it can be used to represent the neutron and photon energy dependence of photon production cross sections. In File 13, however, absolute cross sections in barns are tabulated, and there is no need to refer to the cross sections in File 3.

13.2 Formats

As in File 12, each section in File 13 gives information for a particular reaction type (MT number). Each section always starts with a HEAD record and ends with a SEND record.

The representation of the energy dependence of the cross sections is accomplished by tabulating a set of neutron energy-cross section pairs $\{E, \sigma_k^\gamma(E)\}$ for each discrete photon and for the photon energy continuum. The subscript k designates a particular discrete photon or the photon continuum, and the total number of such sets in NK. For discrete photons, $\sigma_k^\gamma(E)$ is the photon production cross section (barns) for the photon designated by k. For the photon continuum, $\sigma_k^\gamma(E)$ is the cross section, integrated over photon energy, for the photon continuum[1] designated by k. In the continuum case,

$$\sigma_k^\gamma(E) = \int_0^{E_\gamma^{\max}} \frac{d\sigma_k^\gamma}{dE_\gamma}\left(E_\gamma \leftarrow E\right) dE_\gamma \qquad \text{(barns)} \tag{13.1}$$

where E_γ designates photon energy (eV), and $d\sigma_k^\gamma/dE_\gamma(E_\gamma \leftarrow E)$ is the absolute photon energy distribution in barns/eV. The energy distribution can be further broken down as:

$$\frac{d\sigma_k^\gamma}{dE_\gamma}\left(E_\gamma \leftarrow E\right) = \sigma_k^\gamma\left(E\right) f_k\left(E_\gamma \leftarrow E\right) \tag{13.2}$$

[1]There should be no more than one energy continuum for each MT number used. If the decomposition of a continuum into several parts is desired, this can be accomplished in File 15.

which obviously requires that:

$$\int_0^{E_\gamma^{\max}} f_k\left(E_\gamma \leftarrow E\right) dE_\gamma = 1.$$

Any time a continuum representation is used for a given MT number in File 13, the normalized energy distribution, $f_k(E_\gamma \leftarrow E)$, must be given in File 15 under the same MT number.

As a check quantity, the total photon production cross section,

$$\sigma_{tot}^\gamma(E) = \sum_{k=1}^{\mathrm{NK}} \sigma_k^\gamma(E) \qquad \text{(barns)}, \tag{13.3}$$

is also tabulated for each MT number, unless only one subsection is present (*i.e.*, NK=1). The following quantities are defined.

NK Number of discrete photons including the continuum.

ES$_k$ Energy of the level from which the photon originates. If the level is unknown or if a continuous photon spectrum is produced, then ES$_k \equiv 0.0$ should be used.

EG$_k$ Photon energy for LP=0 or 1 or Binding Energy for LP=2. For a continuous photon energy distribution, EG$_k$=0.0 should be used.

LP Indicates whether or not the particular photon is a primary:

- LP=0 origin of photons is not designated or not known, and the photon energy is EG$_k$;
- LP=1 for non-primary photons where the photon energy is again simply EG$_k$;
- LP=2 for primary photons where the photon energy EG$'_k$ is given by:

$$\mathrm{EG}'_k = \mathrm{EG}_k + \frac{\mathrm{AWR}}{\mathrm{AWR}+1} E_n$$

LF Photon energy distribution law number, which presently has only two values defined:
LF=1, a normalized tabulated function (in File 15), and
LF=2, a discrete photon energy.

The structure of a section in File 13 is[2]:

[2] If the total number of discrete photons and photon continua is one (NK=1), this TAB1 record is omitted.

```
[MAT, 13, MT/  ZA, AWR, 0, 0, NK, 0]HEAD
[MAT, 13, MT/ 0.0, 0.0, 0, 0, NR, NP/ E_int / σ^γ_tot(E)]TAB1    (NK>1)
            <subsection for k=1>
            <subsection for k=2>
            -------------------------
            <subsection for k=NK>
[MAT, 13, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

and the structure of each subsection is:

```
[MAT, 13, MT/ EG_k, ES_k, LP, LF, NR, NP/ E_int / σ^γ_k(E)] TAB1,
```

13.3 Procedures

1. The subsections are given in decreasing magnitude of EG_k.

2. The convention is that the subsection for the continuum photons, if present, is last. In this case, $\mathrm{EG}_{NK} \equiv 0.0$.

3. The values of EG_k should be consistent to within four significant figures with the corresponding EG_k values in File 14.

4. ES_k is the energy of the level from which the photon originates, if known. Otherwise $\mathrm{ES}_k \equiv 0.0$.

5. If capture and fission resonance parameters are given in File 2, the corresponding photon production should be given by using Option 1 of File 12, instead of using photon production cross sections.

6. The total photon production cross section table, $\sigma^{\gamma}_{tot}(E)$ should span exactly the same energy range as the combined energy range of all the $\sigma^{\gamma}_{k}(E)$. Within that range,

$$\sigma^{\gamma}_{tot}(E) = \sum_{k=1}^{\mathrm{NK}} \sigma^{\gamma}_{k}(E)$$

   should hold within four significant figures. If only one energy distribution is given, either discrete or continuous (NK=1), the TAB1 record for the $\sigma^{\gamma}_{tot}(E)$ is deleted.

7. The join of all sections in File 12 and 13 combined should represent the photon production data with no redundancy. For example, MT=4 cannot include any photons given elsewhere under MT=51 through 91.

8. The limit on the number of energy points in a tabulation for any photon production subsection is given in Appendix G. This is an upper limit; in practice, the minimum number of points possible should be used. If there is extensive structure, the use of File 12 should be seriously considered, because yields are normally much smoother functions of incident neutron energy than cross sections.

9. The limit on the number of interpolation regions is also given in Appendix G.

10. Tabulations of non-threshold data should normally cover at least the energy range 10^{-5}eV $\leq E \leq 2 \times 10^{7}$eV, where practical. Threshold data should be given from threshold energy up to at least 2×10^{7}eV, where practical.

13.4 Preferred Representations

1. The recommended representation for (n,n'γ) reactions is photon production cross section (File 13) using MT=4. All discrete and continuum γ rays are given in a series of subsections.

2. Photon production cross sections resemble the frequently measured or reported results.

3. The use of MT=4 eliminates confusion about whether the data represent an excitation or de-excitation cross section (see File 11).

4. If for any reason MT=51,52 ... is used, it is understood that these data represent de-excitation and not excitation cross sections (see 3 above). MT=51, 52, ... in File 3, of course, means excitation cross sections.

5. Combined use of MT=4 and MT=51, 52, ... is not allowed.

6. Above a certain energy point probably it will not be possible to separate the various components of the total γ production cross section. When this happens, it is preferable to represent the data as MT=3.

7. Data for all other reactions should be given as photon production cross sections (File 13) using the appropriate MT numbers. The same general rules outlined above should be used.

Chapter 14

File 14: PHOTON ANGULAR DISTRIBUTIONS

14.1 General Description

The purpose of File 14 is to provide a means for representing the angular distributions of secondary photons produced in neutron interactions. Angular distributions should be given for each discrete photon and photon continuum appearing in Files 12 and 13, even if the distributions are isotropic.

The structure of File 14 is, with the exception of isotropic flag (LI), closely analogous to that of File 4. Angular distributions for a specific reaction type (MT number) are given for a series of incident neutron energies in order of increasing neutron energy. The energy range covered should be the same as that for the data given under the corresponding reaction type in File 12 or File 13. The data are given in ascending order of MT number.

The angular distributions are expressed as normalized probability distributions, that is:

$$\int_{-1}^{1} p_k\left(\mu, E\right) d\mu = 1 \ ,$$

where $p_k(\mu, E)$ is the probability that an incident neutron of energy E will result in a particular discrete photon or photon energy continuum (specified by k and MT number) being emitted into unit cosine about an angle whose cosine is μ. Because the photon angular distribution is assumed to have azimuthal symmetry, the distribution may be represented as a Legendre series expansion,

$$p_k(\mu, E) = \frac{2\pi}{\sigma_k^\gamma(E)} \frac{d\sigma_k^\gamma}{d\Omega}\left(\Omega, E\right) \tag{14.1}$$

$$= \sum_{l=0}^{\mathrm{NL}} \frac{2l+1}{2} a_l^k(E) P_l(\mu) \tag{14.2}$$

where

μ cosine of the reaction angle in the laboratory system,

E energy of the incident neutron in the laboratory system,

$\sigma_k^\gamma(E)$ photon production cross section for the discrete photon or photon continuum specified by k, as given in either File 13 or in File 2, 3, and 12 combined,

l order of the Legendre polynomial,

$d\sigma_k^\gamma/d\Omega$ differential photon production cross section in barns/steradian,

$a_l^k(E)$ the lth Legendre coefficient associated with the discrete photon or photon continuum specified by k. It is implicitly assumed that $a_0^k(E) \equiv 1.0$.

$$a_l^k(E) = \int_{-1}^{1} p_k(\mu, E)\ P_l(\mu) d\mu$$

Angular distributions may be given in File 14 by tabulating as a function of incident neutron energy either the normalized probability distribution function, $p_k(\mu, E)$, or the Legendre polynomial expansion coefficients, $a_l^k(E)$. Provision is made in the format for simple flags to denote isotropic angular distributions, either for a block of individual photons within a reaction type or for all photons within a reaction type taken as a group.

If File 14 is used to describe the angular distributions of ***continuum*** spectra, separability of the photon energy and angular distributions is implied. If this is not an adequate representation, File 6 must be used instead.

14.2 Formats

As usual, sections are ordered by increasing reaction type (MT) numbers. The following definitions are required:

LI LI=0, distribution is not isotropic for all photons from this reaction type, but may be for some photons.
LI=1, distribution is isotropic for ***all*** photons from this reaction type.

LTT LTT=1, data are given as Legendre coefficients, where $a_0^k(E) \equiv 1.0$ is understood.
LTT=2, data are given in tabular form.

NK Number of discrete photons including the continuum (must equal the value given in File 12 or 13).

NI Number of isotropic photon angular distributions given in a section (MT number) for which LI = 0, *i.e.*, a section with at least one anisotropic distribution.

NE Number of neutron energy points given in a TAB2 record.

NL$_i$ Highest value of l required at each neutron energy E_i.

ES$_k$ Energy of the level from which the photon originates.
If the level is unknown or if a continuous photon spectrum is produced, then ES$_k$=0.0 should be used.

EG$_k$ Photon energy as given in File 12 or 13.
For a continuous photon energy distribution, EG$_k$,=0.0 should be used.

14.2.1 Isotropic Distribution (LI=1)

If LI=1, then all photons for the reaction type (MT) in question are assumed to be isotropic. This is a flag that the processing code can sense, and thus needless isotropic distribution data are not entered in the file. In this case, the section is composed of a HEAD card and a SEND card, as follows:

```
[MAT, 14, MT/  ZA, AWR, LI, 0, NK, 0]HEAD    (LI=1)
[MAT, 14, 0 / 0.0, 0.0,  0, 0,  0, 0]SEND
```

If LI=0, there are two possible structures for a section, depending upon the value of LTT.

14.2.2 Anisotropic Distribution with Legendre Coefficient Representation (LI=0, LTT=1)

The structure of a section with LI=0 and LTT=1 is:

```
[MAT, 14, MT/ ZA, AWR, LI, LTT, NK, NI]HEAD    (LI=0, LTT=1)
              <subsection for k=1>
              <subsection for k=2>
              ------------------------
              <subsection for k=NK>
[MAT, 14, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The structure of each record in the first block of NI subsections (for the NI isotropic photons) is:

```
[MAT, 14, MT/ EGk, ESk, 0, 0, 0, 0] CONT
```

There is just one CONT record for each isotropic photon. (The set of CONT records is empty if NI=0). The subsections are ordered in decreasing magnitude of EG$_k$ (photon energy), and the continuum, if present and isotropic, appears last, with EG$_k$=0.0.

This block of NI subsections is then followed by a block of NK−NI subsections for the anisotropic photons in decreasing magnitude of EG$_k$. The continuum, if present and anisotropic, appears last, with EG$_k$=0.0. The structure for the last NK−NI subsections is:

```
[MAT, 14, MT/ EG_k, ES_k, 0, 0, NR, NE/ E_int ] TAB2
[MAT, 14, MT/ 0.0, E_1, 0, 0, NL_1, 0/ a_l^k(E_1)] LIST
[MAT, 14, MT/ 0.0, E_2, 0, 0, NL_2, 0/ a_l^k(E_2)] LIST
            -------------------------------------
[MAT, 14, MT/ 0.0, E_NE, 0, 0, NL_NE, 0/ a_l^k(E_NE)] LIST
```

Note that lists of the $a_l^k(E)$ start at $l = 1$ because $a_0^k(E) \equiv 1.0$ is implicitly assumed.

14.2.3 Anisotropic Distribution with Tabulated Angular Distributions (LI=0, LTT=2)

The structure of a section for LI=0 and LTT=2 is:

```
[MAT, 14, MT/ ZA, AWR, LI, LTT, NK, NI] HEAD    (LI=0, LTT=2)
              <subsection for k=1>
              <subsection for k=2>
              ----------------------------
              <subsection for k=NK>
[MAT, 14, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The structure of the first block of NI subsection (where NI may be zero) is the same as for the case of a Legendre representation; *i.e.*, it consists of one CONT record for each of the NI isotropic photons in decreasing magnitude of EG_k. The continuum, if present and isotropic, appears last, with $\mathrm{EG}_k \equiv 0.0$. The structure of the first NI subsections is:

```
[MAT, 14, MT/ EG_k, ES_k, 0, 0, 0, 0] CONT
```

This block of NI subsections is then followed by a block of NK−NI subsections for the anisotropic photons, again in decreasing magnitude of EG_k, with the continuum, if present and anisotropic, appearing last, with $\mathrm{EG}_k \equiv 0.0$. The structure of the last NK−NI subsections is:

```
[MAT, 14, MT/ EG_k, Es_k, 0, 0, NR, NE/ E_int] TAB2
[MAT, 14, MT/ 0.0, E_1, 0, 0, NR, NP/ μ_int / p_k(μ, E_1)] TAB1
[MAT, 14, MT/ 0.0, E_2, 0, 0, NR, NP/ μ_int / p_k(μ, E_2)] TAB1
            ---------------------------------------------------
[MAT, 14, MT/ 0.0, E_NE, 0, 0, NR, NP/ μ_int / p_k(μ, E_NE)] TAB1
```

14.3 Procedures

1. The subsections are given in decreasing magnitude of EG_k within each of the isotropic and anisotropic blocks.

2. The convention is that the subsection for the continuous photon spectrum, if present, appears last in its block. In this case, $\mathrm{EG}_{NK} \equiv 0.0$.

3. The values of EG_k should be consistent within four significant figures with the corresponding EG_k values in File 12 or 13. File 12, Option 2 (transition probability arrays), the values of EG_k are implicitly determined by the level energies.

4. ES_k is the energy of the level from which the photon originates, if known. Otherwise, $ES_k = 0.0$ (as is always the case for the continuum).

5. Data should not appear in File 14 for photons that do not have production data given in File 12 or 13. Conversely, for every photon appearing in File 12 or 13 an angular distribution must be given in File 14. The neutron energy range for which the angular distributions are given should be the same as that for which the photon production data are given in File 12 or 13.

6. For LTT=1 (Legendre coefficients), the value of NL should be the minimum number of coefficients that will reproduce the angular distribution with sufficient accuracy and be positive everywhere. In all cases, NL should be an even number, ≤ 20.

7. The TAB1 records for the $p_k(\mu, E_i)$ within a subsection are given in increasing order of neutron energy, E_i.

8. The tabulated probability functions, $p_k(\mu, E_i)$, should be normalized within four significant figures (to unity).

9. The interpolation scheme for $p_k(\mu, E)$ with respect to E must be linearlinear or loglinear (INT=2 or 4) to preserve normality of the interpolated distributions. It is recommended that the interpolation in μ be linear-linear (INT=2).

10. For LI=1 (isotropic distribution), the parameter NK is the number of photons in that section and should be consistent with the NK values in Files 12 and 13.

11. The minimum amount of data should be used that will accurately represent the angular distribution as a function of both μ and E.

12. If all photons for a reaction type (MT number) are isotropic, the LI=1 flag should be used. The use of LI=0 and NI=NK is strongly discouraged. Likewise, isotropic distributions should not be entered explicitly as a tabulation or as a Legendre expansion with $a_l^k(E) \equiv 0$, $l \geq 1$.

13. Angular distributions for photons must be given for all discrete and continuum photons. This can be done by specifying the data explicitly (by giving distributions) or implicitly by using a flag meaning that all photons for a particular reaction (MT number) are isotropic. Isotropic angular distributions should be specified unless the anisotropy is $\geq 20\%$.

Chapter 15

File 15: CONTINUOUS PHOTON ENERGY SPECTRA

15.1 General Description

File 15 provides a means for representing continuous energy distributions of secondary photons, expressed as normalized probability distributions. The energy distribution of each photon continuum occurring in Files 12 and 13 should be specified in File 15 over the same neutron energy range used in Files 12 and 13. Each section of File 15 gives the data for a particular reaction type (MT number) and the sections are ordered by increasing MT number. The energy distributions, $f(E_\gamma \leftarrow E)$, are in units of eV^{-1} and are normalized so that:

$$\int_0^{E_\gamma^{\max}} f\left(E_\gamma \leftarrow E\right) dE_\gamma = 1 \ ,$$

where E_γ^{max} is the maximum possible secondary photon energy and its value depends on the incoming neutron energy as well as the particular nuclei involved.[1] The energy distributions $f(E_\gamma \leftarrow E)$ can be broken down into the weighted sum of several different normalized distributions in the following manner:

$$f\left(E_\gamma \leftarrow E\right) = \sum_{j=1}^{\mathrm{NC}} p_j(E)\, g_j\left(E_\gamma \leftarrow E\right) \qquad (\mathrm{eV})^{-1} \tag{15.1}$$

where:

NC	the number of partial distributions used to represent $f(E_\gamma \leftarrow E)$,
$g_j(E_\gamma \leftarrow E)$	the jth normalized partial distribution in the units eV^{-1} , and

[1]Note that the subscript k used in describing Files 12 and 13 has been dropped from $f(E_\gamma \leftarrow E)$. This is done because only one energy continuum is allowed for each MT number, and the subscript k has no meaning in File 15. It is, in fact, the NKth subsection in File 12 or 13 that contains the production data for the continuum.

$p_j(E)$ the probability or weight given to the jth partial distribution, $g_j(E_\gamma \leftarrow E)$.

The following condition is imposed.

$$\int_0^{E_\gamma^{\max}} g_j\left(E_\gamma \leftarrow E\right)\, dE_\gamma = 1\ .$$

Thus,

$$\sum_{j=1}^{\mathrm{NC}} p_j(E) = 1\,.$$

The absolute energy distribution cross section, $\sigma^\gamma(E_\gamma \leftarrow E)$, can be constructed from the expression:

$$\sigma^\gamma\left(E_\gamma \leftarrow E\right) = \sigma^\gamma\left(E\right) f\left(E_\gamma \leftarrow E\right) \qquad \text{(b/eV)},$$

where $\sigma^\gamma(E)$ is the integrated cross section for the continuum given either directly in File 13 or through the combination of Files 2, 3, and 12.

The system used to represent continuous photon energy distributions in File 15 is similar to that used in File 5. At present, however, there is only one continuous distribution law activated for File 15, *i.e.*,

$$g_j\left(E_\gamma \leftarrow E\right) = g\left(E_\gamma \leftarrow E\right)\ ,$$

where $g(E_\gamma \leftarrow E)$ represents an arbitrary tabulated function. In the future, new laws (for example, the fission gamma-ray spectrum) may be added.

15.2 Formats

The structure of a section is:

```
[MAT, 15, MT/ ZA, AWR, 0, 0, NC, 0] HEAD
     <subsection for j=1>
     <subsection for j=2>
--------------------------------
     <subsection for j=NC>
[MAT, 15, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

For LF=1, the structure of a subsection is:

```
[MAT, 15, MT/ 0.0, 0.0, 0, LF, NR, NP/ E_int/ p_j(E)] TAB1    (LF=1)
[MAT, 15, MT/ 0.0, 0.0, 0,  0, NR, NE/ E_int ] TAB2
[MAT, 15, MT/ 0.0, E_1,  0,  0, NR, NP/ E_γint/ g(E_γ ← E_1)] TAB1
[MAT, 15, MT/ 0.0, E_2,  0,  0, NR, NP/ E_γint/ g(E_γ ← E_2)] TAB1
     ------------------------------
[MAT, 15, MT/ 0.0, E_NE, 0,  0, NR, NP/ E_γint / g(E_γ ← E_NE)] TAB1
```

Only one distribution law is presently available (tabulated secondary photon energy distribution). Therefore, formats for other laws remain to be defined, but their structures

will probably closely parallel those in File 5 for LF=5, 7, 9, and 11. When histogram representations are used (interpolation scheme, INT=1), 0.25 to 0.5MeV photon energy bands should be used. The incident energy ranges must agree with data given in File 12 and/or 13. Other procedures are the same as those recommended for File 5 data (tabulated distribution).

15.3 Procedures

1. Photon energies, E_γ, within a subsection are given in order of increasing magnitude.

2. The TAB1 records for the $g(E_\gamma \leftarrow E_i)$ within a subsection are given in increasing order of neutron energy, E_i.

3. The tabulated functions, $g(E_\gamma \leftarrow E_i)$, should be normalized to unity within four significant figures.

4. The interpolation scheme for $p_j(E)$ must be either linear-linear or log-linear (INT=1, 2, or 3) to preserve probabilities upon interpolation. Likewise, the interpolation scheme for $(E_\gamma \leftarrow E)$ must be linear-linear or log-linear with respect to E.

5. The neutron energy mesh should be a subset of that used for the $y_{NK}(E)$ tabulation in File 12 or for the $\sigma^\gamma_{NK}(E)$ tabulation in File 13, and the energy ranges must be identical. However, the neutron energy mesh for $p_j(E)$ need not be the same as that for $g(E_\gamma \leftarrow E)$, as long as they span the same range.

6. For an MT number appearing in both File 12 and File 13, a continuous photon energy distribution (LF=1) can appear in only one of those files. Otherwise the distribution as given in File 15 could not in general be uniquely associated with a corresponding multiplicity or production cross section.

7. Use the minimum amount of data that will accurately represent the energy distribution as a function of both E_γ and E. However, do not use too coarse a mesh for E, even if the distributions are slowly varying functions of E, since the interpolated distribution will always have a non-zero component up to the maximum energy at which either of the original distributions has a non-zero component.

8. The limit on the number of neutron energy points for either $p_j(E)$ or $g(E_\gamma \leftarrow E)$ is given in Appendix G.

9. The limit on the number of photon energy points for $g(E_\gamma \leftarrow E)$ is also given in Appendix G.

Chapter 23

File 23: SMOOTH PHOTON INTERACTION CROSS SECTIONS

23.1 General Comments on Photon Production

Photon interaction data are divided into two files. File 23 is analogous to File 3 and contains the "smooth" cross sections. File 27 contains the coherent scattering form factors and incoherent scattering functions (see Chapter 27).

Electron interaction data are divided into two different files. The smooth cross sections for elastic scattering, bremsstrahlung, excitation, and the ionization of different atomic subshells are given in File 23. File 26 is used to give the angular distribution for elastically scattered electrons, the outgoing photon spectra and energy loss for bremsstrahlung, the energy transfer for excitation, and the spectra of the scattered and recoil electrons associated with subshell ionization.

Both photo-atomic and electro-atomic reactions can leave the atom in an ionized state. See Section 28 for a description of the atomic relaxation data needed to compute the outgoing X-ray and electron spectra as an ionized atom relaxes back to neutrality.

23.2 General Description

This File is for the integrated photon and electron interaction crosssections. The reaction type (MT) numbers for photon and electron interaction are in the 500 series. Several common photon and electron interactions have been assigned MT numbers:

MT	Reaction Description
523	Photo-excitation cross sections
526	Electro-atomic elastic scattering
527	Electro-atomic bremsstrahlung
528	Electro-atomic excitation cross section
533	Atomic relaxation data (see Section 28)
534-572	Photo-electric or electro-atomic subshell ionization

Photon cross sections, such as the total cross section, coherent elastic scattering cross section, and incoherent (Compton) cross section, are given in File 23, which has essentially the same structure as File 3. These data are given as a function of energy, E_γ, where E_γ is the energy of the incident photon (in eV). The data are given as energy-cross section pairs.

Similarly, electron cross sections, such as elastic scattering, bremsstrahlung, ionization, and excitation, are given in File 23. These data are given as a function of the electron energy in eV, and they are also given as energy-cross section pairs.

Each section in File 23 contains the data for a particular reaction type (MT number). The sections are ordered by increasing MT number.

23.3 Formats

The following quantities are defined:

ZA,AWR Standard material charge and mass parameters.

EPE Subshell binding energy (equal to the photoelectric edge energy) in eV. The value is zero if MT is not in the 534-599 range.

EFL Fluorescence yield (eV/photoionization).
Value is zero if not a photoelectric subshell ionization cross section.

NR,NP,E$_{int}$ Standard TAB1 interpolation parameters (see Section 1.3.1).

$\sigma(E)$ Cross section (barns) for a photon or electron of energy E given as a table of NP energy-cross section pairs.

The structure of a section is:

```
[MAT, 23, MT/  ZA, AWR, 0, 0,  0,  0] HEAD
[MAT, 23, MT/ EPE, EFL, 0, 0, NR, NP/ E_int / σ(E)] TAB1
[MAT, 23,  0/ 0.0, 0.0, 0, 0,  0,  0] SEND
```

23.4 Procedures

1. Values are usually for elements; hence, except for mono-isotopic elements, ZA=$Z \times 1000.0$; also, AWR should be for the naturally occurring element.

2. Photoelectric edges must not be multi-valued. The edges are defined by two energy points differing in the fourth or fifth significant figure.

3. Interpolation is normally log-log (INT=5).

4. Kerma factor (energy deposition coefficients) libraries will normally be local because there is no universal definition. The application will determine whether annihilation or other radiation fractions are subtracted.

Chapter 26

File 26: SECONDARY DISTRIBUTIONS FOR PHOTO- AND ELECTRO-ATOMIC DATA

26.1 General Description

This file is used to represent the secondary photons or electrons emitted after electro-atomic reactions, energy given to the residual atom, and the energy transfer associated with excitation. It is based on File 6 formats with appropriate simplifications.

Elastic scattering is represented by the normalized angular distribution for the scattered electron given in tabulated form (LAW=2, LANG=12) for scattering cosines ranging from -1 to .999999. Because of the very large mass of the residual atom with respect to the mass of the electron, it is assumed that the electron scatters without a change of energy, and there is no energy transfer to the residual atom.

Bremsstrahlung is represented using two subsections. The electron is assumed to scatter straight ahead with an energy loss described using the LAW=8 format. The photon is assumed to be emitted isotropically with spectra given as tabulated distributions (LAW=1, LANG=1, NA=0). Energy transfer to the residual atom is ignored.

Excitation occurs when the incident electron loses some of its energy by exciting the outer electrons of the atom to higher energy states. The energy transfer to the residual atom is represented using LAW=8. The electron is assumed to continue in the straight-ahead direction.

Ionization is represented by giving a section of File 26 for each sub-shell (MT=534,535,...). There are two electrons coming out of each ionization reaction: the scattered electron and the recoil electron. Because these two particles are identical, it is arbitrarily assumed that the particle with the lower energy is the "recoil" electron, and the one with the higher energy is the "scattered" electron. If E_k is the binding energy for the sub-shell, the energy of the recoil electron varies from 0 to $(E - E_k)/2$, and the energy of the scattered electron varies from $(E - E_k)/2$ to $E - E_k$. Only the distribution for the "recoil" electron is given in File 26. The user can select a recoil energy E_r from the distribution and then generate the corresponding scattered electron with energy $E - E_k - E_r$. The value of E_k is given

in the corresponding section of File 3. It is assumed that both the scattered and the recoil electrons continue in the direction of the incident electron, and that no kinetic energy is transferred to the residual atom.

The relaxation of the residual atom left after ionization results in the emission of additional X-rays and electrons. Those spectra can be computed using the atomic relaxation data described in Section 28.

26.2 Formats

The following quantities are defined:

ZA,AWR Standard material charge and mass parameters

NK Number of subsections in this section (MT).
Each subsection describes one reaction product (in this case, photons or electrons), or a subsection can describe the energy transfer associated with excitation or bremsstrahlung.

ZAP Product identifier: zero for photons, and 11 for electrons.

LAW Distinguishes between different representations of the product distributions:

- LAW=1 continuum distribution (used for bremsstrahlung and ionization);
- LAW=2 two-body angular distribution (used for elastic); and
- LAW=8 energy transfer for excitation (used for excitation and bremsstrahlung).

NR,NP,E$_{int}$ Standard TAB1 interpolation parameters.

$y(E)$ Yield for the particle being described (the yield is always 1 in File 26, but the general format is retained for consistency with File 6).

ET(E) Energy transfer during electro-atomic excitation or bremsstrahlung (eV).

The structure of a section is:

```
[MAT,26, MT/ ZA, 0.0, 0,   0, NK,  0]HEAD
[MAT,26, MT/ZAP, 0.0, 0, LAW, NR, NP/E_int / y(E)] TAB1
   <LAW-dependent structure for product>
   ----------------------------
   repeat TAB1 and LAW-dependent structures
   for the rest of the NK subsections
   ----------------------------
[MAT,26,MT/ 0.0, 0.0, 0,   0,  0,  0]SEND
```

The subsections for bremsstrahlung are given in the order photons, then electrons. The contents of the subsection for each LAW are given below.

26.2.1 Continuum Distribution (LAW=1)

This law is the same as LAW=1 for File 6, except that only LANG=1, NA=0, representing a simple tabulated energy distribution without angle dependence, is allowed.

26.2.2 Two-Body Angular Distribution (LAW=2)

This law is the same as LAW=2 for File 6, except that only LANG=11-15 for linear-linear tabulated angular distributions, is allowed. It is only used for the electro-atomic elastic scattering reaction, and the cosine range is -1 to 0.99999.

26.2.3 Energy Transfer for Excitation (LAW=8)

This law is used to give only the energy transfer during excitation and the energy loss for bremsstrahlung:

[MAT,26, MT/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / ET(E)] TAB1

Chapter 27

File 27: ATOMIC FORM FACTORS OR SCATTERING FUNCTIONS

27.1 General Description

The ENDF system for neutron and photon production data allows two alternatives for storing angular distribution data. One is by probability per unit $\cos(\theta)$ vs. $\cos(\theta)$, and the other is by Legendre coefficients. Actually, neither of these is a "natural" method for photons. The natural method would be atomic form factors or incoherent scattering functions. These are discussed briefly below.

27.1.1 Incoherent Scattering

The cross section for incoherent scattering is given by:

$$\frac{d\sigma_i(E, E', \mu)}{d\mu} = S(q; Z)\frac{d\sigma_i(E, E', \mu)}{d\mu} \ , \tag{27.1}$$

where:

$d\sigma_i/d\mu$ the Klein-Nishina cross section[1] which can be written in a closed form.

$S(q; Z)$ the incoherent scattering function. At high momentum transfer (q), S approaches Z. In the other limit, $S(0, Z) = 0$.

q the momentum of the recoil electron (in inverse angstroms[2]).

$$q = \alpha \left[1 + \left(\frac{\alpha'}{\alpha}\right)^2 - 2\mu\left(\frac{\alpha'}{\alpha}\right)\right]^{1/2} \tag{27.2}$$

[1] O. Klein and Y. Nishina, Z. Phys. 52, 853 (1929).

[2] In ENDF, q is given in inverse angstroms, as customarily reported in the literature. The above equation shows q in m_0c units. See Appendix H for unit conversions.

α $= E_\gamma / m_0 c^2$,

E'_γ scattered photon energy,

μ $\cos\theta$.

The angular distribution can then easily be calculated. Values of $S(q;Z)$ are tabulated as a function of q in File 27. The user presumably will have subroutines available for calculating q for energies and angles of interest and for calculating Klein-Nishina cross sections. The user will then generate the cross sections for the appropriate cases by calculating q's, looking up the appropriate values of S, and substituting them in the above formula.

27.1.2 Cooherent Scattering

The coherent scattering cross section is given by:

$$\frac{d\sigma_{\text{coh}}(E,E',\mu)}{d\mu} = \pi r_0^2 \left(1+\mu^2\right) \left\{ \left[F(q;Z)+F'(E)\right]^2 + F''(E)^2 \right\} , \tag{27.3}$$

where:

q $= \alpha \left[2(1-\mu)\right]^{1/2}$, the recoil momentum of the atom (in inverse angstroms),

r_0 $= e^2/m_0c^2$, the classical radius of the electron.

$F'(E)$ the real part of the anomalous scattering factor.

$F''(E)$ the imaginary part of the anomalous scattering factor.

The quantity $F(q;Z)$ is a form factor, which can be easily tabulated. At high momentum transfer (q), F approaches zero. In the other limit $F(0;Z)$ tends to Z. The anomalous scattering factors are assumed to be isotropic. In addition, they smoothly approach zero at 1.0 MeV and can be assumed to be zero at higher energies.

An alternative way of presenting the photon scattering data would be to tabulate incoherent scattering functions and form factors. Users could then provide processing codes to generate the cross sections from this information. The calculation is quite straightforward and allows the user to generate all his scattering data from a relatively small table of numbers. The incoherent and coherent scattering data should always be presented as scattering functions and form factors, respectively, whether or not data are included in File 6.

27.2 Formats

The structure of a section is very similar to that of File 3 (and 23) and is:

```
[MAT, 27, MT/  ZA, AWR, 0, 0,  0,  0] HEAD
[MAT, 27, MT/ 0.0,   Z, 0, 0, NR, NP/ q_int / H(q;Z)]TAB1
[MAT, 27,  0/ 0.0, 0.0, 0, 0,  0,  0] SEND
```

The general symbol $H(q;Z)$ is used for either $F(q;Z)$ or $S(q;Z)$ for coherent and incoherent scattering, respectively, or for the anomalous factors:

```
[MAT, 27, MT/  ZA, AWR, 0, 0,  0,  0] HEAD
[MAT, 27, MT/ 0.0,   Z, 0, 0, NR, NP/ E_int / F(E)]TAB1
[MAT, 27,  0/ 0.0, 0.0, 0, 0,  0,  0] SEND
```

27.3 Procedures

1. Values of $H(q;Z)$ should be entered in each case for the entire energy range for which integrated coherent and incoherent cross sections are given in File 23. This is true even though the respective values may be 0.0 or Z over most of the (higher) energy range.

2. The value of Z is entered in floating-point format.

Chapter 28

File 28: ATOMIC RELAXATION DATA

28.1 General Description

An atom can be ionized due to a variety of interactions. For example, due to photon or electron interactions the probability of ionizing a particular subshell of the atomic structure (K, L1, L2, *etc.*) is determined by using the subshell cross sections (MT=534-599). For example, if an incident photon of energy E ionizes the K subshell with binding energy E_K, the atom will emit an electron with energy $E - E_K$, and the atomic structure will be left ionized, with a "hole" in the K subshell. One way the atom can proceed to fill this hole is to bring down an electron from a higher energy level, for example L1, with the simultaneous emission of an X-ray of energy $E_K - E_{L1}$. This is a radiative transition. An alternative path is to bring down an electron from a higher level with the simultaneous emission of an electron from that level or a higher one. As an example, you might see an electron of energy $E_K - E_{L1} - E_{M1}$, which fills the vacancy in the K shell and leaves new holes in the L1 and M1 shells. These are called non-radiative transitions. The process will then continue by filling the new holes from higher levels, *etc.*, until all the ionization energy has been accounted for by the emission of X-rays and electrons.

The electrons produced by this atomic relaxation can be used as a source for a subsequent electron transport calculation, or their energy can just be added to the local heating. The X-rays can be transported elsewhere to cause additional photo-atomic reactions. In general, the use of File 28 is indicated when high-Z materials are present and photon energies of less than 1 MeV are of interest.

This file is provided to give the information necessary to compute the emission of X-rays and electrons associated with atomic relaxation cross section. It is based on EADL, the Evaluated Atomic Data Library developed by D. E. (Red) Cullen at the Lawrence Livermore National Laboratory (LLNL).

This file gives the subshell energies, emission energies, transition probabilities, and other quantities needed to compute the X-ray and electron spectra from ionized atoms. It always uses MT=533. It works together with the photoelectric subshell cross sections from MF=23, MT=534-599.

28.2 Formats

The following quantities are defined:

ZA, AWR Standard material charge and mass parameters

NSS Number of subshells

SUBI Subshell designator (see the table below)

SUBJ Secondary subshell designator

SUBK Tertiary subshell designator
(if SUBK is zero for a particular transition, it is a radiative transition; otherwise, it is a non-radiative transition.)

EBI Binding energy for subshell (eV)

ELN Number of electrons in subshell when neutral (given as a floating-point value)

NTR Number of transitions

FTR Fractional probability of transition

ETR Energy of transition (eV)

Table of Subshell Designators

Designator	Subshell		MT
1.	K	(1s1/2)	534
2.	L1	(2s1/2)	535
3.	L2	(2p1/2)	536
4.	L3	(2p3/2)	537
5.	M1	(3s1/2)	538
6.	M2	(3p1/2)	539
etc.			

The structure of a section of File 28 is as follows:

```
[MAT,28,533/   ZA, AWR, 0, 0, NSS,   0]HEAD
[MAT,28,533/SUBI1, 0.0, 0, 0,  NW, NTR/ NW=6*(1+NTR)
            EBI1,   ELN1, 0.0,   0.0, 0.0, 0.0,
            SUBJ1, SUBK1, ETR1, FTR1, 0.0, 0.0,
            ------------------------------------
            SUBJNTR,SUBKNTR,ETRNTR,FTRNTR, 0.0, 0.0]LIST
            ------------------------------------
            [repeat LIST for the rest of the NSS subshells]
            [MAT,28,533/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

28.3 Procedures

Sections with MF=28, MT=533 are used together with either photo-atomic or electro-atomic data evaluations. The value of NSS must be consistent with the number of subshell ionization cross sections given in File 23 (MT=534,535, ...). Note that the subshell cross section MT value equals the subshell designator number SUBI plus 533. Subshell LIST records are given in order of increasing SUBI. Similarly, transitions are given in order of increasing SUBJ first, and increasing SUBK second. This means that radiative transitions appear before non-radiative ones for each subshell.

It is possible to have NTR=0 if there are no allowed transitions from higher subshells to a particular subshell.

Example 1: Atomic Relaxation Data

```
                                                                    10  0    0
 6.000000+3 11.9078164         -1          0          0          0 6001451    1
 0.000000+0 0.000000+0          0          0          0          6 6001451    2
 0.000000+0 0.000000+0          0          0          6          6 6001451    3
 0.000000+0 0.000000+0          0          0          6          2 6001451    4
 6-C -  0 LLNL        EVAL-DEC90 CULLEN                              6001451    5
                      DIST-                                          6001451    6
----ENDF/B-VI        MATERIAL  600                                  6001451    7
-----ATOMIC RELAXATION DATA                                         6001451    8
------ENDF-6 FORMAT                                                 6001451    9
converted from EADL                                                 6001451   10
                               1        451         12          0 6001451   11
                              28        533         17          0 6001451   12
                                                                    6001  0   13
                                                                    6000  0   14
 6.000000+3 11.9078164          0          0          4          060028533   15
 1.000000+0 0.000000+0          0          0         54          860028533   16
 2.910100+2 2.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+060028533   17
 5.000000+0 0.000000+0 2.820200+2 5.614880-4 0.000000+0 0.000000+060028533   18
 6.000000+0 0.000000+0 2.820300+2 1.120600-3 0.000000+0 0.000000+060028533   19
 3.000000+0 3.000000+0 2.558900+2 4.136090-1 0.000000+0 0.000000+060028533   20
 3.000000+0 5.000000+0 2.644600+2 1.361900-1 0.000000+0 0.000000+060028533   21
 3.000000+0 6.000000+0 2.644700+2 2.710990-1 0.000000+0 0.000000+060028533   22
 5.000000+0 5.000000+0 2.730300+2 4.207480-3 0.000000+0 0.000000+060028533   23
 5.000000+0 6.000000+0 2.730400+2 1.100120-1 0.000000+0 0.000000+060028533   24
 6.000000+0 6.000000+0 2.730500+2 6.320080-2 0.000000+0 0.000000+060028533   25
 3.000000+0 0.000000+0          0          0          6          060028533   26
 1.756000+1 2.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+060028533   27
 5.000000+0 0.000000+0          0          0          6          060028533   28
 8.990000+0 6.700000-1 0.000000+0 0.000000+0 0.000000+0 0.000000+060028533   29
 6.000000+0 0.000000+0          0          0          6          060028533   30
 8.980000+0 1.330000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+060028533   31
                                                                  60028  0   32
                                                                  600 0  0   33
                                                                    0 0  0   34
                                                                   -1 0  0   35
```

Example 2: Electron Interaction Data

```
 electron interaction data converted from EEDL                        10  0    0
 6.000000+3 11.9078164         -1          0          0          0 6001451    1
 0.000000+0 0.000000+0          0          0          0          6 6001451    2
 5.438673-4 1.00000+11          0          0        113          6 6001451    3
 0.000000+0 0.000000+0          0          0          6         14 6001451    4
 6-C -  0 LLNL        EVAL-DEC89 CULLEN                              6001451    5
                      DIST-                                          6001451    6
----ENDF/B-VI         MATERIAL  600                                 6001451    7
-----ELECTRO-ATOMIC DATA                                             6001451    8
------ENDF-6 FORMAT                                                 6001451    9
 converted from EEDL                                                 6001451   10
                                1        451         24          0 6001451   11
                               23        526         37          0 6001451   12
                               23        527         31          0 6001451   13
                               23        528         64          0 6001451   14
                               23        534         12          0 6001451   15
                               23        536         14          0 6001451   16
                               23        538         15          0 6001451   17
                               23        539         15          0 6001451   18
                               26        526        353          0 6001451   19
                               26        527        197          0 6001451   20
                               26        534        120          0 6001451   21
                               26        536        151          0 6001451   22
                               26        538        155          0 6001451   23
                               26        539        155          0 6001451   24
                                                                   6001  0   25
                                                                   6000  0   26
 6.000000+3 11.9078164          0          0          0          060023526   27
 0.000000+0 0.000000+0          0          0          1        10160023526   28
        101          2                                             60023526   29
 1.000000+1 3.063510+9 1.258930+1 2.498030+9 1.584890+1 2.036940+960023526   30
 1.995260+1 1.660950+9 2.511890+1 1.354370+9 3.162280+1 1.104370+960023526   31
 3.981070+1 9.008210+8 5.011870+1 7.347880+8 6.309570+1 5.993570+860023526   32
 7.943280+1 4.889770+8 1.000000+2 3.991460+8 1.258930+2 3.258180+860023526   33
 1.584890+2 2.659610+8 1.995260+2 2.171000+8 2.511890+2 1.772160+860023526   34
 3.162280+2 1.447630+8 3.981070+2 1.183030+8 5.011870+2 9.667950+760023526   35
 6.309570+2 7.900840+7 7.943280+2 6.458900+7 1.000000+3 5.282720+760023526   36

...

 6.000000+3 11.9078164          0          0          1          060026526  223
 1.100000+1 5.438673-4          0          2          1          260026526  224
          2          2                                             60026526  225
 1.000000+1 1.000000+0 1.00000+11 1.000000+0                       60026526  226
 0.000000+0 0.000000+0          0          0          1         1660026526  227
         16          2                                             60026526  228
```

```
 0.000000+0 1.000000+1         12          0          4          260026526  229
-1.000000+0 5.000000-1 9.999990-1 5.000000-1                      60026526  230
 0.000000+0 1.000000+3         12          0         54         2760026526  231
-1.000000+0 7.349540-3-6.350000-1 1.014680-2-3.300000-1 1.408430-260026526  232
-7.500000-2 1.996880-2 1.350000-1 2.832790-2 3.000000-1 3.982680-260026526  233
 4.300000-1 5.580130-2 5.350000-1 7.828660-2 6.225000-1 1.108190-160026526  234
 6.925000-1 1.559570-1 7.500000-1 2.204030-1 7.950000-1 3.078220-160026526  235
 8.325000-1 4.339260-1 8.625000-1 6.085020-1 8.875000-1 8.591520-160026526  236
 9.080000-1 1.212620+0 9.250000-1 1.713720+0 9.390000-1 2.413930+060026526  237
 9.510000-1 3.432260+0 9.610000-1 4.874960+0 9.690000-1 6.802370+060026526  238
 9.760000-1 9.598280+0 9.820000-1 1.360430+1 9.870000-1 1.914880+160026526  239
 9.915001-1 2.744700+1 9.956001-1 4.014720+1 9.999990-1 6.259920+160026526  240
 0.000000+0 2.000000+3         12          0         64         3260026526  241
-1.000000+0 3.008670-3-9.000000-1 3.301630-3-5.350000-1 4.906250-360026526  242

...

 6.000000+3 11.9078164          0          0          1          060026534  775
 1.100000+1 5.438673-4          0          1          1          260026534  776
          2          2                                           60026534  777
 2.910100+2 1.000000+0 1.00000+11 1.000000+0                      60026534  778
 0.000000+0 0.000000+0          1          2          1          760026534  779
          7          2                                           60026534  780
 0.000000+0 2.910100+2          0          0          4          260026534  781
 1.000000-2 1.111110+1 1.000000-1 1.111110+1                      60026534  782
 0.000000+0 2.973140+2          0          0          4          260026534  783
 3.152220-2 3.265060-1 3.152220+0 3.143760-1                      60026534  784
 0.000000+0 1.995260+3          0          0         28         1460026534  785
 1.000000-1 7.771360-3 6.309570+0 7.133700-3 1.412540+1 6.229690-360026534  786
 3.162280+1 5.440240-3 6.309570+1 4.054250-3 8.912520+1 3.138130-360026534  787
 1.258930+2 2.429030-3 1.778280+2 1.605960-3 2.511890+2 1.061790-360026534  788
 3.162280+2 7.491710-4 3.758380+2 5.767510-4 4.869680+2 3.895820-460026534  789
 6.309570+2 2.631530-4 8.521260+2 2.098710-4                      60026534  790
 0.000000+0 3.981070+4          0          0         70         3560026534  791
 1.000000-1 7.237010-3 6.309570+0 6.655140-3 1.412540+1 5.837310-360026534  792
 3.162280+1 5.119990-3 6.309570+1 3.846900-3 8.912520+1 2.990940-360026534  793
 1.258930+2 2.325440-3 1.496240+2 1.886340-3 1.938660+2 1.378130-360026534  794

...

 2.06836+10 4.46563-21 2.51189+10 3.13693-21 3.16228+10 2.30613-2160026539 1357
 3.98107+10 1.69536-21 5.00000+10 1.51523-21                      60026539 1358
                                                                  60026   0 1359
                                                                  600 0   0 1360
                                                                    0 0   0 1361
                                                                   -1 0   0 1362
```

Chapter 29

INTRODUCTION TO DATA COVARIANCE FILES

29.1 General Comments

The inclusion of uncertainty estimates is intrinsic to any evaluation of physical constants because the practical utility of a "constant" depends on whether the true magnitude of the quantity is sufficiently close to the quoted best value. The need is now accepted to include uncertainties in evaluated nuclear cross section files in order that the propagated uncertainties in nuclear analytic results can be estimated. The resulting files are called "covariance files" as shorthand for a more complete name such as "files of nuclear variance and covariance data." The priority for development of formats and evaluation of covariance data is highest where the sensitivity of important calculated results to the quantities in the associated cross section file is high.

Until ENDF/B-IV, the only means available to evaluators for communicating the estimated uncertainties in the evaluated data was through publication of the documentation of the evaluations. During the preparation of ENDF/IV and -V, a Data Covariance Subcommittee of CSEWG was formed to coordinate the efforts at standardizing statements made about the data uncertainties and correlations.

One of the important aspects of nuclear data and of cross sections in particular is that the various data tend to be correlated to an important degree through the measurement processes and the different corrections made to the observable quantities to obtain the microscopic cross sections. In many applications when one is interested in estimating the uncertainties in calculated results due to the cross sections, the correlations among the data play a crucial role.

In principle, the uncertainties in the results of a calculation due to the data uncertainties can be calculated, provided one is given all of the variances in and covariances among the data elements. In practice, in addition to the uncertainties due to the basic data, the results of calculations have uncertainties due to imperfections in the calculational models used. In some situations "modeling uncertainties" may dominate the uncertainties in computed results; in others they are negligible compared to the effects of microscopic data uncertainties. In principle improving the models may reduce "modeling uncertainties", although sometimes at a large cost. The data uncertainties may also be reduced, often at large costs, by performing better measurements, new kinds of measurements, or sometimes a more refined analysis of existing data.

One of the requirements of the uncertainty information is that it be easily processed to yield the (variances and) covariances for the multigroup or other "data" used directly in the calculations.

For ENDF/B-IV, the principle of having the uncertainty information on the data file was adopted and a trial formalism was developed. This formalism has the virtue that the information is in such a form that it can be easily processed with minor modification to existing processing codes. Only a few evaluations of ENDF/B-IV were issued with data covariance information in this format. Since then, considerably more work has been done in trying to quantify data covariances within the ENDF formalism and using the information for purposes of sensitivity studies. These sensitivity studies have been made in three different areas where the data covariances play a crucial role: propagation of uncertainties to final calculated results, adjustment of data sets incorporating information from some integral measurements, and determination of data accuracies needed to meet targeted uncertainties in results. The formalism and formats for representing data covariances in ENDF/B-V were extended to cover all neutron cross section data in the files.

Formats and procedures exist in ENDF-6 for representing the data covariances in fission neutron multiplicity (File 1), resonance parameters (File 2), neutron cross sections (Files 3 and 10), angular distributions (File 4) and energy distributions (File 5). There is also the capability to represent data covariances obtained from parameter covariances and sensitivities. The ability to represent cross section uncertainties is rather complete, while for other parameters in the ENDF files there may be restrictions. In cases such as inelastic scattering one may employ the subterfuge of pseudo-discrete levels to treat a continuum using the formats and procedures of Files 3 and 33.

Since covariance files may be incomplete, the absence of covariance data in a file in ENDF-6 formats does not imply that the uncertainty component of interest has been evaluated as zero. Evaluators should not unintentionally enter explicit zero covariance components into a file, since these would imply to a user that the uncertainty or correlation has been evaluated as negligibly small.

The dominant reason for the inclusion of covariance files in the ENDF system is to enable estimation of nuclear data contributions to the uncertainties in calculated results for nuclear systems having broad (neutron) spectra. Therefore, in developing the ENDF formats the highest priority was given to attaining this goal. The ENDF covariance files are structured to enable processing them to any energy group structure. As is explained most fully in Chapter 33, except for LB=8 and 9 sub-subsections, the stored quantities are defined to yield the covariances between point cross sections. To simplify processing, the magnitudes of these components are constant between the points on the defined energy grid.

The files have a histogram appearance, but the quantities have a precise definition that can lead to incorrect inferences if the encoded values are used for other than the primary purpose of uncertainty propagation with broad particle energy spectra. For example, File 33 (except for LB=8 and 9) sub-subsections literally implies that the cross sections at any two points within the same energy grid interval are perfectly correlated, and that the uncertainty is no larger for a cross section averaged over a tiny energy interval than if it were averaged over the whole interval between grid points. The LB=8 and 9 formats allow the evaluator to avoid this unrealistic implication. A broadly spaced energy grid was usually chosen in the past to achieve the primary purpose without attempting to provide greater covariance data detail than is warranted by the available information.

As indicated above, the main purpose of the covariance information in ENDF-6 formats is to permit the propagation of nuclear data uncertainties for applications with broad neutron spectra. Users of the file should interpret the files as they were designed. If modifications to the covariance data must be made by users to place the data on a finer grid without reconsideration of the uncertainties in the underlying data, those modifications should be designed so that the original evaluator's covariance data is recovered if the modified results are collapsed to the evaluator's energy grid.

Modifications of covariance files to a finer grid have been required in the past by users who employ the adjustment equations to update an existing evaluation by "adding" new data and their associated covariances. To minimize the extent to which such users will be tempted to make *ad hoc* changes to covariance files, covariance evaluators for reactions of particular importance should employ relatively fine energy meshes to reduce the difficulties to be encountered by future evaluators/users of the covariance files. Overlapping structures in energy and other techniques should be used to reduce the occurrence of large changes in correlation as one crosses any arbitrary energy boundary. The File 30 format provides an alternate way to avoid the effects of artificial energy boundaries.

It is appropriate to define uncertainty quantities[1]. Each cross section or related quantity in an ENDF file represents a physical quantity that has a definite, though unknown true magnitude. The knowledge of each such quantity X is summarized by its density function defined so that $f(X)\ \Delta X$ is the probability that the true numerical value of X lies in the range ΔX about X. The marginal density function $f(X)$ is the average over all other independent variables Y, Z, *etc.* of the overall multivariate density function for the cross section data base. The shape of a density function depends on the experiments that have been performed, relevant to estimating the true values of the data elements. The density function has unit normalization for each variable.

The "expected value", $\langle g(X)\rangle$, of any function $g(X)$ is given by the average value of that function over the marginal density function. The simplest example is the expected value of the quantity itself:

$$\langle X\rangle = \int X\ f(X)\ dX\ . \tag{29.1}$$

In practice, one often uses the same symbol for a physical quantity, its expected value, and its value in a particular data set. In the notation used in this Chapter, the true value of the physical quantity is equal to $X = \langle X\rangle + \delta X$, where $\langle \delta X\rangle = 0$. In this language the cross section, *etc.*, quantities in ENDF files are expected values.

The width of the density function reflects the scatter among experimental cross section results and/or the uncertainties ascribed to the values by the experimenters. That width is a property of the experiments, not of the cross section quantity, so one cannot in the usual sense "measure" nuclear covariance data. The width arises from the ambiguity with which each underlying experimental result defines the true value. These ambiguities are quantified as "errors" with modifiers like "systematic" or "statistical" to indicate the origin of the ambiguities and modifiers like "standard" or "relative" to indicate the normalization of the uncertainty quantities. Since both systematic errors and statistical counting errors broaden the density functions of evaluated quantities, evaluated uncertainty data must combine both types. The systematic uncertainties are harder to estimate, and are larger than statistical counting uncertainties in most modern nuclear experiments.

The ENDF-6 formats deal only with the expected values of quantities and the second-degree moments of the joint density function describing the evaluator's knowledge of the true value of the nuclear data vector. It is not necessary to assume that the density functions are normal in shape, or otherwise, unless one must estimate the probability that the true value lies within a certain range of the expected value. The ENDF-6 covariance quantities are not intended to represent, and cannot well represent, any known difference between ENDF-6 formatted cross section and some more-recently realized "better" evaluation, or any cross-section imprecision induced by ENDF-6

[1]The treatment below is paraphrased from R. Peelle, Sensitivity and Uncertainty Analysis of Reactor Performance Parameters, Advances in Nuclear Science and Technology, Vol. 14, pp 11, Lewins and Becker, Eds., Plenum Press, New York, 1982.

procedures, or the widths of any physical distributions such as the fission neutron multiplicity distribution $P(\nu)$.

The following quantities are defined that relate to the second moments of the density function. Here $\langle X \rangle$ and $\langle Y \rangle$ are cross section or related quantities in a file using ENDF-6 formats. The quantity $f(X, Y)$ is the full density function averaged over all variables other than X and Y. Recall that $\delta X = X - \langle X \rangle$.

The frequently used quantities are the covariance between X and Y:

$$\begin{aligned} \mathrm{Cov}(X, Y) &= \langle \delta X \; \delta Y \rangle \\ &= \int\int (X - \langle X \rangle)(Y - \langle Y \rangle) \; F(X, Y) \; dX \; dY, \end{aligned}$$

the variance of X:

$$\mathrm{Var}(X) = \mathrm{Cov}(X, X) = \langle \delta X^2 \rangle \; ,$$

the standard error or uncertainty in $\langle X \rangle$:

$$s(X) = [Var(X)]^{1/2}$$

and the correlation coefficient between X and Y

$$\rho(X, Y) = \mathrm{Cov}(X, Y) / \left[s(X) \; s(Y) \right] \; .$$

The relative standard error, $s(X)/\langle X \rangle$, the relative variance $\mathrm{Var}(X)/\langle X \rangle^2$ and the relative covariance, $\mathrm{Rcov}(X, Y) = \mathrm{Cov}(X, Y)/(\langle X \rangle \langle Y \rangle)$ are also often used.

Knowledge of the covariance is crucial to the joint application of the quantities X and Y; for example, the standard error in the sum $X + Y$ can lie anywhere between $s(X) + s(Y)$ and $|s(X) - s(Y)|$ depending upon the degree of correlation between X and Y. A nonzero covariance between two quantities can arise from a partial dependence of one upon the other or from a common dependence upon some third uncertain quantity.

Chapter 30

File 30. DATA COVARIANCES OBTAINED FROM PARAMETER COVARIANCES AND SENSITIVITIES

30.1 General Comments

File 30 is provided as a means of describing the covariances of tabulated cross sections, multiplicities, and energy-angle distributions that result from propagating the covariances of a set of underlying parameters (for example, the input parameters of a nuclear model code) using an evaluator-supplied set of parameter-covariances and sensitivities. Whenever nuclear data are evaluated primarily through the application of nuclear models, the covariances of the resulting data can be described very adequately, and compactly, by specifying the covariance matrix for the underlying nuclear parameters, along with a set of sensitivity coefficients giving the rate of change of each nuclear datum of interest with respect to each of the model parameters. Although motivated primarily by these applications of nuclear theory, use of File 30 is not restricted to any one particular evaluation methodology. It can be used to describe data covariances of any origin, so long as they can be formally separated into a set of parameters with specified covariances and a set of data sensitivities.

The need for a covariance format of this type became clear in connection with the R-matrix analysis of the ENDF/B-VI light-element standards. The key parameters here are the parameters of a few high-energy resonances in the relevant compound systems. Another area where this format is expected to find early application is in representing the covariances of cross sections and secondary-particle emission spectra and angular distributions due to neutron interactions in the 0.1 - 20 MeV range, when the data are obtained primarily from the optical model and statistical pre-equilibrium theory. Relevant parameters here include the optical parameters, level-density prescription, pre-equilibrium matrix elements, and gamma-ray strength functions.

It is shown below that multigroup averages of parameter sensitivities are identical to the parameter sensitivities of the corresponding multi-group data. It is the latter that are actually needed in most applications. (See Section 30.4) To take maximum advantage of this equivalence, sensitivity information is represented in File 30 in a format that is as close as possible to the format for the actual data, so that the sensitivities can be retrieved and integrated by processing codes with the

least possible modification.

It should be emphasized that File 30 is ***not*** intended as a repository for complete "evaluations of parameters." In fact, to limit the bulk of the files and to minimize processing costs, evaluators are encouraged to reduce the number of parameters and the number of sensitivities per parameter to the minimum necessary to describe data uncertainties of practical importance. In defining the format for File 30, no attempt is made to pre-judge the parameter definitions or types of nuclear theory that may be most appropriate or useful. Discussion of such points is obviously encouraged in the printed documentation, but the format itself is deliberately kept totally general. One advantage of this generality is that the results of a wide variety of evaluation methodologies can be described using a single format. As discussed in Section 30.3 below, this generality also facilitates various mathematical operations, such as diagonalizing the parameter covariance matrix.

30.1.1 Definitions

In the context of File 30 the word "sensitivity" is defined as the derivative of an evaluated quantity, call it σ, with respect to the logarithm of one of the parameters, α_i,

$$\sigma_i' \equiv \frac{\partial \sigma}{\partial (\ln \alpha_i)} = \alpha_i \frac{\partial \sigma}{\partial \alpha_i}. \tag{30.1}$$

An advantage of employing such derivatives is that σ_i' is expressed in exactly the same units as σ, whether it be an actual cross section or a distribution (energy distribution, angle distribution, double-differential quantity, *etc.*). This means, among other things, that integrations over energy and angle can be performed with minimal changes in multi-group processing codes. The use of derivatives with respect to the logarithms of the parameters also meshes nicely with the use of relative parameter covariance matrices, as shown below in equation (30.7).

As discussed in detail in Section 30.2.1, a ***subsection*** of one section of File 30 is employed to store the sensitivities of the data in one ***section*** (called the **r*eferenced*** section) of a file elsewhere in the material of interest.

It should be emphasized that normally there will not be a direct, one-to-one correspondence between the energy or angular grid in a subsection of File 30 and that used in the referenced section. This follows from the fact that the derivatives in File 30 are not actually the derivatives of individual data values. Rather, the collection of data in one such subsection should form an adequate representation of the energy and angle-dependence of the relevant derivative function, making effective use of the standard interpolation laws.

File 30 does not permit the representation of the uncertainty in independent variables (the floating-point numbers that define the energy and angle grids of an ENDF section). This would seriously complicate the calculation of the uncertainty in averaged quantities, as discussed below. Further, if σ is thought of as the output of a model calculation, quantities such as the incident energy or the outgoing angle are specified by the model-code user and have no meaningful uncertainty.

In addition, File 30 may not be used to represent uncertainty of any integer, nor the uncertainty of standalone (untabulated) quantities that affect energy or angle grids, such as masses, Q-values, and the boundaries of energy ranges. Thus, it is understood that the data fields normally used to store probability information (cross sections, multiplicities, or normalized distributions) are used in File 30 to record sensitivity information, but that other quantities have standard (MF$\neq$30) ENDF definitions.

30.1.2 Treatment of Various Data Types

Following the general guidelines stated above, subsections of File 30 describing cross-section (as opposed to multiplicity or distribution) sensitivities would have the same mechanical structure as sections of File 3. Of course, since sensitivities are derivatives, many more negative numbers would appear in the floating-point data fields than one normally expects to see in File 3. One can treat $\overline{\nu}$ data in File 1 in the same way as cross sections.

Some interesting points arise with respect to distributions, for example tabulated angular distribution data in File 4 for elastic scattering. If the derivatives of the normalized angular distribution $p(\theta)$ with respect to a given parameter are large, they should be described in a subsection with (MFSEN,MTSEN)=(4,2) (see Section 30.2.1).

Note that since $p(\theta)$ is normalized to unity by definition, the angle integral of the sensitivities (equal to the parameter-derivative of the angle integral) should be zero. A second important aspect of the use of two separate functions to build the actual desired data is that, in order to build the corresponding sensitivities, the product rule is employed. For example, the differential elastic cross section $\gamma(\theta)$ (barns/steradian) at angle θ is formed as a product,

$$\gamma(\theta) \equiv \frac{d\sigma}{d\Omega} = \sigma p(\theta) \ , \tag{30.2}$$

so that

$$\frac{\partial \gamma(\theta)}{\partial \alpha_i} = \sigma \frac{\partial p(\theta)}{\partial \alpha_i} + p(\theta) \frac{\partial \sigma}{\partial \alpha_i} \ . \tag{30.3}$$

Multiplying both sides of equation (30.3) by α_i, and recalling the notation of equation (30.1), one gets,

$$\gamma_i'(\theta) = \sigma p_i'(\theta) + \sigma_i' p(\theta) \ . \tag{30.4}$$

Equation (30.4) shows, then, how the sensitivity $\gamma_i'(\theta)$ is constructed from the data in two different subsections (σ_i' and p_i') of File 30, plus data (σ and p) from Files 3 and 4, respectively. The generalizations needed to treat three or more separate factors are obvious.

Both to reduce the bulk and to reduce processing costs, evaluators should simply omit reference to sections in the main evaluation that exhibit little sensitivity to a given parameter. Such omissions will be treated as if zeroes had been entered explicitly. For example, if the angular distributions are omitted from File 30, then the first term on the right in equation (30.4) will be omitted.

Just as one is permitted to employ a Legendre representation of $p(\theta)$ in File 4, one is permitted in File 30 to use a Legendre expansion to represent $p_i'(\theta)$. In fact, if it reduces the size of the files, it is preferable to use Legendre moments for $p_i'(\theta)$, even if $p(\theta)$ itself is given in tabular form. As mentioned above $p_i'(\theta)$ must integrate to zero, so the magnitude of the implied zeroth Legendre moment of $p_i'(\theta)$ is zero, not unity. These considerations of File 4-type sensitivities can be extended in an obvious way to treat neutron spectra in File 5, isomer ratios in File 9, photon-production multiplicities in File 12, fission-product yields, *etc.*

No fundamental new problems are introduced by considering double-differential data, as represented in File 6. In that case, p becomes a function $p(E', \theta)$ of both the final energy and angle of the outgoing particle. The only complication that this adds is that p_i' in equation (30.4), for example, is also doubly differential, $p_i' = p_i'(E', \theta)$. It is conceivable that p_i' for some parameter will exhibit more severe angle-energy correlations than $p(E', \theta)$

itself, so it is permitted to represent the emission sensitivities for a given reaction in File 6 format in File 30, even though the angle and energy distributions for that reaction are given separately in Files 4 and 5. In this case, the entry MFSEN=6 in the File 30 dictionary really points to both File 4 and File 5 in the main evaluation. Since the File 6 type matrix information will in general occupy more space than the approximate treatment in Files 4 and 5, this option should be exercised only on those parameters (*i.e.*, in those sections) where it is crucial.

30.1.3 Multigrouped Sensitivities

Multigroup operations on the data in an evaluation can be summarized as the performance of certain weighted integrations over incident energy, secondary particle type, secondary energy, and secondary angle. Although these operations are very complicated, there is no commonality between variables (or limits) of integration and the parameters of concern in File 30. One can take advantage of this in calculating the derivatives of multigroup-averaged data with respect to the parameters. If we introduce g as a generic group-averaged quantity (such as a single Legendre moment of one element of a multigroup scattering matrix), which corresponds to a differential quantity γ, then:

$$g = \int dE\, dE'\, d\Omega\, \gamma_i(E, E', \theta)\, \omega(E, E', \theta)\ , \tag{30.5}$$

where ω is some weighting function. As discussed below, one frequently is interested in the uncertainty in such multigroup quantities, and to obtain this uncertainty, one will first need to calculate the derivative of g with respect to the parameter α_i:

$$g_i' = \frac{\partial g}{\partial(\ln \alpha_i)} = \alpha_i \int dE\ dE'\ d\Omega\ \frac{\partial \gamma(E, E', \theta)}{\partial \alpha_i}\, \omega(E, E', \theta)\ ,$$

or

$$g_i' = \int dE\ dE'\ d\Omega\ \gamma_i'(E, E', \theta)\, \omega(E, E', \theta)\ . \tag{30.6}$$

Comparing equations (30.5) and (30.6), we obtain the useful result that the sensitivity of a multigroup value to a given parameter is equal to the multigroup average of the (energy and angle dependent) parameter sensitivity. Thus an ENDF processing program that calculates multigroup cross sections can use equation (30.5), with few modifications, to calculate the parameter sensitivity of multigroup constants, given by equation (30.6). As mentioned in the General Description above, this is the motivation for storing the sensitivities γ_i' in a format that is as close as possible to the format of the data γ.

30.2 Formats

File 30 is divided into sections identified by the value of MT. (In File 30, MT does not refer to a reaction type). Each section of File 30 begins with a HEAD record and ends with a SEND record.

30.2.1 Directory and Correspondence Table (MT=1)

The first section, MT=1, of File 30 consists of a "directory" that displays the contents and ordering of information in other sections of the file, plus an optional, cross-material "correspondence table", described below. The following quantities are defined.

NP Total number of distinct parameters.

NDIR Number of CONT records in the MF=30 directory, including the internal datablock "marker" records described below, but excluding both the correspondence table and the SEND record.

NCTAB Number of CONT records in the correspondence table, excluding the SEND record.

MP$_i$ Parameter index.

MFSEN$_i$**, MTSEN**$_i$ If nonzero, location of a section of data in the main body of the evaluation (the referenced data) that are sensitive to parameter MP$_i$.
MFSEN and MTSEN determine the formats to be used to represent the energy and angle-dependence of the sensitivities. For example, if the referenced section describes a normalized angular distribution, MFSEN=4, then any of the formats described in Chapter 4 of this manual may be employed to describe the sensitivity of the distribution in (MFSEN,MTSEN) to parameter MP$_i$.

NC$_i$ Number of records used to represent this sensitivity information. These NC records constitute a single subsection of a later section of File 30.

LIBF$_i$ Sublibrary number.

MATF$_i$ Material number.

MPF$_i$ Parameter number.

A section with MT=1 has the following structure:

```
[MAT,30,1/  ZA, AWR,   0,     0,     0,   NP] HEAD
[MAT,30,1/ 0.0, 0.0,   0,     0,  NDIR,NCTAB] CONT
[MAT,30,1/ 0.0, 0.0, MP1, MFSEN1, MTSEN1, NC1] CONT
[MAT,30,1/ 0.0, 0.0, MP2, MFSEN2, MTSEN2, NC2] CONT
     -------------------------------------
     -------------------------------------
[MAT,30, 1/ 0.0, 0.0, MPNDIR,MFSENNDIR,MTSENNDIR, NCNDIR] CONT
[MAT,30, 1/ 0.0, 0.0, MP1, LIBF1, MATF1, MPF1] CONT
[MAT,30, 1/ 0.0, 0.0, MP2, LIBF2, MATF2, MPF2] CONT
     -------------------------------------
     -------------------------------------
[MAT,30, 1/ 0.0, 0.0,MPNCTAB,LIBFNCTAB, MATFNCTAB,MPFNCTAB] CONT
[MAT,30, 1/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The directory serves as a guide for the processing codes and provides, in addition, a detailed, eye-readable list of the files and sections elsewhere in the current evaluation that are significantly sensitive to the parameters under consideration. As shown above, this information is presented in a format that is similar to the main index for this material in (MF,MT) = (1,451).

In general, a given parameter will affect the data in several different sections, so the same value of MP will appear in several consecutive entries in the dictionary. MP is higher in the ENDF hierarchy than MFSEN, which is in turn higher that MTSEN. Within the File 30 framework, then, MP can be considered an index to a "sub-material". The first value of MP_1 must be 1, the next new, non-zero value must be 2, and so on. Except for marker records, MP, MFSEN, and MTSEN must occur in normal ENDF ascending order.

Unlike the main directory in (MF,MT)=(1,451) the File 30 directory contains internal file-end and sub-material-end "markers". That is, within the range of records describing a given parameter MP, and following the final reference to a given value of MFSEN, an explicit directory entry with MFSEN=0 is given in order to indicate the end of information concerning MFSEN-type sensitivities for parameter MP.

```
[MAT,30, 1/ 0.0, 0.0, MP, 0, 0, 0] CONT
```

Similarly, following the final reference to a given value of MP in the directory, a directory entry with MP=0 is given to indicate the end of information concerning the current parameter.

```
[MAT,30, 1/ 0.0, 0.0, 0, 0, 0, 0] CONT
```

It may occur that the evaluated data for two different materials are sensitive to the same parameter, or to a common set of parameters. Here "sensitive to the same parameter" means that the same numerical value of some particular quantity was employed in generating both evaluations. If, in addition, the numerical value thus employed has a substantial uncertainty, then this would imply substantial cross-material and/or cross-library data covariances. These covariances may be important in some applications, for example, in uncertainty analyses involving physical mixtures of the materials in question. In order to represent these cross-library or cross-material covariances, the evaluator may include a correspondence table in the first section of MF=30 to identify the common set. The covariances of these parameters must be given in both evaluations, and the covariances must be identical. However, since the parameter-numbering scheme need not be the same the two evaluations, the correspondence table is also used to specify the relationship of the numbers assigned to these parameters in the two evaluations.

The index parameter NCTAB indicates the number of CONT records appearing in the correspondence table of the current evaluation. NCTAB may be zero, in which case the table is omitted. If present, the table includes, in the format shown above, the sub-library number LIBF, the material number MATF, and the parameter number MPF of a parameter in some external, or "foreign" evaluation that is identical to parameter MP of the current evaluation. A value of LIBF=0 is entered if the foreign sub-library is the same as that of the current evaluation. The correspondence table should be ordered (in ascending order) first on MP, then on LIBF, then MATF, and then MPF. No internal "marker" records are included in the correspondence table.

30.2.2 Covariance Matrix (MT=2)

The second section of File 30, MT=2, contains the NP(NP+1)/2 unique, relative covariances Rcov(I, J) of the Ith parameter with the Jth parameter in the form of NP separate LIST records. This structure permits the inclusion of a large number of parameters without requiring excessive computer storage during routine data handling. There is one such LIST record for each MP value. The structure of MT=2 is as follows:

```
[MAT,30, 2/    ZA, AWR, 0, 0,   0, NP]HEAD
[MAT,30, 2/ PARM1, 0.0, 0, 0, NCS1, 1/ {Rcov(1,K  ), K=1,NCS1}]LIST
[MAT,30, 2/ PARM2, 0.0, 0, 0, NCS2, 2/ {Rcov(2,K+1), K=2,NCS2}]LIST
[MAT,30, 2/ PARM3, 0.0, 0, 0, NCS3, 3/ {Rcov(3,K+2), K=3,NCS3}]LIST
   ------------------------------------------------
   ------------------------------------------------
[MAT,30, 2/ PARMNP, 0.0, 0, 0, 1, NP/ {Rcov(NP,NP)}] LIST
[MAT,30, 2/    0.0, 0.0, 0, 0, 0,  0] SEND
```

Since the filling of the MPth row of covariance matrix begins with the diagonal element, Rcov(MP,MP), the number of matrix elements NCS$_{MP}$ explicitly given in the list must be less than or equal to (NP-MP+1). If the number given is smaller than this, the remaining covariances in that row are taken to be zero. Evaluators can take maximum advantage of this zero-suppression feature by assigning consecutive MP-values to members of groups of strongly correlated parameters. The numerical value PARM$_{MP}$ of the MPth parameter (or optionally just a zero) is entered in the first floating-point field of the LIST.

30.2.3 Sensitivities (MT=11-999)

Sections MT≥11 contain the sensitivities. A single section in this range of MT-values is the collection of all sensitivities (or subsections) relevant to a given parameter MP. The section number is determined by the parameter index, using the relation (MT=MP+10). While evaluators should employ the minimum number of parameters necessary, no particular limit is placed on MP, other than the obvious one that MT may not exceed 999. The structure of a section with MT≥11 is as follows:

```
[MAT,30,MT/  ZA, AWR,   0,   0,   0,  NL]HEAD   MT=MP+10
          <subsection for NSUB=1>
          <subsection for NSUB=2>
          ----------------------------
          ----------------------------
          <subsection for NSUB=NL>
[MAT,30, 0/ 0.0, 0.0,   0,   0,   0,   0]SEND
```

NL in the HEAD record is the number of subsections in the current section. In other words, NL is the number of referenced sections for the current parameter. The format of a subsection of a section with MT≥ 11 is, with very few exceptions, the same as the format of the referenced section in the main body of the evaluation. Certain minor "bookkeeping"

changes are unavoidable; for example, the MF and MT positions of a data record will contain 30 and (MP+10), respectively, not MFSEN and MTSEN.

Of necessity, the subsections of a section of File 30 are simply abutted to one another without intervening SEND of FEND records. In a sense, the roles of the usual SEND and FEND records in defining data-type boundaries are taken over here by the contents of the File 30 directory. (See Section 30.2.1) For example, by reading a copy of the directory in parallel with the reading of the subsections of a single File 30 "source section" with MT≥11, a processing code could create a new ENDF-formatted evaluation on a third file from the information encountered, with MFSEN and MTSEN written into the usual MF and MT positions, and with the required SEND, FEND, and MEND records inserted.

Each subsection of the source section must be constructed so that the sensitivity information in section (MFSEN,MTSEN) of a new evaluation created in this way will comply, in all mechanical details, with the correct, current ENDF formats, as described in the chapter of this manual devoted to data of the type (MFSEN,MTSEN). Of course, requirements of completeness (for example, the requirement that MT=2 must appear in File 4 if MT=2 appears in File 3) do not apply in this context, since the absence of such information simply indicates small sensitivities.

Because of the application of the product rule, as described in Section 30.1.2 above, each ***subsection*** of a section with MT≥ 11 leads in principle to a complete multigroup, multi-Legendre table "transfer" matrix in which the sensitivities corresponding to the referenced section are combined with regular data from the other sections of the evaluation. These NL matrices, when summed, give the net sensitivity of all multigroup data to parameter MP, as in equation (30.4).

30.3 Additional Procedures

30.3.1 Relation of MP-values to Physical Parameters

Since the actual parameter definitions will vary from one evaluation to the next, it is clear that choices concerning:

a) the assignment of particular MP-values to different physical parameters, and

b) what physical parameters to omit altogether,

are left to the evaluator.

30.3.2 Parameter Values

Because many models are non-linear, the actual numerical values of the parameters PARM_n may be included in the file, in order to record the point in parameter space where the sensitivities were calculated. See the discussion of this item in Section 30.2.2 The value of PARM_n has no effect on propagated data uncertainties, so the units of PARM_n are given only in the printed documentation. At the evaluator's option, a zero may be entered in place of the actual parameter value.

30.3.3 Eigenvalue Representation

By use of eigenvalue methods[1], it is straightforward to find a linear transformation that diagonalizes a given covariance matrix. This is a useful method of locating blunders (indicated by the existence of negative eigenvalues) and redundancies (indicated by zero eigenvalues) and is recommended as a general procedure prior to submission of any covariance evaluation. Moreover, once having performed such a diagonalization of a parameter covariance matrix, one could report in MT=2 of File 30 only the eigenvalues of the matrix and, in MT=11 and above, sensitivities of the data to variations in the effectively-independent linear combinations of the parameters (as summarized in the eigenvectors). If it proves feasible in individual evaluation situations, and if it leads to a substantial reduction in the overall size of the file, evaluators are encouraged to employ this technique.

30.3.4 Thinning of Sensitivity Information

The collection of sensitivities in one subsection should form an adequate representation of the energy- and angle-dependence of the relevant derivative function, making effective use of the standard interpolation laws. "Thinning" the sensitivity information (that is, removing intermediate grid points) is encouraged, in order to reduce the size of the file, but, as a general guide, such thinning should not induce changes greater than about 10% in the reconstructed covariances.

30.3.5 Cross-file Correlations

The information in File 30 is considered to describe sources of uncertainty that are independent of those described in Files 31-40. Thus, for a given set of multigroup cross sections, the multigroup covariance matrix obtained from File 30 should be added, in a matrix addition sense, to such a matrix derived from the other files. This is the only level on which File 30 "communicates" with the other files.

A complication that can occur with respect to cross-file correlations is that there may exist strong correlations (due to normalization procedures, for example) between certain low-energy cross sections that are evaluated directly from measurements and the parameters employed to calculate the evaluated data at higher energies. If the evaluator wishes to describe these correlations, the covariances for the low-energy normalization reaction (and those for other reactions strongly correlated to it) can be "moved" from File 33 to File 30. A possible method for accomplishing this is to consider the moved data to have been evaluated by multiplying a well-known reference cross section by an uncertain, energy-dependent, correction factor. The correction factor can be assumed to have been evaluated on some fixed, coarse energy grid, with linear interpolation applied between grid points. In this case the "parameters" would be the values of the correction factors at the coarse-grid points EG_i . The sensitivities [see Eq. (30.1)] of the "experimentally evaluated" cross sections σ to these new parameters would be a series of triangular "hat" functions, with peak values $\sigma(\mathrm{EG}_i)$. (Alternative approaches exist.)

[1] For example, the SSIEV routine described in B.T. Smith, et. al., Matrix Eigenvalue Routines EISPACK Guide, 1976.

30.4 Multigroup Applications of Parameter Covariances

Given the relative covariances, $\mathrm{Rcov}(\alpha_i, \alpha_j) \equiv \mathrm{Cov}(\alpha_i, \alpha_j)/(\alpha_i \alpha_j)$, from (MF30, MT2), and the multigrouped sensitivities g'_{mi} from equation (30.6), it is straightforward to obtain the covariance between one multigroup datum g_m and another g_n. It is necessary to add the additional index to keep track of the multiplicity of data types, as well as the possible multiplicity of materials. (See discussion of the latter point at the end of Section 30.2.1) Making the usual approximation that g_m is not an extremely nonlinear function of the parameters, we expand in a Taylor series and retain only the first term,

$$\begin{aligned} \mathrm{Cov}(g_m, g_n) &= \sum_{ij} \frac{\partial g_m}{\partial \alpha_i} \frac{\partial g_n}{\partial \alpha_j} \mathrm{Cov}(\alpha_i, \alpha_j) \\ &= \sum_{ij} \alpha_i \alpha_j \frac{\partial g_m}{\partial \alpha_i} \frac{\partial g_n}{\partial \alpha_j} \mathrm{Cov}(\alpha_i, \alpha_j)/(\alpha_i \alpha_j) \\ &= \sum_{ij} g'_{mi}\, g'_{nj}\, \mathrm{Rcov}(\alpha_i, \alpha_j)\ . \end{aligned} \tag{30.7}$$

Equation (30.7) gives the desired multigroup covariance matrix in terms of the multigrouped (logarithmic) sensitivities from equation (30.6) and data read directly from the second section of File 30.

In addition to providing a direct route to the calculation of the uncertainty of multigroup cross sections due to parameter uncertainties, data provided in File 30 format have the potential for additional kinds of application, not involving straightforward application of equation (30.7). Since these issues relate to computing requirements, it is necessary to deal with specific examples. In situations presently foreseen, the number of nuclear parameters might be in the range of 10 to 100, so we take 50 as typical. On the other hand, it is easy to imagine neutronics applications where the number of individual multigroup constants exceeds 10000. For example, if there are 3 high-threshold neutron-emitting reactions for a given material, the number of individual cross section items might be 3 reactions × 10 "source" groups × 80 "sink" groups × 4 Legendre tables = 9600. In such cases, the data covariance matrix $\mathrm{Cov}(g_m, g_n)$ becomes prohibitively large (10^8 items), while the sensitivity matrix g'_{mi} (containing 500 000 items) and parameter covariance matrix $\mathrm{Rcov}(\alpha_i, \alpha_j)$ (with 2500 items) remain fairly manageable. Since, according to equation (30.7), all covariance information content is already contained in the latter two items, it seems likely that multigroup libraries for high-energy neutronics applications will store these items separately, rather than in the expanded product form.

Further efficiencies are possible if the ultimate aim is to calculate the uncertainties in a set of predicted integral quantities (dose, radiation damage, fuel-breeding ratio, *etc.*), which can be denoted by a column vector, $\boldsymbol{y}$. A typical number of such quantities might also be around 50. The covariance matrix $\mathbf{D}(\boldsymbol{y})$ for the integral quantities is related (again in the first-order approximation) to the cross section covariance matrix $\mathbf{D}(\boldsymbol{g})$, with elements given

by equation (30.7), by the familiar propagation of errors relation,

$$\mathbf{D}(\boldsymbol{y}) = \mathbf{S}\,\mathbf{D}(\boldsymbol{g})\,\mathbf{S}^T \tag{30.8}$$

where $\mathbf{S}$ is the 50×10000 sensitivity matrix relating the integral quantities $\boldsymbol{y}$ to the multigroup cross sections $\boldsymbol{g}$. Matrix $\mathbf{S}$ can be obtained from standard neutronics analyses. If we introduce a 10000×50 matrix $\mathbf{R}$, having elements g'_{mi} that define the sensitivities of multigroup constants to a set of parameters $\boldsymbol{\alpha}$ in the file, equation (30.7) can be rewritten in matrix form,

$$\mathbf{D}(\boldsymbol{g}) = \mathbf{R}\,\mathbf{D}(\boldsymbol{\alpha})\mathbf{R}^T \tag{30.9}$$

Equation (30.8) then becomes

$$\mathbf{D}(\boldsymbol{y}) = \mathbf{S}\left[\mathbf{R}\,\mathbf{D}(\boldsymbol{\alpha})\,\mathbf{R}^T\right]\mathbf{S}^T = \mathbf{T}\,\mathbf{D}(\boldsymbol{\alpha})\,\mathbf{T}^T \tag{30.10}$$

The product matrix $\mathbf{T} = \mathbf{SR}$, which contains the direct sensitivity of the integral data $\boldsymbol{y}$ to the nuclear-model parameters $\boldsymbol{\alpha}$, is very compact, having about the same size as the covariance matrix $\mathbf{D}(\boldsymbol{\alpha})$. Note that in evaluating the matrix products in equation (30.9) one actually never needs to calculate the full $10\,000 \times 10\,000$ cross section covariance matrix.

In cases where the evaluator chooses to use File 33 for certain data and File 30 for others, there is no logical problem with adding together integral covariances $\mathbf{D}_{33}(\boldsymbol{y})$ based on conventional sensitivity and uncertainty analysis (*i.e.*, based on Files 3 and 33 only) with analogous data $\mathbf{D}_{30}(\boldsymbol{y})$ obtained from File 30, using equation (30.9), because the data covariances due to the parameter covariances are, by definition, independent of those described in the other covariance files.

Chapter 31

File 31. COVARIANCES OF THE AVERAGE NUMBER OF NEUTRONS PER FISSION

31.1 General Comments

For materials that fission, File 31 contains the covariances of the average number of neutrons per fission, given in File 1. MT=452 is used to specify $\overline{\nu}$, the average total number of neutrons per fission. MT=455 and MT=456 may be used to specify the average total number of delayed neutrons per fission, $\overline{\nu}_d$, and the average number of prompt neutrons per fission, $\overline{\nu}_p$, respectively.

The average number of neutrons per fission is given as a function of incident energy for particle-induced fission. This energy dependence may be given by tabulating the values as a function of incident particle energy or (if MT=452 alone is used) by providing the coefficients for a polynomial expansion as a function of incident neutron energy. Whichever method is used, the result is that the quantities are specified as a function of incident neutron energy and in this sense are similar to the data given in File 3. Therefore, the problems associated with representing the covariances of the average number of neutrons per fission are identical to those in File 33.

For spontaneous fission, in the sub-library for a radioactive decay, the average multiplicities are given by zero-order terms in polynomial expansions, and the lack of any energy dependence is recognized in the formats.

31.2 Formats

Particle-induced fission formats for fission neutron multiplicity in File 31, MT=452, 455, and 456, are directly analogous to those for File 33 given in Section 33.2.

Spontaneous fission formats for neutron multiplicity in File 31, MT=452, 455 and 456, are modified from those in Section 33.2 because there is no energy dependence to express for $\overline{\nu}$ or its covariance components. There, NC and NI-type subsubsections for spontaneous

fission neutron multiplicity have no energy variables present.

"NC-type" subsubsections for spontaneous fission $\overline{\nu}$, MT=452, 455, or 456, have the following structure, using definitions given in Section 33.2:

For LTY=0:

```
[MAT,31, MT/ 0.0, 0.0,    0, LTY,     0,   0]CONT    (LTY=0)
[MAT,31, MT/ 0.0, 0.0,    0,   0, 2*NCI, NCI/ {CI,XMTI}]LIST
```

For LTY=1, 2, or 3:

```
[MAT,31, MT/ 0.0, 0.0,    0, LTY,    0,    0] CONT
[MAT,31, MT/ 0.0, 0.0, MATS, MTS,    4,    1/
            ------(XMFS,XLFSS)(0.0, Weight) ]LIST
```

"NI-type" subsubsections for spontaneous fission neutron multiplicity are allowed with LB=0 and LB=1, and have the structure:

```
[MAT,31, MT/ 0.0, 0.0, 0, LB, 2, 1/(0.0,F)] LIST
```

where F gives the absolute or relative covariance component depending on whether LB=0 or LB=1. (See Section 33.2 of this manual for notation.)

31.3 Procedures

All procedures given in Section 33.3 concerning the ordering and completeness of sections of File 33 apply to sections of File 31: $\overline{\nu}$ (MAT,31,452), $\overline{\nu}_d$ (MAT,31,455) and $\overline{\nu}_p$ (MAT,31,456). Note that in File 1 $\overline{\nu}$ (MT=452), $\overline{\nu}_d$ (MT=455) and $\overline{\nu}_p$ (MT=456) satisfy the relation:

$$\overline{\nu}(E) = \overline{\nu}_d(E) + \overline{\nu}_p(E) \ . \tag{31.1}$$

Therefore, if one of these quantities is "derived" in terms of the other two, it is permissible to use NC-type subsections with LTY=0 to indicate that it is a "derived redundant cross section". See Section 33.2.2.1 for an explanation of this format.

If a section of File 31 is used with MT=456, there must also be a section of File 31 with MT=452.

When a section of File 31 for either MT=452, 455 or 456 is used for induced fission, there must be a section in File 33 for the fission cross sections, *i.e.*, section (MAT,33,18).

Note:

1. Since $\overline{\nu}_d$ is much smaller than $\overline{\nu}_p$, it should never be evaluated by subtracting $\overline{\nu}_p$ from $\overline{\nu}$.

2. When a polynomial representation is used to describe the data in File 1 MT=452, the covariance file applies to the tabular reconstruction of the data as a function of energy and not to the polynomial coefficients.

3. The ENDF-6 formats do not provide for covariance references between different sublibraries except by use of File 30. Therefore, it is not possible to express the covariances between, for example, the $\overline{\nu}$ for spontaneous fission of ^{252}Cf and the $\overline{\nu}(E)$ for the major fissile materials by use of NC-type subsubsections with LTY=1, 2, and 3.

4. In ENDF-6 formats there is no provision to express uncertainty in MT=455 for the decay constants for the various precursor families.

Chapter 32

File 32. COVARIANCES OF RESONANCE PARAMETERS

32.1 General Comments

File 32, MT=151, contains the variances and covariances of the resonance parameters given in File 2, MT=151. The resonance parameters, used with the appropriate resonance formulae, provide an efficient way to represent the complicated variations in the magnitudes of the different resonant partial cross sections, compared to the use of File 3 alone. Similarly for File 32, the use of the covariances of the resonance parameters of individual resonances provides an efficient way of representing the rapid variation over the individual resonances of the covariances of the partial cross sections. The covariance data of the processed cross sections include the effects of both File 32 and File 33 within a given energy region, similar to the way the cross sections themselves are the sum of contributions from File 2 and File 3.

In the resonance region, the covariances of the partial cross sections are often characterized by

a) "long-range" components that affect the covariances over many resonances, and

b) "short-range" components affecting the covariances of the different partial cross sections in the neighborhood of individual resonances.

The former often can best be represented in File 33, while the latter can be given in File 32.

When the material composition is dilute in the nuclide of concern and the cross sections are to be averaged over an energy region that includes many resonances, the effects of "short-range" components are unimportant and the covariances of the averaged cross sections can be well represented by processing the long-range components given in File 33. Therefore, the covariances of the cross sections in the unresolved resonance energy region should be given entirely by means of File 33 unless resonance self-shielding in this energy region is thought to be of practical significance for a particular nuclide. For many nuclides these conditions may also be valid in the high-energy portion of the resolved resonance energy region.

In the resolved resonance region it may be necessary to calculate covariances for the resonance self-shielding factors to obtain the uncertainty in the Doppler effect. As another

example, one may require group cross-section covariances where the groups are narrow compared to the resonance width or where only a few resonances are within a group. In these cases File 32 should be used. Because this situation may be important only in the lower energy portion of the resolved resonance region, File 32 need not include the whole set of resonances given in File 2. File 33 remains available for use in combination with File 32.

The ENDF-6 formats for File 32 are structured to maintain compatibility with those of ENDF/B-V, and there are new features to permit representation of covariance components among the parameters of different resonances. Covariances between resonance energies and widths are now also allowed. While File 32 was limited in ENDF/B-V to the Breit-Wigner representations (LRF=1 or 2), in ENDF-6 formats covariances may also be given for the Reich-Moore (LRF=3), Adler-Adler (LRF=4) and R-Matrix Limited (LRF=7) formulations. A limited representation is offered for unresolved resonance parameter covariance data. The conventions are retained that the cross section covariances for the resonance region are combined from covariance data in File 32 and File 33, and that relative covariances given in File 33 apply to the cross sections reconstructed from File 2 plus File 3 when that option is specified in File 2. (There is a partial exception for LRF=4.) Since the ENDF-6 formats do not allow a continuous range of values for the total angular momentum J of a resonance, covariance data for the resonance spin are no longer recognized.

Note that File 32 formats retain many restrictions. For example, there is no provision for representing covariances between the parameters of resonances in two different materials or in two isotopes within the same elemental evaluation. Since File 32 can become cumbersome if many resonances are treated, evaluators will do so only for nuclides of greatest practical importance. (The LCOMP=2 format is available for use in the case of very many resonances; this format provides a compact but approximate representation for the resonance parameter covariance matrix. Details are given in Section 32.2.3).

The strategy employed for File 32 is similar to that for smooth cross sections in that the variance of a resonance parameter or the covariance between two such parameters can be given as a sum of several components. Some contributions can be labeled by resonance energy and parameter type, while others can arise from long-range covariances among parameters of the same type for different resonances in the same isotope. The latter are labeled by energy bands, and the same uncertainty characteristic is applied to the indicated parameter of all the File 2 resonances in a given band.

The idea of assigning the same relative covariance to all parameters of a given type in an energy region has limited validity. One limit arises because long-range uncertainties in reaction yields don't generally carry over proportionately to uncertainties in the corresponding reaction widths. However, gamma-ray widths are sometimes known only for resonances at low neutron energy, and then the average of these values is used for the resonances at higher energies. This situation motivates formats resembling File 33 except that a relative uncertainty in the file applies to the indicated parameter (*e.g.*, Γ_γ) of every resonance in the indicated energy range. The approach here is to allow the long range correlations to extend over any energy interval in which consistent resolved resonance formulations are utilized.

The definitions of common quantities are as given in Chapter 2.

Caveat: Resonance parameter covariance matrices reported in File 32 are written in terms of parameters given in File 2 listing; this is true even when a given parameter is not the

actual quantity used in the calculation. In particular, if the value GAM given in File 2 for the partial width is negative, the negative sign is to be associated with the reduced width amplitude γ_{λ_c} rather than with Γ_{λ_c} (since Γ_{λ_c} is always a positive quantity). More specifically, $\Gamma_{\lambda_c} = |\text{GAM}|$ and $\gamma_{\lambda_c} = \text{sign}(\text{GAM} \times \sqrt{|\text{GAM}|/2P})$, with P evaluated at the energy of the resonance. In this case the covariance matrix is written in terms of GAM rather than Γ_{λ_c}. [See Section 2.2.1 for details; the rule applies for LRF=1, 2 and 3, as well as for LRF=7].

32.2 Formats

The format for File 32, MT=151, parallels the format for File 2, MT=151, with the restriction to LRF=1,2,3,4 or 7 for LRU=1 (resolved parameters) and to LRF=1 for LRU=2 (unresolved parameters). The File 32 format for LRU=1, LRF=7 may omit some of the File 2 information. The general structure of File 32 is as follows:

```
[MAT,32,151/  ZA, AWR,   0,   0, NIS,    0]HEAD
[MAT,32,151/ ZAI, ABN,   0, LFW, NER,    0]CONT  (isotope)
[MAT,32,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
       <subsection for the first energy range for the first isotope>
[MAT,32,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
       <subsection for the second energy range for the first isotope>
            ------------------------------
            ------------------------------
[MAT,32,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
       <subsection for the last energy range for the first isotope>
            ------------------------------
            ------------------------------
[MAT,32,151/ ZAI, ABN,   0, LFW, NER,    0]CONT  (isotope)
[MAT,32,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
       <subsection for the first energy range for the last isotope>
            ------------------------------
            ------------------------------
[MAT,32,151/  EL,  EH, LRU, LRF, NRO, NAPS]CONT  (range)
       <subsection for the last energy range for the last isotope>
            ------------------------------
            ------------------------------
[MAT,32, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
[MAT, 0, 0/ 0.0, 0.0, 0, 0, 0, 0] FEND
```

Data are given for all ranges for a given isotope, then for successive isotopes. The data for each isotope start with a CONT (isotope) record; those for each range with a CONT (range) record. File segments need not be included for all isotopes represented in the corresponding File 2.

If the "range" record preceding a subsection has NRO≠0, indicating that the energy dependence of the scattering radius is given in File 2, the initial file segment within the

subsection has the form:

```
[MAT,32,151/ 0.0, 0.0, 0, 0, 0, NI]CONT
        <NI subsubsections as defined in Section 33.2.1 for the
        energy-dependent covariances of the scattering radius>
```

The next record of a subsection (the first record if NRO=0) has the form:

```
[MAT,32,151/ SPI, AP, 0, LCOMP, NLS, 0]CONT.
```

If the compatibility flag, LCOMP, is zero, NLS is the number of L-values for which lists of resonances are given in a form compatible with that used in ENDF/B-V, as described in Section 32.2.1. If LCOMP=1, then NLS=0 and subsection formats are as shown in Sections 32.2.2. If LCOMP=2, the covariance matrix is expressed in compact form as described in Section 32.2.3.

32.2.1 Compatible Resolved Resonance Format (LCOMP=0)

This format differs from that used for ENDF/B-V only in that covariances of the resonance spin are all zero. It is applicable only for resolved parameters (LRU=1) and for the Breit-Wigner formalisms (LRF=1 or 2). No long-range covariances can be defined. The following covariance quantities are defined:

DE^2	Variance of the resonance energy in units eV^2.
DN^2	Variance of the neutron width GN in units eV^2.
DNDG	Covariance of GN and GG in units eV^2.
DG^2	Variance of the gamma-ray width in units eV^2
DNDF	Covariance of GN and GF in units eV^2.
DGDF	Covariance of GG and GF in units eV^2.
DF^2	Variance of the fission width GF in units eV^2.
DJDN	(null) covariance of resonance J-value and GN.
DJDG	(null) covariance of resonance J-value and GG.
DJDF	(null) covariance of resonance J-value and GF.
DJ^2	(null) variance of resonance J-value.

A complete subsection for LCOMP=0 has the following form:

```
        <If NRO≠ 0, a control record and NI subsubsections for
        energy-dependent covariances of the scattering radius>
[MAT,32,151/ SPI,  AP, 0, LCOMP,    NLS,   0]CONT   (LCOMP=0)
[MAT,32,151/AWRI, 0.0, L,     0, 18*NRS, NRS/
            ER1, AJ1, GT1, GN1, GG1, GF1,
            DE1^2, DN1^2, DNDG1, DG1^2, DNDF1, DGDF1,
            DF1^2, DJDN1, DJDG1, DJDF1, DJ1^2,    (DJDN1,DJDG1,DJDF1=0.0)
      <three physical records for each resonance through NRS> ]LIST
      <a similar list record for each value of L through NLS>
```

Note that in this compatible format no covariance can be given between parameters of different resonances even if they overlap. This format therefore permits only a relatively crude approximation to the true resonance parameter covariance matrix.

32.2.2 General Resolved Resonance Formats (LCOMP=1)

Following the record that starts with the target spin, SPI, if it states LCOMP=1, the next card of a subsection defines for that isotope and energy range, how many (NSRS) subsections will occur for covariances among parameters of specified resonances and how many (NLRS) subsections are to contain data on long-range parameter covariances. The complete structure of an LCOMP=1 subsection is as follows:

```
        <If NRO≠0, a control record and NI subsubsections for energy
         dependent covariances of the scattering radius are given>
[MAT,32,151/ SPI,  AP, IFG, LCOMP,  NLS,    0]CONT   (LCOMP=1,NLS=0)
[MAT,32,151/AWRI, 0.0,   0,     0, NSRS, NLRS]CONT
      <NSRS subsubsections each giving covariances among specified
      parameters of enumerated sets of resonances>
      <NLRS subsubsections each giving long-range covariances
      contributions for stated energy regions for a particular type
      of resonance parameter>
```

The formats here differ from the LCOMP=0 formats of Section 32.2.1 in that covariance between parameters of different resonances appear, resonance representations LRF=1,2,3,4 and 7 are allowed, there is no segregation by L-value (or by J and parity for LRF=7), and the number of parameters considered per resonance is declared in each sub-subsection primarily to avoid tabulating zero covariances for fission widths in files concerning structural materials. The listed resonances must be present in File 2, but there is no requirement that all resonances be included in File 32 that are given in File 2.

The formats for the short-range covariances (NSRS-type) depend on the resonance formalism, while the format for the long-range covariances (NLRS-type) is general.

The following paragraphs cover the formats for the NSRS-type covariances for the various resonance formulations (LRF=1,2,3,4 and 7) for resolved parameters (LRU=1). For LRF=7, parameter NLS is is to be interpreted as NJS. Parameter IFG is relevant only for LRF=7 and its meaning is the same as in File 2, described in Section 2.2.1.6.

32.2.2.1 SLBW and MLBW (LRF=1 or 2)

These cases have the same formats. All the resonances for which covariances are to be included are divided into blocks. Covariances between parameters can only be included for resonances in the same block. (A given resonance can appear in more than one block.) A sub-subsection covers the data for a block. Within each such block, the parameters are given of those resonances for which covariances are included, and the upper triangular representation of the parameter covariance matrix is included for the whole block of resonances. For each block one specifies the number MPAR of parameters to be included for each listed resonance in the block, since for most cases there is, for example, no fission width and the size of the covariance matrix can therefore be minimized. The NSRS-type subsections have the form below for LRF=1 and 2:

```
[MAT,32,151/ 0.0, 0.0, MPAR, 0, NVS+6*NRB, NRB/
    <Parameters for each resonance for which there are
     covariance data>
          ER1, AJ1, GT1, GN1, GG1, GF1
          -----------
          -----------
          ERNRB, AJNRB, GTNRB, GNNRB, GNNRB, GGNRB, GFNRB,
    <Resonance parameter variances and covariances for
      all resonances listed>
          V1,1, V1,2, ....  V1,MPAR*NRB, V2,2,
          ---, V2,MPAR*NRB, V3,3,
          ---, VMPAR*NRB,MPAR*NRB, 0.0, 0.0] LIST
```

Note that the record first lists all the parameters of resonances in the group, for positive identification, and then lists the covariance terms. The parameters have the following meaning:

MPAR Number of parameters per resonance in this block which have covariance data (In order: ER, GN, GG, GF, GX, indices 1-5)

NVS Number of covariance elements listed for this block of resonances, NVS = [NRB×MPAR×(NRB×MPAR+1)]/2.

NRB Number of resonances in this block and for which resonance parameter and covariance data are given in this subsection.

ER Lab system energy of the kth resonance (in this block).

AJ$_k$ Floating-point value of the spin for the kth resonance.

GT$_k$ Total width (eV) for the kth resonance. GT=GN+GG+GF+GX.

GN$_k$ Neutron width of the kth resonance.

GG$_k$ Gamma width for the kth resonance.

GF$_k$ Fission width of the kth resonance.

V$_{mn}$ Variance (eV^2) or covariance matrix element, row m and column, $n \geq m$. If $j \leq$MPAR is the parameter index ($j = 4$ for fission width) for the kth resonance in the block, $m = j + (k-1) \times$ MPAR. The indexing is the order defined above under MPAR.

32.2.2.2 Reich-Moore (LRF=3)

The representation for the Reich-Moore resonance formulation is very similar. The listing of the parameters among which covariance terms are allowed takes the form used in File 2, namely:

ER, AJ, GN, GG, GFA, GFB.

Similarly, in interpreting the indices for the covariance matrix of the parameters in a given block of resonances, the order when LRF=3 is ER, GN, GG, GFA, GFB and the largest possible value of MPAR is 5.

32.2.2.3 Adler-Adler (LRF=4)

The Adler-Adler resonance representation includes background constants as well as resonance parameters. The uncertainty in the background constants is to be treated indirectly just as the smooth background given in File 3. (That is, in the energy region EL, EU for LRF=4 any relative uncertainty data in File 33 applies to the sum of the cross section in File 3 and the contribution of the cross sections computed from the Adler-Adler background constants. Great care will be required if this uncertainty representation for Adler-Adler fits is used in other than single-isotopes evaluations.) The inherent assumption is that covariance data will be detailed for the largest resonances, and those representing the Adler-Adler backgrounds. It is assumed that LI=7.

An LRF=4 NSRS subsubsection takes the following form, using the previous definitions where possible:

```
[MAT,32,151/ 0.0, 0.0, MPAR, 0, NVS+6*NRB, NRB/
          DET1, DWT1, GRT1, GIT1, DEF1, DWF1
    <Parameters for each reference in the block>
          GRF1, GIF1, DEC1, DWC1, GRC1, GIC1
          -----------
          -----------
          DETNRB, DWTNRB, GRTNRB, GITNRB, DEFNRB, DWFNRB,
          GRFNRB, GIFNRB, DECNRB, DWCNRB, GRCNRB, GICNRB,
    <Resonance parameter variances and covariances for
      all resonances listed>
          V1,1, V1,2, ....  V1,MPAR*NRB, V2,2,
          ---, V2,MPAR*NRB, V3,3,
          ---, VMPAR*NRB,MPAR*NRB, 0.0, 0.0] LIST
```

The Adler-Adler parameters of the selected list of resonances are given in the same redundant style indicated in Section 2.2.1.3. For LRF=4 the maximum value of MPAR is 8 and for a given resonance the covariance matrix indexing is in the order:

μ = DET = DEF = DEC, ν = DWT = DWF = DWD, GRT, GIT, GRF, GIF, GRC, GIC

32.2.2.4 R-Matrix Limited Format (LRF=7)

No long-range subsections are allowed for LRF=7. For each short-range section, it is not sufficient to give merely the number of resonances in the block (as is done for LRF=3, for

example). Instead, because the LRF=7 format permits different numbers of channels for different spin-and-parity (J^π) groups, both the number of spin groups in the block and the number of channels for each spin group must be specified. As with the other LRF values, not all resonances need to be included in this listing; further, not all J^π groups need to be included here. NJSX is the number of J^π groups that are included in this short-range section; the format for specifying NJSX is:

```
[MAT,32,151] 0.0, 0.0, NJSX, 0, 0, 0]CONT
```

For each spin group the number of channels (NCH), the number of included resonances (NRB), and the number of lines per resonance (NX) must be specified. In addition, the number of values to be read (6 times the number of lines) must also be given in the LIST record, along with the resonance parameters:

```
[MAT,32,151] 0.0, 0.0, NCH, NRB, 6*NX, NX/
             ER_1, GAM_{1,1}, GAM_{2,1}, GAM_{3,1}, GAM_{4,1}, GAM_{5,1},
             GAM_{6,1}, ------ GAM_{NCH,1},
             ER_2, GAM_{1,2}, GAM_{2,2}, GAM_{3,2}, GAM_{4,2}, GAM_{5,2},
             GAM_{6,2}, ------ GAM_{NCH,2},
             ER_{NRB}, GAM_{1,NRB}, GAM_{2,NRB}, GAM_{3,NRB}, GAM_{4,NRB}, GAM_{5,NRB},
             GAM_{6,NRB}, GAM_{NCH,NRB}]LIST
```

The above two (CONT and LIST) records are repeated, once for each included J^π group.

Parameters are numbered in the order in which they appear in the listing; the total number of parameters (NPARB) is the sum (over all included J^π values) of (NCH+1)*NRB, where NRB is the number of resonances from this J^π group in the covariance block. Following the final resonance for the final J^π group in this block, the triangular half of the covariance matrix is presented as a LIST record with N entries, where N=(NPARB*(NPARB+1))/2. The covariance matrix is given in the following format:

```
[MAT,2,151] 0.0, 0.0,   0,   0,   N, NPARB/
          V_{1,1}, V_{1,2}, ....  V_{1,NPARB}, V_{2,2},
          ---, V_{2,NPARB}, V_{3,3},
          -----------------, V_{NPARB,NPARB}] LIST
```

32.2.2.5 Format for Long-Range Covariance Subsubsections (LRU=1)

Here are described the forms that the formats may take to represent long-range (in energy) covariances among parameters of a given type. The strategy is to use formats that resemble those for File 33 but refer to a particular parameter and equally to all resonances of a given isotope within the indicated energy regions.

Each subsubsection must identify the resonance parameter considered (Γ_n, Γ_γ, *etc.*) via the parameter IDP, indicate the covariance pattern via a value of LB, and give the energy regions and covariance components. The list below defines the permitted values of LB. Note the definition of one LB value not defined in File 33, and that LB=3 and 4 are not employed in File 32 because of LB=5 is typically much more convenient. The term $\mathrm{Cov}[\Gamma_{\alpha(i)}, \Gamma_{\alpha(j)}]$ is defined as the covariance between the Γ_α parameters for two different resonances (indexed i and j) in the same nuclide.

LB=-1 Relative variance components entirely uncorrelated from resonance-to-resonance but having constant magnitude within the stated energy intervals:

$$\mathrm{Cov}\left[\Gamma_{\alpha(i)}\Gamma_{\alpha(j)}\right] = \delta_{ij} \sum_{k=1}^{\mathrm{NE}-1} \mathcal{S}_i^k F_{\alpha(k)}^{(-1)} \Gamma_{\alpha(i)}^2$$

LB=0 Absolute covariance components correlated only within each energy interval.

$$\mathrm{Cov}\left[\Gamma_{\alpha(i)}\Gamma_{\alpha(j)}\right] = \sum_{k=1}^{\mathrm{NE}-1} \mathcal{P}_{j,k}^{i,k} F_{\alpha(k)}^{(0)}$$

LB=1 Relative covariance components correlated only within each energy interval.

$$\mathrm{Cov}\left[\Gamma_{\alpha(i)}\Gamma_{\alpha(j)}\right] = \sum_{k=1}^{\mathrm{NE}-1} \mathcal{P}_{j,k}^{i,k} F_{\alpha(k)}^{(1)} \Gamma_{\alpha(i)} \Gamma_{\alpha(j)}$$

LB=2 Fractional covariance components fully correlated over all energy intervals with variable magnitude.

$$\mathrm{Cov}\left[\Gamma_{\alpha(i)}\Gamma_{\alpha(j)}\right] = \sum_{k,k'=1}^{\mathrm{NE}-1} \mathcal{P}_{j,k'}^{i,k} F_{\alpha(k)}^{(2)} F_{\alpha(k')}^{(2)} \Gamma_{\alpha(i)} \Gamma_{\alpha(j)}$$

LB=5 Relative covariance components in an upper triangular representation of a symmetric matrix.

$$\mathrm{Cov}\left[\Gamma_{\alpha(i)}\Gamma_{\alpha(j)}\right] = \sum_{k,k'} \mathcal{P}_{j,k'}^{i,k} F_{\alpha(k,k')}^{(5)} \Gamma_{\alpha(i)} \Gamma_{\alpha(j)}$$

Note that the $F^{(-1)}$, $F^{(1)}$, and $\mathrm{F}^{(5)}$ parameters have the dimensions of relative covariances, the $F^{(0)}$ are absolute covariances, and the $F^{(2)}$ are relative standard deviations.

The $\mathcal{S}$ and $\mathcal{P}$ are dimensionless operators defined in Section 33.2.

The format for LB=-1, 0, 1, or 2 is:

`[MAT,32,151/ 0.0, 0.0, IDP, LB, 2*NE, NE/ {` E_k`,` $\mathrm{F}^{(LB)}$`}] LIST`

For LB=5 the requisite format is:

`[MAT,32,151/ 0.0, 0.0, IDP, LB, NT, NE/ {` E_k `}, {`$\mathrm{F}_{kk'}^{(5)}$`}] LIST  (LB=5)`

In the above, the parameters have the following meaning:

LB Indicator of covariance pattern as defined above.

NE Number of energies in the parameter table for a given subsection.

NT = NE*(NE+1)/2.

IDP Identification number of a resonance parameter type. This index depends on the resonance formulation used, as summarized in the table below. This table is consistent with the order of parameters used in the NSRS-type sub-subsections to define the parameter covariances included, the first NPAR parameters in the list for the given LRF value.

	LRF			
IDP	**1**	**2**	**3**	**4**
1	E_r	E_r	E_r	$E_r = \mu$
2	Γ_n	Γ_n	Γ_n	ν
3	Γ_γ	Γ_γ	Γ_γ	GRT
4	Γ_f	Γ_f	Γ_f	GIT
5	Γ_x	Γ_x	Γ_x	GRF
6				GIF
7				GRC
8				GIC

For LB=0, ±1, 2, and 5 the energy values in the tables are monotonically increasing and cover the range EL to EH. For LB=5 the F-values are given in the upper triangular representation of a symmetric matrix by rows, *i.e.* $F_{1,1}$, $F_{1,2}$, ..., $F_{1,NE-1}$; $F_{2,2}$, $F_{2,NE-1}$; $F_{NE-1,NE-1}$

32.2.3 Resolved Resonance Compact Covariance Format (LCOMP=2)

This format was developed in order to provide a means of communicating the actual resonance-parameter covariance matrix (as determined during the data-evaluation process) in a compact, legible, and accurate form, for those situations in which it is not practical to provide the entire covariance matrix using the LCOMP=1 format. The covariance matrix is specified as uncertainties plus correlation matrix. The correlation coefficients (whose values range from -1 to 1) are presented in a compact representation as an integer with NDIGIT digits plus a sign; each approximated correlation coefficient differs from the original value by at most $0.5 \times 10^{-\mathrm{NDIGIT}}$ (0.005 if NDIGIT = 2). Allowed values for NDIGIT are 2 through 6.

If the covariance matrix element connecting parameter number i with parameter number j is denoted by V_{ij}, the uncertainty on parameter i by D_i, and the correlation coefficient by C_{ij}, then these quantities are related by

$$D_i^2 = V_{ii} \qquad ; \qquad V_{ij} = D_i \, C_{ij} \, D_j$$

Values for C_{ij} range from -1 to +1; values for D_i are always positive. Note that the diagonal elements of C_{ij} (*i.e.* those for which $i = j$) are always exactly 1.0 and therefore are never specified explicitly. Compacting the off-diagonal correlation coefficients is accomplished as follows:

1. Drop (set to zero) all values of C_{ij} between between $-10^{-\mathrm{NDIGIT}}$ and $+10^{-\mathrm{NDIGIT}}$.
2. Multiply the remaining coefficients by 10^{NDIGIT}.
3. Map all positive values greater than K and less than or equal to K+1 to the integer K.
4. Map all negative values less than –K and greater than or equal to –K–1 to the integer –K.

The reverse mapping takes the integer to the center of the range. For example, with NDIGIT=2, the positive integer 87 (which corresponds to original correlation coefficients in the range from 0.87 up to and including 0.88) maps to 0.875. The negative integer –12 (which corresponds to original correlation coefficients in the range from –0.12 inclusive down to –0.13 exclusive) maps to correlation coefficient -0.125.

In the LCOMP=2 format, parameters for one resonance are given first (on one line in a LIST record), followed directly by the uncertainties on those parameters, followed by values and uncertainties for the next resonance. After parameters and uncertainties for all resonances have been specified, the correlation coefficients are given.

Two types of records are used for the mapped correlation coefficients. A CONT record reads NDIGIT (the number of digits), NNN (the number of parameters), and NM (the number of lines of INTG records that follow). NDIGIT can have any of the values 2, 3, 4, 5, or 6; the corresponding number NROW of correlation coefficients that can be displayed on one INTG record is 18, 13, 11, 9, and 8, respectively.

The information stored in the INTG records may be summarized as follows: Let i and j represent two of the parameters in the numbering scheme defined above, with $i > j$. All those correlation coefficients mapped to non-zero integers K_{ij} are printed in File 32; zero-valued K_{ij} are printed (as blanks or zeros) only when they occur on the same record with non-zero values. Each line (record) in the file begins by specifying the location (i.e., by specifying i and j, with $i > j$); other K's on the same line correspond to $(i, j+1)$, $(i, j+2)$, ... $(i, j+NROW-1)$ [so long as $j+NROW-1 < i$]. If there are more non-zero K's for the same i, they are given on another line, again beginning with the next non-zero K.

The following FORTRAN statement sequence can be used to read the mapped correlation coefficients and reconstruct the correlation matrix:

```
C CORR is the full correlation matrix of dimensions NNN x NNN
C MXCOR is the maximum dimension of CORR (NNN.LE.MXCOR)
      PARAMETER (MXCOR=1000)
      DIMENSION KIJ(18), CORR(MXCOR*MXCOR)
C Read the CONT record:
C NNN is the dimension of CORR(NNN,NNN),
C NM is the number of lines to follow in the file
C NDIGIT is the number of digits for the covariance matrix
      READ (LIB,10) C1,C2,NDIGIT,NNN, NM, NX, MAT, MF, MT, NS
   10 FORMAT (2F11.0, 4I11, I4, I2, I3,I5)
      IF(NNN.GT.MXCOR) STOP 'MXCOR Limit exceeded'
```

```
C     Preset the correlation matrix to zero
      NN2=NNN*NNN
      DO I=1,NN2
        CORR(I)=0
      END DI
C     Preset the diagonal to one
      DO I=1,NNN
        CORR(I+(I-1)*NNN)=1
      END DO
      DO M=1,NM
C Read the INTG record
        IF(NDIGIT.EQ.2) THEN
          NROW=18
          READ (LIB,20) II, JJ, (KIJ(N),N=1,NROW), MAT, MF, MT, NS
   20     FORMAT (I5, I5, 1X, 18I3, 1X, I4, I2, I3, I5)
        ELSE IF(NDIGIT.EQ.3) THEN
          NROW=13
          READ (LIB,30) II, JJ, (KIJ(N),N=1,NROW), MAT, MF, MT, NS
   30     FORMAT (I5, I5, 1X, 13I4, 3X, I4, I2, I3, I5)
        ELSE IF(NDIGIT.EQ.4) THEN
          NROW=11
          READ (LIB,40) II, JJ, (KIJ(N),N=1,NROW), MAT, MF, MT, NS
   40     FORMAT (I5, I5, 1X, 11I5,     I4, I2, I3, I5)
        ELSE IF(NDIGIT.EQ.5) THEN
          NROW= 9
          READ (LIB,50) II, JJ, (KIJ(N),N=1,NROW), MAT, MF, MT, NS
   50     FORMAT (I5, I5, 1X,  9I6, 1X, I4, I2, I3, I5)
        ELSE IF(NDIGIT.EQ.6) THEN
          NROW= 8
          READ (LIB,20) II, JJ, (KIJ(N),N=1,NROW), MAT, MF, MT, NS
   60     FORMAT (I5, I5,      8I7,     I4, I2, I3, I5)
        ELSE
          STOP 'ERROR - Invalid NDIGIT'
        END IF
C Interpret the INTG record and fill the covariance matrix
        JP = JJ - 1
        Factor =10**(NDIGIT)
        DO N=1,NROW
          JP = JP + 1
          IF(JP.GE.II) GO TO 30
          IF(KIJ(N).NE.0) THEN
            IF(KIJ(N).GT.0) THEN
              CIJ = ( KIJ(N)+0.5)/Factor
            ELSE
```

```
            CIJ =-(-KIJ(N)+0.5)/Factor
          END IF
        JJII = JJ + (II-1)*NNN
        IIJJ = II + (JJ-1)*NNN
        CORR(JJII)= CIJ
        CORR(IIJJ)= CIJ
        END IF
      END DO
30    CONTINUE
   END DO
```

The general structure of the formats has already been described at the beginning of this section. Formats for the individual subsections differ depending on the value of LRF, and are discussed below.

In the format descriptions to follow, the notation is as defined in Chapter 2. Uncertainties are denoted by parameters whose names begin with "D", but are otherwise identical to the parameter of Chapter 2. For example, ER represents the resonance energy in the laboratory system, in units of eV. Therefore, DER represents the uncertainty (square root of the variance) associated with the resonance energy; DER has the same units as ER.

Parameters which are not variables (that is, which are not searchable parameters in the analysis process) do not have uncertainties associated with them. For example, the total spin of a resonance, denoted by parameter AJ, has no associated uncertainty DAJ. In File 32, the value 0.0 is given instead of DAJ (for LRF = 1,2,3).

For LRF = 1 and 2, the redundant parameter GT (which is equal to GN + GG + GF) has no corresponding uncertainty DGT specified explicitly. Instead, if needed, DGT may be calculated using values for DGN, DGG, and DGF, and the correlation matrix.

During the evaluation process, not all potential variables are treated as searchable parameters. For example, if no capture cross section data were available, the evaluator might choose to set all capture widths GG to a constant value. The associated uncertainty DGG is then specified in File 32 as 0.0, indicating that this parameter's uncertainty is not known. (The proper procedure to be used in evaluating the effect of these unvaried parameters on the final covariance matrix remains an open question, and is not addressed in this document.)

In order to express the correlation matrix as compactly as possible, the resonance parameters (those which may be varied during the evaluation process) are implicitly numbered, in the order in which they occur in the listing of File 2. For LRF = 1, 2, or 3, the non-searchable parameter AJ is included in the list but is NOT included in this numbering, nor (for LRF=1 or 2) is the redundant parameter GT. Parameters whose value is given but whose uncertainty is unknown (as described in the previous paragraph) are nevertheless included in the numerical ordering. For completely non-fissile nuclides, fission widths are not included in the numbering scheme; likewise, for fissile or fissionable nuclides for which the evaluator chose to use only one fission width, the second fission width (for LRF = 3) would not be counted.

Notation used here but not previously defined:

NRSA For LRF=1,2, or 3, the total number of resonances (for all L values) to be included in the covariance matrix.
For LRF=7, the number of resonances from a particular J^π group to be included in the covariance matrix.

NJSX For LRF=7 only, the number of J^π groups with resonances to be included in the covariance matrix.

NDIGIT Number of digits to be used in writing the LCOMP=2 type INTG record.

32.2.3.1 SLBW and MLBW (LRF=1 or 2)

The structure of the *subsection* (assuming NRO=0) is as follows:

```
[MAT,32,151/ SPI,    AP,       0,  LCOMP,        0,       0]CONT
[MAT,32,151/AWRI,    QX,       0,    LRX,  12*NRSA,    NRSA/
             ER1,    AJ1,     GT1,    GN1,      GG1,     GF1,
            DER1,   0.0,     0.0,   DGN1,     DGG1,    DGF1,
             ER2,    AJ2,     GT2,    GN2,      GG2,     GF2,
            DER2,   0.0,     0.0,   DGN2,     DGG2,    DGF2,
            ----------------------------------------------
         ERNRSA, AJNRSA, GTNRSA,  GNNRSA, GGNRSA,  GFNRSA,
        DERNRSA,    0.0,    0.0, DGNNRSA, DGGNRSA, DGFNRSA]LIST
[MAT,32,151/ 0.0,   0.0, NDIGIT,      NNN,      NM,      0 ]CONT
[MAT,32,151/  II,    JJ,    KIJ]INTG
[MAT,32,151/  II,    JJ,    KIJ]INTG
     < Continue until a total of NM of INTG-type records are read>
```

Note that NNN is the total number of unique resonance parameters included in this listing, not including AJ or GT. For fissile nuclides, NNN=NRSA×4; for non-fissile nuclides, NNN=NRSA×3.

32.2.3.2 Reich-Moore (LRF=3)

The structure of the *subsection* is:

```
[MAT,32,151/ SPI,    AP,     LAD,   LCOMP,       0,       0]CONT
[MAT,32,151/AWRI,   APL,       0,       0, 12*NRSA,    NRSA/
              ER1,   AJ1,     GN1,     GG1,    GFA1,     GFB1,
             DER1,   0.0,    DGN1,    DGG1,   DGFA1,    DGFB1,
              ER2,   AJ2,     GN2,     GG2,    GFA2,     GFB2,
             DER2,   0.0,    DGN2,    DGG2,   DGFA2,    DGFB2,
          ----------------------------------------------------
          ERNRSA,AJNRSA,  GNNRSA, GGNRSA, GFANRSA, GFBNRSA,
         DERNRSA,    0.0, DGNNRSA,DGGNRSA,DGFANRSA,DGFBNRSA]LIST
[MAT,32,151/ 0.0,    0.0,  NDIGIT,     NNN,     NM,       0 ]CONT
[MAT,32,151/  II,     JJ,     KIJ]INTG
[MAT,32,151/  II,     JJ,     KIJ]INTG
< Continue until a total of NM of INTG records are read>
```

Note that NNN is the total number of resonance parameters in this listing (again not including AJ). For non-fissile nuclides, NNN=NRSA×3. For fissile nuclides, NNN=NRSA×4 if only one fission channel is used, and NNN=NRSA×5 if both are used.

32.2.3.3 R-Matrix Limited Format (LRF=7)

The structure of the *subsection* is:

```
[MAT,32,151/ 0.0,     0.0,       IFG,   LCOMP,      NJS,   KRL ]CONT
[MAT,32,151/ 0.0,     0.0,       NPP,    NJSX,   12*NPP, 2*NPP/
             MA1,     MB1,        ZA1,     ZB1,      IA1,    IB1,
              Q1,    PNT1,       SHF1,     MT1,      PA1,    PB1,
             MA2,     MB2,        ZA2,     ZB2,      IA2,    IB1,
              Q2,    PNT2,       SHF2,     MT2,      PA2,    PB1,
            ------------------------------------------------
          MANPP,  MBNPP,     ZANPP,   ZBNPP,    IANPP, IBNPP,
           QNPP, PNTNPP,    SHFNPP,   MTNPP,    PANPP, PBNPP]LIST
[MAT,32,151/ AJ,      PJ,       0,         0,    6*NCH,    NCH/
           IPP1,       L1,     SCH1,     BND1,      APE1,    APT1,
           IPP2,       L2,     SCH2,     BND2,      APE2,    APT2,
             ------------------------------------------------
        IPPNCH,    LNCH,   SCHNCH,  BNDNCH,   APENCH, APTNCH]LIST
             ------------------------------------------------
[MAT,32,151/0.0,      0.0,        0,     NRSA,     12*NX,      NX/
            ER1,    GAM1,1,     GAM2,1,    GAM3,1,     GAM4,1,    GAM5,1,
          GAM6,1, ...  ...  ...  ...  ...  ...  ...  .  ,  GAMNCH,1,
           DER1,   DGAM1,1,    DGAM2,1,   DGAM3,1,    DGAM4,1,   DGAM5,1,
         DGAM6,1, ...  ...  ...  ...  ...  ...  ...  .  , DGAMNCH,1,
            ER2,    GAM1,2,     GAM2,2,    GAM3,2,     GAM4,2,    GAM5,2,
          GAM6,2, ...  ...  ...  ...  ...  ...  ...  .  ,  GAMNCH,2,
           DER2,   DGAM1,2,    DGAM2,2,   DGAM3,2,    DGAM4,2,   DGAM5,2,
         DGAM6,2, ...  ...  ...  ...  ...  ...  ...  .  , DGAMNCH,2,
             ------------------------------------------------
         ERNRSA,GAM1,NRSA, GAM2,NRSA, GAM3,NRSA, GAM4,NRSA, GAM5,NRSA,
        GAM6,NRS, ...  ...  ...  ...  ...  ...  ...  .  , GAMNCH,NRS,
        DERNRSA,DGAM1,NRSA,DGAM2,NRSA,DGAM3,NRSA,DGAM4,NRSA,DGAM5,NRSA,
     DGAM6,NRSA, ...  ...  ...  ...  ...  ...  .  , DGAMNCH,NRSA]LIST
           <The above two list records are repeated until each of
           the NJS Jπ states has been specified.>
[MAT,32,151/ 0.0,    0.0,  NDIGIT,     NNN,        NM,        0 ]CONT
[MAT,32,151/  II,     JJ,     KIJ ]INTG
[MAT,32,151/  II,     JJ,     KIJ ]INTG
           < Continue until a total of NM of INTG records are read >
```

For LRF=7 (unlike other formats), the number of channels may vary from one spin group to another. The number of resonance parameters NNN is therefore given by the sum (from 1 to NJS) of (NCH×NRSA).

32.2.4 Unresolved Resonance Format (LRU=2)

For the unresolved resonance region a simplified covariance formulation is permitted. For the purposes of covariance representation, no energy dependence is specified for the average parameter relative covariances, even though in File 2 the unresolved region may be represented with energy-dependent average Breit-Wigner parameters using LRF=2. Relative covariance elements are tabulated, unlike the cases above.

If the evaluator wishes to represent the relative covariance of the unresolved resonance parameters, the subsection for a given isotope has the following form.

```
[MAT,32,151/  SPI,  AP,    0,   0,   NLS,   0]CONT
[MAT,32,151/ AWRI, 0.0,    L,   0, 6*NJS, NJS/
               D1,  AJ1, GNO1, GG1,   GF1, GX1,
             ------------------------------------
             DNJS, AJNJS, GNONJS, GGNJS, GFNJS, GXNJS]LIST
       <NJS card images for each L value in successive LIST records>
[MAT,32,151/ 0.0, 0.0, MPAR, 0,(NPAR*(NPAR+1))/2,NPAR/
             RV11, RV12, -------------------------,
             -----------, RV1,NPAR,--------, RNNAPR,NPAR]LIST
```

MPAR is the number of average parameters for which relative covariance data are given for each L and J, in the order D, GNO, GG, GF, and GX, for a maximum of 5. That is, relative covariance values for the first MPAR of these are tabulated for each (L,J) combination. If MPAR is given as 4 when LFW=0 on the CONT (isotope) record, then the four covariance matrix indices per (L,J) combination represent D,GNO, GG, and GX.

NPAR=MPAR*(sum of the values of NJS for each L).

The LSSF flag is defined in Section 2.3.1.

RV_{ij}, the relative covariance quantities among these average unresolved parameters for the given isotope. The final LIST record contains the upper triangular portion of the symmetric relative covariance matrix by rows.

32.3 Procedures

As indicated earlier, it is desirable to utilize File 32 when self-shielding is important or when only a few resonances fall within an energy group of the processed cross sections. It is believed that in most cases the covariances the evaluator needs to represent will not use many of the available File 32 options. One does not expect to find covariance data in File 32 for all the resonance parameters in File 2.

Correspondence Between Files 2 and 32. Completeness of File 32.

1. The overall energy range for a given isotope in File 32 is nested within the corresponding range of File 2. In either case, there may be several energy range control records. The following rules apply separately for each isotope:

   (a) The smallest lower range limit EL for Files 2 and 32 must agree.

   (b) The highest upper range limit EH for File 32 may be smaller than or equal to that for File 2.

   (c) In File 32 as in File 2, the energy ranges of the subsections may not leave gaps. Subsections with LRU=1 may overlap if consistent resonance formulations are referenced (LRF=1 or 2).

   (d) An unresolved energy region (LRU=2) may be used in File 32 if one is employed in File 2. If one is used, its lower energy range limit must equal the corresponding limit for File 2.

2. In a File 32 LCOMP=0 subsection, any selection of the resonances shown in File 2 with LRF=1 or 2 must be listed in order of increasing energy. The resonance energy given in File 32 shall agree with that in File 2 for the same resonance to a relative tolerance of $\leq 10^{-5}$ to assume positive identification.

3. In LCOMP=1, LRU=1 subsections, any selection of the resonances shown in File 2 for consistent resonance formulations may be listed in NSRS-type subsections. The listed resonances should be in order of increasing energy within each block, and the blocks should be arranged by order of increasing energy for the lowest-energy resonance in the block. A given resonance may appear in more than one block. The resonance energy given in File 32 shall agree with that in File 2 for the same resonance to a relative tolerance of $\leq 10^{-5}$.

4. The energy identifiers of every long-range (NLRS-type) subsection must cover the entire energy range (EL,EH) of the subsection. However, any desired covariance components may be null.

5. Long-range subsections may be included in any order in LCOMP=1, LRU=1 subsections.

Obtaining Cross Section Covariances From File 32 and File 33.

1. Outside the combined energy range covered by File 32, whether in part or all of the energy range covered by File 2, the covariance data in File 33 refers to the cross sections reconstituted from File 2 plus File 3 according to the value of the LSSF flag.

2. In LCOMP=0 subsections a nonzero variance or covariance involving the resonance spin J (AJ) will be treated as null.

3. When File 32 is present for a resolved resonance range (LRU=1), the covariances among the effective cross sections in the region are obtained by combining data from Files 32 and 33.

   (a) A resonance parameter covariance matrix is developed by summing all the contributions for each resonance from the File 32 subsections with LRU=1.

   (b) The resonance parameter covariance file is processed to obtain the covariance data of effective cross sections implied by File 32. (This data will in general be a function of isotopic dilution and temperature.) Covariance for the various isotopes are summed with appropriate weights if the evaluation is an elemental one.

   (c) Covariances derived from File 32 are summed with those given in File 33. With one exception, relative covariances given in File 33 apply to the effective cross sections reconstituted from File 2 and File 3. In that exception, when the Adler-Adler (LRF=4) resonance formulation is employed, any relative covariances in File 33 for that energy region apply to the sum of the cross section from File 3 with the smooth background given for the LRF=4 resonance data.

4. When File 32 is present for the unresolved resonance range (LRU=2), covariance data for the region are obtained as follows:

   (a) File 33 covariance data for this energy region are taken to represent the covariances of evaluated average cross sections for "infinite isotopic dilution."

   (b) To obtain covariances among effective cross sections for material dilutions such that uncertainties in self shielding can become important, the effects of the unresolved resonance parameter covariances in File 32 and the evaluated average cross section covariances in File 33 are to be combined. A means for this combination was described by deSaussure and Marable [Ref. 1]. (Note that covariances of the effective cross sections in one test case were not much affected by uncertainties in average parameters. See B.L. Broadhead and H.L. Dodds [Ref. 2].)

Example For Fictitious MAT 3333, ZA 99280

The nucleus of concern in this example has resonances represented by LRF=2 for the energy range 1 to 50 eV. Five (5) resonances are given in File 2, one of which lies at negative energy, but the resonance at 15 eV is considered only relative to long-range uncertainties. Example 32.1 shows the File 2 and Example 32.2 shows the corresponding File 32.

In File 32, three NSRS-type subsections and four NLRS-type subsections are included. Of the former, the first refers only to the negative energy resonance and indicates the following parameter covariance contribution for that resonance, in eV^2.

r	1	2	3	4
E_r	1.0	-1.5	0	-0.2
Γ_n	-1.5	4.0	0	-1.0
Γ_γ	0	0	0	0
Γ_f	-0.2	-1.0	0	0.8

This block is mostly to express the negative correlation between neutron width and apparent resonance energy for this guessed resonance.

The second subsection refers only to the 5 eV resonance, and conveys the following covariance contribution:

r	1	2	3	4
E_r	0.5×10^{-6}	0	0	0
Γ_n		1.0×10^6	1×10^6	0.2×10^6
Γ_γ		1.0×10^6	0.0	2.0×10^6
Γ_f		0.2×10^6	2×10^6	4.0×10^6

The third block covers Γ_n covariances for the 30 and 40 eV resonances.

The first NLRS subsection gives the Γ_γ uncertainty correlated among all the resonances. The value is assumed to have been determined solely by analysis of the 5 eV resonance. Note that the variance for the 5 eV resonance generated by the subsection fills the "hole" in the table just above (with the value 16×10^{-6}). The second subsection expresses the expected resonance-to-resonance uncorrelated fluctuation in Γ_γ. The third and fourth subsections cover long-range uncertainties in Γ_n and Γ_f the example for the former might be hard for the evaluator to defend for a real nuclide.

Example 32.1. File 2 for Sample File 32

```
 99.280+3   2.70+2        0        0    NIS=1       0333332151 HEAD
 99.280+3   1.00+0        0    LFW=0    NER=1       0333332151 CONT
   1.00+0   5.00+1    LRU=1    LRF=2    NRO=0  NAPS=0333332151 CONT
   1.00+0   0.60+0        0        0    NLS=1       0333332151 CONT
   2.70+2   0.00+0      L=0    LRX=0 6*NRS=30   NRS=5333332151
   1.00+0   1.50+0  4.04 +0  3.0  +0  0.04 +0  1.0 +0333332151
   5.00+0   1.50+0  0.07 +0  0.01 +0  0.04 +0  0.02+0333332151
   1.50+1   0.50+0  0.08 +0  0.01 +0  0.04 +0  0.03+0333332151
   3.00+1   1.50+0  7.04 +0  1.0  +0  0.04 +0  6.0 +0333332151
   4.00+1   1.50+0  6.04 +0  5.0  +0  0.04 +0  1.0 +0333332151 LIST
   0.00+0   0.00+0        0        0        0        0333332 0 SEND
   0.00+0   0.00+0        0        0        0        03333 0 0 FEND
```

Example 32.2. Sample File 32

```
 99.280+3  2.700+2        0        0    NIS=1       0333332151 HEAD
 99.280+3  1.000+0        0    LFW=0    NER=1       0333332151 CONT
 1.0000+0  5.000+1    LRU=1    LRF=2    NRO=0  NAPS=0333332151 CONT
 1.0000+0  0.600+0        0  LCOMP=1    NLS=0       0333332151 CONT
 2.7000+2  0.000+0        0        0   NSRS=3  NLRS=4333332151 CONT
 0.0000+0  0.000+0   MPAR=4        0     M*16   NRB=1333332151
-1.0000+0  1.500+0  4.040+0  3.000+0  0.040+0  1.00+0333332151
 1.0000+0 -1.500+0   0.00+0 -0.200+0  4.000+0  0.00+0333332151
-1.0000+0  0.000+0   0.00+0  0.800+0  0.000+0  0.00+0333332151 LIST
 0.0000+0  0.000+0   MPAR=4        0     M*16   NRB=1333332151
 5.0000+0  1.500+0  0.070+0   0.01+0   0.04+0  0.02+0333332151
 0.5000-6  0.000+0  0.000+0   0.00+0   1.00-6 -1.00-6333332151
-0.2000-6  0.000+0 -2.000-6   4.00-6   0.00+0  0.00+0333332151 LIST
 0.0000+0  0.000+0   MPAR=2        0     M*22   NRB=2333332151
 3.0000+1  1.500+0  7.040+0   1.00+0   0.04+0  6.00+0333332151
 4.0000+1  1.500+0  6.040+0   5.00+0   0.04+0  1.00+0333332151
 2.0000-3  0.000+0   0.00+0   0.00+0   1.00-3  0.00+0333332151
-0.5000-4  2.000-3   0.00+0   2.00-3   0.00+0  0.00+0333332151 LIST
 0.0000+0  0.000+0    IDP=3     LB=1   2*NE=4    NE=2333332151
-2.0000+0  1.000-2   5.00+1   0.00+0   0.00+0  0.00+0333332151 LIST
 0.0000+0  0.000+0    IDP=3     LB=1   2*NE=8    NE=4333332151
-2.0000+0  1.000-2   1.00+0   0.00+0   1.00+1  1.00-2333332151 LIST
 5.0000+1  0.000+0   0.00+0   0.00+0   0.00+0  0.00+0333332151 LIST
 0.0000+0  0.000+0    IDP=2     LB=5     NT=6    NE=3333332151
 1.0000-5  2.000+1   5.00+1   1.00-4   1.00-4  2.00-4333332151 LIST
 0.0000+0  0.000+0    IDP=4     LB=1   2*NE=4    NE=2333332151
 1.0000-5  4.000-4   5.00+1   0.00+0   0.00+0  0.00+0333332151 LIST
 0.0000+0  0.000+0        0        0        0       0333332  0 SEND
 0.0000+0  0.000+0        0        0        0       03333 0  0 FEND

M  =NVS+6*NRB
NVS=NRB*MPAR*(NRB*MPAR+1)/2.
```

References for Chapter 32

1. G. DeSaussure and Marable, ***Nucl. Sci. Eng.*** **101**, 285 (1989)

2. B. L. Broadhead and H. L. Dodds, ***Trans. Am. Nucl. Soc.*** **39**, 929 (1981)

Chapter 33

File 33, COVARIANCES OF NEUTRON CROSS SECTIONS

33.1 General Comments

File 33 contains the covariances of neutron cross section information appearing in File 3. It is intended to provide a measure of the "uncertainties and their correlations" and does not indicate the precision with which the data in File 3 are entered. However, it should be stressed that for most practical applications to which the files are intended, the data will be processed into multigroup variance-covariance matrices. When generating File 33, it should be remembered that major aims are to represent adequately:

i. the variances of the group cross sections,

ii. the correlations between the cross sections of the several adjacent groups, and

iii. the long-range correlations among the cross sections for many groups.

Table 33.1 illustrates a typical relation of these three covariances with experimental uncertainties[1].

Table 33.1: Analogies Between File 33 Covariances Within One Section and Uncertainties in a Hypothetical Experiment.

File 33	**Experimental**	**Energy Dependence**
Short range	Statistical	Rapid variation
Medium range	Detector Efficiency, Multiple Scattering, In/Out Scattering	Slowly varying
Long range	Geometry Background Normalization	More or less constant

[1] As with all analogies, this should be used with care. It is designed to show in a familiar way of thinking how the covariances within a section are related.

These primary considerations and the inherent difficulties associated with quantifying uncertainties should dictate the level of detail given in File 33.

In the resolved resonance region, some of the covariances of the cross sections may be given through the covariances of the resonance parameters in File 32. In this case, the long-range components of the covariance matrix of the cross sections, which span many resonances, may be given in File 33, since often the most important components of the matrix are long-range.

Example:
Consider a case with the following sources of uncertainty:

- 2% uncertainty due to statistics (short-range),
- 2% due to multiple scattering (medium-range), and
- 1% due to geometry (long-range),

we would cite the uncertainties as:

- 3% uncertainty for a discrete measurement (one group covering a small energy range, calculated as the square root of the squares of individual contributions $\sqrt{2^2 + 2^2 + 1^2}$);
- ≈2.5% over an energy range encompassing several measurements (several groups which together cover a 1 to 2 MeV range, calculated as above, but the statistical component becomes smaller than 2% due to the averaging procedure over the energy interval); and
- ≈ 1% average over the entire energy range (long- and medium-range terms disappear).

33.2 Formats

File 33 is divided into sections identified by the values of MT. Within a section defined by (MAT,33,MT), several subsections may appear. Each section of File 33 starts with a HEAD record, ends with a SEND record. The following quantities are defined:

ZA,AWR Standard material charge and mass parameters.

MTL Non-zero value of MTL is used as a flag to indicate that reaction MT is one component of the evaluator-defined lumped reaction MTL, as discussed in paragraphs at the end of Section 33.2 and 33.3 below; in this case, no covariance information subsections are given for reaction MT and NL=0.

NL Number of subsections within a section.

The structure of a section is:

```
[MAT, 33, MT/  ZA, AWR, 0, MTL, 0, NL] HEAD
            <subsection for n = 1>
            <subsection for n = 2>
            <subsection for n = NL>
[MAT, 33,  0/ 0.0, 0.0, 0,   0, 0,  0] SEND
```

33.2.1 Subsections

Each subsection of the section (MAT,33,MT) is used to describe a single covariance matrix. It is the covariance matrix of:

- 1st set of energy-dependent cross sections given in section (MAT,3,MT) and
- 2nd set of energy-dependent cross sections given in section (MAT1,MF1,MT1) when MF1=3 or (MAT1,MF1,MT1.LFS1) when MF1=10 (see definitions below).

The values of MAT1, XMF1, MT1 (and XLFS1, if MF=10) are given in the CONT record which begins each subsection. Each File 33 subsection is therefore identified with a unique combination of values (MAT,MT) and (MAT1,MF1,MT1[.LFS1]), and we may use the notation (MAT,MT; MAT1,MF1,MT1[.LFS1]) to specify a subsection.

Each subsection may contain several sub-subsections. Two different types of sub-subsections may be used; they are referred to as "NC-type" and "NI-type" subsections. Each sub-subsection describes an independent contribution (called a component) to the covariance matrix given in the subsection. The total covariance matrix given by the subsection is made up of the sum of the contributions from the individual sub-subsections. The following quantities are defined:

XMF1 Floating point equivalent of the MF for the 2nd energy-dependent cross section of the pair, for which the correlation matrix is given. If MF1=MF, XMF1=0.0 or blank.

XLFS1 Floating point equivalent for the final excited state of the 2nd energy-dependent cross section. For MF1=10, XLFS1 = 10; if MF1$\neq$10, XLFS1=0.0 or blank.

MAT1 MAT for the 2nd energy-dependent cross section

MT1 MT for the 2nd energy-dependent cross section

NC Number of NC-type sub-subsections which follow the CONT record.

NI Number of NI-type sub-subsections which follow the NC-type sub-subsections.

The structure of a subsection describing the covariance matrix of the cross sections given in (MAT,3,MT) and (MAT1,MF1,MT1.[LFS1]) is:

```
[MAT,33,MT/ XMF1, XLFS1, MAT1, MT1, NC, NI]CONT
          <sub-subsection for n =1>
          <sub-subsection for n =2>
           -----------------------------
           -----------------------------
          <sub-subsection for n =NC>
          <sub-subsection for n =1>
          <sub-subsection for n =2>
           -----------------------------
           -----------------------------
          <sub-subsection for n = NI>
```

33.2.2 Sub-Subsections

NC-type and NI-type sub-subsections have different structures.

NC-type sub-subsections may be used to indicate that some or all of the contributions to the covariance matrix described in the subsection are to be found in a different subsection of the ENDF tape. The major purpose of the NC-type sub-subsections is to eliminate from the ENDF tape a large fraction of the mostly redundant information, which would otherwise be needed if only NI-type sub-subsections were used.

NI-type sub-subsections are used to describe explicitly various components of the covariance matrix defined by the subsection.

33.2.2.1 NC-type Sub-Subsections

NC-type subsections may be used to describe the covariance matrices in energy ranges where the cross sections in (MAT,3,MT) can be described in terms of other evaluated cross sections in the same energy range. In the context of File 33, and for purposes of discussing NC-type sub-subsections, we define an "evaluated" cross section in a given energy range as one, for which the covariance matrix in that energy range is given entirely in terms of NI-type sub-subsections. The covariance matrices involving the "derived" cross sections may be obtained in part in terms of the covariance matrices of the "evaluated" cross sections given elsewhere in File 33. The following quantity is defined:

LTY Flag used to indicate the procedure used to obtain the covariance matrix. The values of LTY can be from 0 to 4, as explained below.

<u>LTY=0, "Derived Redundant Cross Sections"</u>
In File 33, the evaluator may indicate by means of an LTY=0 sub-subsection that in a given energy range the cross sections in (MAT,3,MT) were obtained as a linear combination of

other "evaluated" cross sections having the same MAT number but different MT values. By the definition of "evaluated covariances" the covariances of these cross sections are given in File 33 wholly in terms of NI-type sub-subsections.[2] The following additional quantities are defined:

E1, E2 Energy range (eV) where the cross sections given in the section (MAT,3,MT) were "derived" in terms of other "evaluated" cross sections given in the sections (MAT,3,MTI)s.

NCI Number of pairs of values in the array {CI, XMTI}[3].

{CI, XMTI} Array of pairs of numbers, each pair consisting of the coefficient CI and a value of XMTI, (*i.e.* the MTI number given in floating point representation). The pair of numbers indicates that, in the energy range E1 to E2, the cross sections in file (MAT,3,MT), were obtained in terms of the cross sections in files (MAT,3,MTI), as follows:

$$\sigma_{\mathrm{MT}}^{\mathrm{MAT}}(E) = \sum_{i=1}^{\mathrm{NCI}} C_i \times \sigma_{\mathrm{MT_i}}^{\mathrm{MAT}}(E) \ .$$

[At the minimum, the use of an LTY=0 sub-subsection implies that the evaluator wishes the corresponding covariance components to be derived as if this expression were valid.]

In this expression we have written the CI's as C_i, and XMTI's as MT_i. The numbers CI are constant numbers over the whole range of energy E1 and E2, usually ±1.

The structure of an NC-type sub-subsection with LTY=0 is:

```
[MAT,33,MT/ 0.0, 0.0,   0, LTY=0,     0,   0]CONT
[MAT,33,MT/  E1,  E2,   0,     0, 2*NCI, NCI/{CI, XMTI}]LIST
```

Note: In general, each subsection describes a single covariance matrix. However, when an NC-type sub-subsection with LTY=0 is used in a subsection, portions of NCI+1 covariance matrices are implied and these are not explicitly given as subsections in the File 33 (see procedure in Section 33.3.2 item a.3). In such cases the subsection may be thought of as describing in part several covariance matrices.

LTY=1, 2 and 3, "Covariances of Cross Sections Derived via Ratios to Standards"

Many important cross sections in ENDF files are based on measurements of cross sections ratios to standard cross sections. When an evaluated cross section is obtained from such measurements, covariances so generated between the cross sections for the two reactions may

[2]In general the linear relationship given in an LTY=0 sub-subsection applies not only to the range of energies specified, but also over the whole range of the file.

[3]The Notation {AI,BI} stands for A1, B1; A2, B2; ...; Ai, Bi in a list record.

become important. This is the primary origin of ENDF covariances linking cross sections for different materials. As seen below, these covariances depend on the covariances of the standard cross section and on the covariances of the evaluated cross section ratios. When the resulting multigroup covariance files are utilized, the covariances of the ratios themselves play an important role if the performance of some system depends on the relative magnitude of two cross sections.

In order to represent efficiently in File 33 the covariances that depend on "absolute" ratio measurements to standards, evaluators may use NC-type sub-subsections with LTY=1, 2 or 3 in appropriate File 33 subsections. [In other cases of covariance components induced by ratio measurements, it is necessary for the evaluator to explicitly represent the covariance components that arise and may be found in the literature.[4]]

First we identify the covariances induced if an evaluator obtains cross section $\sigma_a(E)$ for (MAT,MT) within the interval [E1,E2] entirely from ***absolute*** ratio measurements to a cross section standard $\sigma_S(E)$ for (MATS,MTS). That is,

$$\sigma_a(E) = \alpha(E)\ \sigma_S(E)\ ,\ \text{for (E1} \leq E < \text{E2)}\ .$$

The evaluated ratio $\alpha(E)$ itself is assumed to be independent of the standard cross section evaluation because the relevant measurements are similarly independent. If so, then:

$$\begin{aligned}
\text{Rvar}[\sigma_a(E)] &= \text{Rvar}[\alpha(E)] + \text{Rvar}[\sigma_S(E)]\ ,\text{for (E1} \leq E < \text{E2)} \\
\text{Rcov}[\sigma_a(E), \sigma_a(E')] &= \text{Rcov}[\alpha(E), \alpha(E')] + \text{Rcov}[\sigma_S(E), \sigma_S(E')] \\
&\quad \text{for (E1} \leq E < \text{E2) and (E1} \leq E' < \text{E2)} \\
\text{Rcov}[\sigma_a(E), \sigma_S(E')] &= \text{Rcov}[\sigma_S(E), \sigma_S(E')] \\
&\quad \text{for (E1} \leq E < \text{E2) and (E1} \leq E' < \text{E2)}\ .
\end{aligned}$$

Rvar and Rcov are the relative variance and relative covariance defined in Chapter 30, and the values generated by the specified ratio evaluation are zero outside the specified ranges. The variance and covariance terms in (MAT,MT) depend on those for both the standard and the ratio, and only for energies in ranges where the cross section is specified to depend on this standard. However, the covariance matrix between the cross sections (MAT,MT) and (MATS,MTS) does not depend on the covariances of the ratio determination but spans all values of the energy E'.

A cross section $\sigma_a(E)$ may be obtained from measurements relative to the standard (MATS,MTS) in the energy region (E1 $\leq E \leq$ E2) and cross section $\sigma_b(E')$ relative to another standard (MATS',MTS') in the energy region (E1' $\leq E' \leq$ E2'). If the cross sections for the two standards are correlated and the two sets of ratio measurements are uncorrelated, then one obtains the additional results:

[4] W. P. Poenitz, "Data Interpretation, Objective Evaluation Procedures, and Mathematical Techniques for the Evaluation of Energy-Dependent Ratio, Shape, and Cross Section Data", BNL-NCS-51363, Conf. on Nuclear Data Evaluation and Techniques, p. 264, B. A. Magurno and S. Pearlstein, eds. (March, 1981)

$$\begin{aligned}
\mathrm{Rcov}[\sigma_a(E), \sigma_b(E')] &= \mathrm{Rcov}[\sigma_S(E), \sigma_{S'}(E')] \text{ for (E1} \leq E \leq \text{E2) , (E1'} \leq E' \leq \text{E2')} \\
&\quad \text{zero otherwise;} \\
\mathrm{Rcov}[\sigma_a(E), \sigma_{S'}(E')] &= \mathrm{Rcov}[\sigma_S(E), \sigma_{S'}(E')] \text{ for (E1} \leq E \leq \text{E2) and all } E', \\
&\quad \text{zero otherwise;} \\
\mathrm{Rcov}[\sigma_S(E), \sigma_b(E')] &= \mathrm{Rcov}[\sigma_S(E), \sigma_{S'}(E')] \text{ for (E1'} \leq E' \leq \text{E2') and all } E, \\
&\quad \text{zero otherwise.}
\end{aligned}$$

Note that the above expressions apply when $\sigma_a(E)$ and $\sigma_b(E')$ refer to the same (MAT,MT) for which cross sections are obtain by ratios to different standards in the two energy regions.

The most far-reaching relationship correlates $\sigma_a(E)$ with all cross sections correlated to the standard relative to which it was measured. That is:

$$\begin{aligned}
\mathrm{Rcov}[\sigma_a(E), \sigma_x(E')] &= \mathrm{Rcov}[\sigma_S(E), \sigma_x(E')] \text{ for (E1} \leq E < \text{E2) and all } \sigma_x(E'), \\
&\quad \text{zero otherwise.}
\end{aligned}$$

The right side may be non-zero for many (MATX,MTX), and discretion may be required to avoid in cross section processing the generation of negligible but non-zero multigroup covariance matrices.

Let the cross sections in (MAT,3,MT) be strictly "derived" in the energy range E1 to E2 through the evaluation of ratio measurements to the "evaluated" cross sections given in (MATS,MFS,MTS[.LFSS]), referred to also as the "standard" cross sections for this "ratio evaluation". Then, in the subsection (MAT,3,MT;MAT,3,MT) of the File 33 for the material MAT, an LTY=1 sub-subsection must be used to describe, in part, the covariance matrix in the energy range E1 to E2. (LFSS=0 when MF=3). The part, or component, of the covariance matrix represented by the LTY=1 sub-subsection is obtained by the user from the covariance matrix of the "standard" cross sections in the File (MFS+30) subsection (MATS,MTS[.LFSS]; MATS,MFS,MTS[.LFSS]) of the material MATS. The other part, or component, of the covariance matrix comes from the evaluation of the "ratios" and is given explicitly, over the range E1 to E2, by means of NI-type sub-subsections in the File 33 subsection (MAT,3,MT;MAT,3,MT).

This method of evaluation introduces a covariance of the "derived" cross sections in (MAT,3,MT) over the energy range E1 to E2 and the "standard" cross section over its complete energy range. Therefore, in File 33 of the material MAT, in subsection containing the covariance of the "standard" cross section, there must be an LTY=2 sub-subsection to represent this covariance matrix. This LTY=2 sub-subsection [which contains the same information as the previously given LTY=1 sub-subsection in the subsection (MAT,3,MT; MAT,3,MT)] refers to a different covariance matrix than the LTY=1 sub-subsection previously mentioned, but it can also be derived from the covariance matrix of the "standard" cross sections in File MFS+30 subsection of the standard material MATS.

Finally, as a consequence of the evaluation of the cross sections in (MAT,3,MT) in the energy range E1 to E2, as a "ratio" to the "standard" cross sections, there must be in the subsection (MATS,MFS,MTS[.LFSS]; MAT,MF,MT) of the File (MFS+30) of the

"standard" material MATS and LTY=3 sub-subsection in the File 33 subsection (MAT,MT; MAT,3,MT)] which serves in the material MATS the same role as the LTY=2 sub-subsection in the material MAT since they describe the same covariance matrix. In addition, the LTY value of 3 serves as a "flag" to the user, and the processing codes, to indicate existence of any additional covariances among cross sections using the same "standard" cross sections, covariances not explicitly given in the covariance files. These additional covariance matrices can be derived from the appropriate LTY=3 sub-subsections and the covariance matrix of the "standard" cross sections in the File (MFS+30) subsection. The following quantities are defined:

E1, E2 Energy range where the cross sections given in the section (MAT,3,MT) were obtained to a significant extent in terms of ratio measurements to "standard" cross sections.

NEI Number of energies that demarcate (NEI1) regions where this standard was employed in measurements with WEI.

WEI Fractional evaluated weight.

The structure of NC-type sub-subsections with LTY=1,2 and 3 is:

```
[MAT,33,MT/ 0.0, 0.0,    0, LTY,       0,   0]CONT
[MAT,33,MT/  E1,  E2, MATS, MTS, 2*NEI+2, NEI/
            (XMFS,XLFSS), {EI,WEI}           ]LIST
```

The number of items in the list record is 2*NEI+2. The file number that contains the standard cross sections is the integer equivalent of XMFS, except that XMFS=0.0 is entered when MFS=3. The value of XLFSS is always zero unless MFS=10.

The use of the format LTY=1, 2 and 3 is allowed when the cross sections given in (MAT,3,MT) are only partially determined from ratio measurements to the "standard" cross section. In such cases the list {EI,WEI} indicates the fractional weight of the ratio measurements to this standard in the evaluation of the cross sections in (MAT,3,MT). That fractional weight is W_i of WEI in the interval $E_i \leq E < E_{i+1}$ of EI. The first value of E_i in the sub-subsection shall equal the E1 given, and E_{NEI} =E2.

Note A: LTY=1, 2 and 3 sub-subsections are all used as flags in subsections to represent relative covariance matrix components obtained from the relative covariance matrix of the "standard" cross sections that is given in a File 33, 31, or 40. There is, however, as seen in the formulae above, a major difference between covariance matrices obtained with LTY=1 sub-subsections and those obtained from LTY=2 and 3 sub-subsections. This difference results from the definition of their use given above. LTY=2 and 3 sub-subsections are always used in subsections where one of the cross sections involved is the "standard" cross section used. The LTY=2 subsection appears in the File 33 [in the present case] of the material whose cross sections are "derived," whereas the LTY=3 sub-subsection appears in the File (MFS+30) of the material whose cross sections are the "standard"; LTY=1 sub-subsections always appear in subsections describing covariance matrices of cross sections "derived" from a "standard"

and no LTY=2 or 3 sub-subsections may appear in such subsections. An LTY=1 sub-subsection represents a covariance matrix which in principle is a "square matrix" covering the ranges E1 to E2. An LTY=2 or 3 subsection describes in principle a "rectangular matrix": the covariance matrix of the "derived" cross sections over the energy range E1 or E2 and of the "standard" cross sections over their complete energy range.

In general, if cross sections in (MAT,3,MT) are "derived," over an energy range E1 to E2, by "ratios" to "standard" cross sections, there will be three NC-type sub-subsections with LTY=1, 2 and 3 generated in the covariance files. The LTY=1 sub-subsection is given in the subsection (MAT,MT; MAT,3,MT); the LTY=2 sub-subsection is given in the subsection (MAT,MT; MATS,MFS,MTS[.LFSS]). Both of these subsections are given in the File 33 of the material MAT of the "derived" cross sections (MAT,3,MT). The LTY=3 sub-subsection is given in the subsection (MATS,MFS,MTS[.LFSS] ; MAT,3,MT) which is in the File (MFS+30) of the material MATS of the "standard" cross sections.

There are, however, some instances, such as the one taken in the Example 33.1, where other cross sections, such as those in (MAT,3,MTI), are "indirectly derived" from the cross sections in (MATS,3,MT) through evaluation of ratios of the cross sections in (MAT,3,MTI) to those in (MAT,3,MT). In such cases, an LTY=1 sub-subsection will also be used in the subsections (MAT,MT1,MAT,MT1) and (MAT,MT; MAT,MT1) and LTY=2 sub-subsection will also be used in the subsection (MAT,MT1; MATS,MFS,MTS[.LFSS]). All three of these subsections are in File 33 of the material MAT. Corresponding to the LTY=2 sub-subsection in the subsection (MAT,MT1; MATS,MFS,MTS[.LFSS]) of the File 33 of the material MAT, there will also be an LTY=3 sub-subsection in the subsection (MATS,MTS[.LFSS]; MAT,MT1) of the File (MFS+30) of the material MATS.

Note B: For purposes of discussing the covariance matrices of cross sections derived through evaluation of ratio measurements, the label "standard" cross sections is used for the cross sections relative to which the ratio measurements were made. The cross sections for which the label "standard" was used may be any "evaluated" cross sections of an ENDF library and are not restricted to the special set of "standard cross sections" library. The "standard cross sections" are the preferred ones to use for ratio measurements in order to minimize the magnitude of the covariance matrix elements obtained from LTY=1, 2 and 3 sub-subsections. However, they may not always be the ones that were used in the data available to evaluators to perform evaluations.

33.2.2.2 NI-type Sub-Subsections

NI-type sub-subsections are used to describe explicitly the various components of the covariance matrix given in the subsection. In each NI-type sub-subsection there is an LB flag. The numerical value of LB indicates whether the components are "relative" or "absolute," the kinds of correlations as a function of energy represented by the components in the sub-subsection, and the structure of the sub-subsection. The following quantity is defined:

LB Flag whose numerical value determines the meanings of the numbers given in the arrays $\{E_k, F_k\}\{E_l, F_l\}$.

Flag LB= 0 to 4
The following additional quantities are defined:

NP Total number of pairs of numbers in the arrays $\{E_k, F_k\}\{E_l, F_l\}$.

NT Total number of numbers in the LIST record; NT=2*NP.

LT Number of pairs of numbers in the second array, $\{E_l, F_l\}$.
If LT=0, the table contains a single array $\{E_k, F_k\}$.
If LT$\neq$ 0, the table contains two arrays; the first array, $\{E_k, F_k\}$, has $(NP - LT)$ pairs of numbers in it.

$\{E_k, F_k\}\{E_l, F_l\}$ two arrays of pairs of numbers; each array is referred to as an "E-table," so the "E_k-table" and the "E_l-table" are defined.

In each E-table the first member of a pair is an energy, E_n; the second member of the pair, F_n, is a number associated with the energy interval between the two entries E_n and E_{n+1}

For values of the LB flag from 0 through 4, NI-type sub-subsections have the following structure:

`[MAT,33,MT/ 0.0, 0.0, LT, LB, NT, NP/` $\{E_k, F_k\}\{E_l, F_l\}$`]LIST`

The E_k-table, and the E_l-table, when present, must cover the complete energy range of the File 3 for the same (MAT,MT). The first energy entry in an E-table must therefore be 10^{-5} eV, or the reaction threshold, and the last one 20×10^6 eV unless a large upper-energy limit has been defined for the evaluation. Some of the F_k's, or F_l's, may be zero, and the last value of F in an E-table must be zero.

We now define the meaning of the F values entered in the E-tables for different values of LB. [Note that the units of F vary]. Let X_i refer to the cross sections in (MAT,3,MT) at energies E_i and Y_j refer to the cross sections in (MAT1,3,MT1) at energies E_j. The contribution of the sub-subsection to the covariance matrix $\mathrm{Cov}(X_i, Y_j)$, having the units of "barns squared," is defined as follows for the different values of LB:

LB=0 Absolute components correlated only within each E_k interval

$$\mathrm{Cov}\,(X_i, Y_j) = \sum_k \mathcal{P}^{i;k}_{j;k} F_{xy;k}$$

LB=1 Fractional components correlated only within each E_k interval

$$\mathrm{Cov}\,(X_i, Y_j) = \sum_k \mathcal{P}^{i;k}_{j;k} F_{xy;k} X_i Y_j$$

LB=2 Fractional components correlated over all E_k intervals

$$\mathrm{Cov}\,(X_i, Y_j) = \sum_{k,k'} \mathcal{P}^{i;k}_{j;k'} F_{xy;k} F_{xy;k'} X_i Y_j$$

LB=3 Fractional components correlated over E_k and E_l intervals

$$\mathrm{Cov}\,(X_i, Y_j) = \sum_{k,l} \mathcal{P}^{i;k}_{j;l} F_{x;k} F_{y;l} X_i Y_j$$

LB=4 Fractional components correlated over all E_l intervals within each E_k interval

$$\mathrm{Cov}\,(X_i, Y_j) = \sum_{k,l,l'} \mathcal{P}^{i;k,l}_{j;k,l'} F_k F_{xy,l} F_{xy,l'} X_i Y_j$$

For LB=0, 1 and 2 we have LT=0, *i.e.*, only one E_k table. For LB=3 and LB=4 we have LT$\neq$ 0, *i.e.*, two E-tables, the E_k and the E_l-tables.

The dimensionless operators $\mathcal{P}$ in the above definitions are defined in terms of the operator $\mathcal{S}$ as follows:

$$\mathcal{P}^{i;k,l,\ldots}_{j;m,n,\ldots} \equiv \mathcal{S}^k_i \mathcal{S}^l_i \ldots \mathcal{S}^m_j \mathcal{S}^n_j \ldots,$$

where

$\mathcal{S}^k_i \equiv 1$ when $E_k \leq E_i \leq E_{k+1}$ and

$\mathcal{S}^k_i \equiv 0$ when the energy E_i is outside the range of E_k to E_{k+1} of an E_k-table.

Flag LB=5

It is often possible during the evaluation process to generate the relative covariance matrix of some cross sections averaged over some energy intervals. Such relative covariance matrices may be suitable for use in File 33. Although the use of LB=3 sub-subsections allows the representation of such matrices one row (or one column) at a time, this method of representation is very inefficient. One sub-subsection must be used for each row (or column) and the same energy mesh is repeated in the E_k-table (or E_l-table) of every sub-subsection. Often, in addition, such relative covariance matrices are symmetric about their diagonal and there is no way to avoid repeating almost half of the entries with LB=3 sub-subsections. In order to allow such relative covariance matrices to be entered into the files efficiently, LB=5 sub-subsections may be used. The following definition applies for LB=5 sub-subsections:

$$\mathrm{Cov}\,(X_i, Y_j) = \sum_{k,k'} \mathcal{P}^{i;k}_{j;k'} F_{xy;k,k'} X_i Y_j$$

A single list of energies $\{E_k\}$ is required to specify the energy intervals labeled by the indices k and k'. The numbers $F_{xy;k,k}$ represent fractional components correlated over the energy intervals with lower edges E_k and $E_{k'}$.

Since there is no need for E_k-tables with pairs of numbers (E_k, F_k) like those found in sub-subsections with LB<5, a new structure is required for LB=5 sub-subsections. The following quantities are defined:

NT Total number of entries in the two arrays $\{E_k\}$ and $\{F_{k,k'}\}$.

NE Number of entries in the array $\{E_k\}$ defining (NE-1) energy intervals.

LS Flag indicating whether the $F_{k,k'}$, matrix is symmetric or not.

The structure of an LB=5 sub-subsection is:

`[MAT,33,MT/ 0.0, 0.0, LS, LB=5, NT, NE/` $\{E_k\}\{F_{k,k'}\}$`] LIST.`

LS=0 Asymmetric matrix:
The matrix elements $F_{k,k'}$, are ordered by rows in the array $\{F_{k,k'}\}$:

$$\{F_{k,k'}\} \equiv F_{1,1}, F_{1,2}, ..., F_{1,NE-1}; F_{2,1}, ..., F_{2,NE-1}; F_{NE-1,1}, ..., F_{NE-1,NE-1}$$

There are (NE –1)^2 numbers in the array $\{F_{k,k'}\}$ and

$$\text{NT} = \text{NE} + (\text{NE} - 1)^2 = \text{NE(NE+1)} + 1$$

LS=1 Symmetric matrix:
The matrix elements $F_{k,k'}$ are ordered by rows starting from the diagonal term in the array $\{F_{k,k'}\}$:

$$\{F_{k,k'}\} \equiv F_{1,1}, F_{1,2}, ..., F_{1,NE-1}; F_{2,2}, ..., F_{2,NE-1}; F_{NE-1,NE-1}$$

There are [NE*(NE – 1)]/2 numbers in the array $\{F_{k,k'}\}$ and

$$\text{NT} = \text{NE} + [\text{NE (NE} - 1)]/2 = [\text{NE (NE+1)}]/2$$

Flag LB=6
A covariance matrix interrelating the cross sections for two different reaction types or materials generally has different energy grids for its rows and columns. The LB=6 format described below allows efficient representation of a rectangular (not square) matrix in one LIST record with no repetition of energy grids. The following definition applies for LB=6 sub-subsections:

$$\text{Cov}\,(X_i, Y_j) = \sum_{k,l} \mathcal{P}^{i;k}_{j;l} F_{xy;k,l} X_i Y_j$$

where

X_i as before refers to the cross sections at E_i in (MAT,3,MT) and

Y_j refers to the cross section at E_j in (MAT1,MF1,MT1[.LFS1]).

The dimensionless operator $\mathcal{P}$ is as defined for other LB's. A single "stacked" list of energies $\{E_{k,l}\}$ is required to specify the energy intervals with lower boundaries labeled by the indices k and l. That is, a single array contains the energies for the rows (E_k) and then the columns (E_l) of the matrix with the energies corresponding to the rows given first: (ER_1, ER_2, ..., ER_{NER}, EC_1, EC_2, ..., EC_{NEC}). The numbers $F_{xy;k,l}$ represent fractional components correlated over the energy intervals with lower boundaries E_k and E_l. The following quantities are defined:

NT Total number of entries in the two arrays $\{E_{k,l}\}\{F_{k,l}\}$. See below.

NER Number of energies corresponding to the rows of the matrix and defining (NER – 1) energy intervals.

NEC Number of energies corresponding to the columns of the matrix and defining (NEC – 1) energy intervals. NEC may be inferred from NT and NER.

The structure of an LB=6 sub-subsection is:

`[MAT,33,MT/ 0.0, 0.0, 0, LB=6, NT, NER/` $\{E_{kl}\}\{F_{k,l}\}$`]LIST`

The matrix elements $F_{k,l}$ are ordered by rows in the array $\{F_{k,l}\}$:

$$\{F_{k,l}\} = F_{1,1}, F_{1,2}, ..., F_{1,NEC-1}; F_{2,1}, ..., F_{2,NEC-1}; ...; F_{NER-1,1}, F_{NER-1,2}, ..., F_{NER-1,NER-1}$$

There are (NER – 1)(NEC – 1) numbers in the array $\{F_{k,l}\}$. Therefore, the total number of entries in the two arrays $\{E_{kl}\}$ and $\{F_{k,l}\}$ is:

$$\text{NT} = \text{NER} + \text{NEC} + (\text{NER} - 1)(\text{NEC} - 1) = 1 + \text{NER*NEC}.$$

Hence

$$\text{NEC} = (\text{NT} - 1)/\text{NER}.$$

Flag LB=8 or 9, Short Range Variance Representation

A short range self-scaling variance component should be specified in each File 33 subsection of the type (MAT,MT; 0,MT) by use of an LB=8 or 9 sub-subsection, unless the cross section is known to be free from unresolved underlying structure. (See section 33.3.3). The following quantities are defined:

NP Total number of pairs of numbers in the array $\{E_k, F_k\}$.

NT Total number of numbers in the LIST record. NT=2*NP

{E_k, F_k} Array of pairs of numbers; the first member of a pair is an energy, E_n; the second member of the pair, F_n, is a number associated with the energy interval between the two entries E_n and E_{n+1}.

The format of an LB=8 or 9 sub-subsection is (just as for LB=0):

`[MAT,33,MT/ 0.0, 0.0, LT, LB, NT, NP/` $\{E_k, F_k\}$`]LIST  (LT=0,LB=8 or 9)`

Only one E_k table is required. The F_k values for LB=8 or 9 have the dimension of squared cross sections. The magnitude of the resulting variance component for a processed average cross section depends strongly on the size of the energy group as well as on the values of F in the sub-subsection. For the simplest case of a multigroup covariance matrix processed on the energy grid of this sub-subsection with a constant weighting function, the variance

elements Var_{kk} are just F_k for the LB=8 component and zero for the LB=9 component; the off diagonal elements are zero in both cases.

In general, each F_k characterizes an uncorrelated contribution to the absolute variance of the indicated cross section averaged over any energy interval (subgroup) ΔE_j that includes a portion of the energy interval ΔE_k. Sub-subsections corresponding to LB=8 and LB=9 differ in the definition of the contribution to the processed group variance for the energy group (E_j, E_{j+1}).

The variance contribution $\mathrm{Var}(X_{jj})$ from an LB=8 sub-subsection to the processed group variance for the energy group (E_j, E_{j+1}) is <u>inversely</u> proportional to its width ΔE_j when (E_j, E_{j+1}) lies within (E_k, E_{k+1}) and is obtained from the relation:

$$\mathrm{Var}(X_{jj}) = F_k \frac{\Delta E_k}{\Delta E_j},$$

where $E_k \leq E_j \leq E_{j+1} \leq E_{k+1}$. This form is applicable in the resonance range where the covariances in the other sub-subsections define "average" coarse energy-grid uncertainties, while the actual pointwise cross-section values may fluctuate by orders of magnitude. The evaluator must be aware that the actual uncertainty in the cross sections depends on the user's energy-grid. The user should be aware of possible processing problems, for example when the union grid of the user's energy group structure and the covariance grid *nearly* coincide at some energy. The LB=8 variances should not be used to specify the uncertainty on the actual value of pointwise cross sections.

The variance contribution $\mathrm{Var}(X_{jj})$ from an LB=9 sub-subsection to the processed group variance for the energy group (E_j, E_{j+1}) is <u>directly</u> proportional to the width ΔE_j when (E_j, E_{j+1}) lies within (E_k, E_{k+1}). It is obtained from the relation:

$$\mathrm{Var}(X_{jj}) = F_k \left[1 - \frac{\Delta E_j}{\Delta E_k}\right],$$

where $E_k \leq E_j < E_{j+1} \leq E_{k+1}$. This form is applicable in cases when experimental evidence suggests the possibility of structure in the cross sections, but the experimental resolution is not sufficient to determine the detailed shape, which is then approximated by a smooth curve. The LB=9 option defines the maximum uncertainty in the cross section due to possible fine-structure, which vanishes when the user's energy grid is equal or coarser than the covariance grid. The physical consequence of this property is that it increases the absolute variance when the user defines an energy grid more refined than the covariance grid (thus avoiding zero-eigenvalue problems), but will not affect any coarse energy-group uncertainties. The increase in the variance remains finite (limited to F_k) and is applicable to defining the uncertainties of pointwise cross sections.

Note that the $\mathrm{Var}(X_{jj})$ are variances in average cross sections. This rule suffices for arbitrary group boundaries if subgroup boundaries are chosen to include all the E_k. No contributions to off-diagonal multigroup covariance matrix elements are generated by LB=8 or 9 sub-subsections.

33.2.3 Lumped Reaction Covariances

A lumped reaction is an evaluator-defined "redundant" cross section, defined in File 33 for the purpose of specifying the uncertainty in the *sum* of a set of cross sections, such as those for a set of neighboring discrete inelastic levels. The uncertainty in a lumped-reaction cross section, as well as its correlations with other reactions, are given in the usual way using the formats described above. On the other hand, the uncertainties and correlations of the individual parts or components of a lumped reaction are not given.

The File 33 section for one component of a lumped reaction consists of a single HEAD record that contains, in the second integer field, the section number MTL of the lumped reaction to which the component contributes. (See definition of the HEAD record at the beginning of this Section.)

```
[MAT, 33, MT/ ZA, AWR, 0, MTL, 0, NL=0]HEAD
```

The value of MTL must lie in the range 851-870, which has been reserved specifically for covariance data for lumped reactions. These MT-numbers may not be used in Files 3, 4, 5 or 6, so the net cross section and net scattering matrix for a lumped reaction must be constructed at the processing stage by summing over the reaction components.

A list of the components of a given lumped reaction is given only indirectly, namely, on the above-mentioned HEAD records. These special HEAD records, with MTL$\neq$ 0 and NL=0, form a kind of index that can be scanned easily by the processing program in order to control the summing operation.

Except for the need to sum the cross-section components during uncertainty processing, lumped reactions are "normal" reactions, in that all covariance formats can be used to describe their uncertainties in MF=33, MT=MTL. For example, one expects in general that the covariances of a lumped reaction with other reactions, including other lumped reactions, will be given by the evaluator. Also, a lumped reaction may be represented, using an NC-type subsection with LTY=0, as being "derived" from other reactions, including other lumped reactions. However, since uncertainties are not provided for the separate component reactions, a lumped reaction may not be represented as being "derived" from its components.

33.3 Procedures

Although it is not necessary to have a section in File 33 for every section in File 3, the most important values of MT for the applications to which the evaluation was intended should have a section in File 33.

33.3.1 Ordering of Sections, Subsections and Sub-Subsections

a.) Sections

The sections in File 33 are ordered by increasing value of MT.

b.) Subsections

Within a section, (MAT,33,MT), the subsections are ordered in a rigid manner. A subsection of File 33 is uniquely defines the covariances by the set of numbers: (MAT,MT;

MAT1,MF1,MT1[.LFS1]); the first pair of numbers indicates the section to which the subsection refers and the second set of numbers is the one that appears in the appropriate fields, XMF1, XLFS1, MAT1 and MT1, of the CONT record which begins every subsection. [When MT$\neq$ 10, XLFS1=0.0.]

1. The subsections within a section are ordered by increasing values of MAT1. In order to have the covariance matrices of the cross sections for which MAT1=MAT appear first in a section, the value MAT1=0 shall be used to mean MAT1=MAT in the CONT record which begins the subsection.

2. When there are several subsections with the same value of MAT1 in a section, these subsections shall be ordered by increasing values of XMF1. When MF1=MF – 30, the XMF1 field shall be entered as blank or zero. Therefore, within a given section and for a given MAT1, the subsections for MF1=MF – 30 will always appear before those for other MF1 values.

3. When there are several subsections with the same value of MAT1 and MF1 in a section, these subsections shall be ordered by increasing values of MT1 given in CONT record which begins the subsections.

4. According to the procedure in Section 33.3.1, item b.2, MAT1=0 means that MAT1=MAT; similarly, XMF1=0.0 means MF1=MF – 30. Only subsections for which MT1>MT need to be be given.

5. When there are several subsections with the same values of MAT1, MF1=10, and MT1 in a section, these subsections shall be ordered by increasing values of LFS1.

When both NC-type and NI-type sub-subsections are present in a subsection, the format requires that the NC-type sub-subsections be given first.

NC-type subsections: Several NC-type sub-subsections may be given in a subsection. When more than one is given, these must be ordered according to the value of the energy range lower endpoint E1 given in the LIST record. We note that by definition, if several LTY=0 NC-type sub-subsections are given in a subsection, the energy ranges E1 to E2 of the these different sub-subsections cannot overlap with each other or with any LTY=1 sub-subsections. However, in ENDF-6 formats it is permitted to have overlapping (E1,E2) ranges for LTY$\geq$ 1, provided that the sum of the WEI values in one subsection is no greater than unity at any energy. The value of the LTY flag of NC-type sub-subsections does not affect the ordering of the sub-subsections within a subsection.

NI-type sub-subsections: There is no special ordering requirement of NI-type sub-subsections within a subsection. However, it often happens that the full energy range of the file is covered by different sub-subsections, the F-values being set to zero in the E-tables outside the different ranges. The readability of the files is enhanced if these different sub-subsections are grouped together by the energy range effectively covered in the sub-subsections.

33.3.2 Completeness

As previously stated, there is presently no minimum requirement on the number of sections and subsections in File 33. Lack of a File 33 for a reaction does not imply zero uncertainty. However, the presence of some subsections in a File 33, as well as the presence of some sub-subsections in a subsection, implies the presence of other subsections either in the same File 33 or the File 33 (or 31 or 40) of another material. In what follows we shall identify the File 33 subsections by their value of the sextet: (MAT,MT; MAT1,MF1,MT1[.LFS1])

a.) Subsections for which MAT1=0

By subsections for which MAT1=0, we mean the subsections of the class:
(MAT,MT; 0,MF1,MT1[.LFS1]),
which according to the procedure in Section 33.3.1, item b.1 implies that MAT1=MAT.

1. If there is a File 33 subsection (MAT,MT; 0,MF1,MT1[.LFS1]) with MT1≠MT, there must be within the same material the two subsections: (MAT,MT; 0,3,MT) in File 33 and (MAT,MT1; 0,MF1,MT1[.LMF1]) in File MF1+30. Note that the converse is not necessarily true since the two cross sections (MAT,3,MT) and (MAT,MF1,MT1[.LMF1]) may have zero covariances between them, which are not required to be explicitly stated in the files. (However, see the discussion in Section 33.3.2 item b. below concerning the desirability of explicitly representing some zero covariances.) This procedure and procedure in Section 33.3.1 item b.4 guarantee that every section of File 33, (MAT,33,MT), starts with the subsection (MAT,MT; 0,3,MT).

2. In a subsection (MAT,MT; 0,3,MT,0), if there is an NC-type sub-subsection with LTY=0, it contains a list of MTI given in the NC-type sub-subsections.

3. NC-type sub-subsections with LTY=0 must be given only in subsections of the type (MAT,MT; 0,3,MT), *i.e.* with MT1=MT. NC-type sub-subsections with LTY=0, for derived redundant cross sections, imply many covariance matrices of the "derived" cross sections and of the "evaluated" cross sections. It is a task of the processing code to generate these covariance matrices from the information given in the File 33.

4. In a subsection (MAT,MT; 0,3,MT) if there is an NC-type sub-subsection with LTY=1, this sub-subsection contains values of (MATS,MFS,MTS[.LFSS]). In the same File 33, there must be a sub-subsection (MAT,MT; MATS,MFS,MTS[.LFSS]). There must be another material MATS with a File (MFS+30) containing the subsection (MATS, MTS[.LFSS]; 0,MFS,MTS[.LFSS]). Note that according to procedure in Section 33.3.3 item a., given below, MATS must be different from MAT in an "NC-type sub-subsection with LTY=1.

5. In a subsection (MAT,MT; 0,3,MT), if there is an NC-type sub-subsection with LTY=1 which covers the energy range E1 to E2, in the same subsection there must be at least one NI-type subsections represent the relative covariance matrix of the evaluated ratio measurements. In the energy range where WEI is the relative weight given to the evaluated ratio to the indicated standard cross section, the processing code takes into account the value of WEI when it applies the standards covariances. The evaluator

is responsible for multiplying the covariances of the evaluated ratios by WEI^2 before entry into the NI-type sub-subsections. Note that, where the weight is not unity in a given energy region, the NI-type sub-subsections that represent the covariance data for the ratios are mixed together without identification in File 33.

b.) Subsections for MAT1≠0

If there is a File 33 subsection (MAT,MT; MAT1,MF1,MT1[.LFS1]) with MAT1≠ 0, by analogy with the procedure in Section 33.3.2, item a.1., there must also be a subsection (MAT,MT; 0,3,MT) in the same File 33. There must also be two sub-subsections, (MAT1,MT1[.LFS1]; 0,MF1,MT1[.LFS1]) and (MAT1,MT1[.LFS1]; MAT,3,MT) in the File (MF1+30) for material MAT1.

33.3.3 Other Procedures

1. NC-type sub-subsections with LTY=1 shall only be used with MATS=MAT. The use of LTY=1 sub-subsections is reserved for covariance matrix components arising out of ratio measurements of cross sections of different nuclides, *i.e.*, different values of MAT.

2. If a single NC-type sub-subsection with LTY=0 is used in a subsection and there are no NI-type sub-subsections, the value of E1 must be 10^{-5} eV, or the reaction threshold, and the value of E2 must be the highest energy for which the corresponding cross section is given, at least 2×10^7 eV.

3. As a consequence of the definition of NC-type sub-subsections with LTY=0, if there are any NI-type sub-subsections in the same subsection, the F-values in their E-tables must be zero within the range E1 to E2 of these NC-type LTY=0 sub-subsections.

4. NI-type sub-subsections with LB=0 shall in general be avoided and forbidden in the case of cross sections relative to which ratio measurements have been evaluated. [Therefore, the acknowledged "standard cross sections" shall not have LB=0, NI-type sub-subsections.] The use of LB=0 NI-type sub-subsections should be reserved for the description of covariance matrices of cross sections which fluctuate rapidly and for which details of the uncertainties in the deep valleys of the cross sections are important.

5. The formats of File 33 allow for the possibility of great details to be entered in the files if needed. The number of NI-type sub-subsections and the number of energy entries in their E_k and E_l-tables will be a function of the details of the covariance matrices available and the need to represent them in such detail. However, good judgement should be used to minimize as much as possible the number of different entries in the E_k and E_l-tables. An important quantity to note is the union of all of the E values in the E_k and E_l-tables of a File 33. A reasonable upper limit of the order of a few hundred different E values for the union of all energy entries in all of the E_k and E_l-tables in a File 33 should be considered.

   Note that the evaluator's covariance values will be most readily recognized in a processed multigroup covariance matrix when the energies in the E_k and E_l-tables can be

chosen from the set of standard multigroup energy boundaries. If in the File 33 the uncertainties in a cross section are represented using LB=0 or 1 in regions of width ΔE_i, and if the File is processed to give a multigroup covariance library with group width in that energy region ΔE_a such that $\Delta E_i > \Delta E_a$, the correlation patterns in ENDF-6 are defined so that the processed group uncertainties are lowest and the inter-group correlations greatest when an energy group of the processed covariance matrix is evenly split by a covariance file E value. This behavior has alarmed some users. However, because of the correlation pattern set up, no big anomalies arise in the uncertainty projected for an integral quantity that is sensitive to a broad spectrum of incident particle energies. The magnitude of the effect can be reduced by using narrower intervals in LB=0, 1 files, or more favorably by using overlapping files with staggered energy edges.

6. The ground rules above (see 33.2, under LT=1 sub-subsections) state that if cross sections are obtained by evaluating ratio measurements to a "standard cross section," the latter cross section should be "evaluated" in the sense that there are no NC-type sub-subsections with LTY=0 or 1 describing the covariance data for that cross section. This leads to procedural requirements.

   (a) Evaluators of established standard cross sections should endeavor to avoid the use of any LTY=0 or LTY=1 sub-subsections. If the physics of an evaluation problem should require that this rule be broken, the CSEWG should be informed and the text documentation should call attention to the situation.

   (b) If an evaluated cross section is best obtained as the ratio to a cross section in another material that is not an established standard, than an evaluator needs to contact the evaluator of that material to be reassured that NC-type sub-subsections will not appear in the files for the reference cross section for the energy region of concern.

   Such communication is required in any case to encourage the evaluation of the covariance data for that reference cross section, without use of LB=0 sub-subsections, and to assure that the required LTY=3 sub-subsection will be entered. To aid the review process, a written form of this communication should be sent to the CSEWG.

7. The ENDF-6 formats allow the evaluator to recognize the partial dependence of a cross section on a standard cross section. This means that it is possible to recognize in the covariance files an evaluation that utilizes some absolute data as well as ratio data to one or more standard cross sections. Use of this capability is expected to be necessary to properly represent some covariance information. Since processing complexity is thereby induced, evaluators are urged to use this capability with caution, and in no case to represent the dependence of a cross section in a given energy region on ratio measurements to more than two standard cross sections.

8. The discussion of the covariance terms that arise from evaluated cross section ratio measurements was based entirely on so-called absolute ratio measurements. Evaluators should note that various types of cross section "shape" measurements induce additional

covariance terms that can be derived for specific situations. Within ENDF-6 formats the evaluator must include them in NI-type sub-subsections in the covariance files of the derived cross section.

9. When cross section A is correlated to B, and cross section C is also correlated to B even though A is uncorrelated to C, evaluators should include the file segments that express this zero correlation to signify to reviewers and users that an unusual case is recognized. This is the exception to the general rule that zero covariances need not be openly expressed in the covariance files.

10. The lumping of reactions for uncertainty purposes will be useful mainly in connection with discrete-level inelastic scattering cross sections. However, other reactions, such as (n,n'p), (n,n'), and (n,n'$_{\text{continuum}}$), may also be treated in this way.

11. In order not to lose useful uncertainty information, reactions lumped together should have similar characteristics. Ordinarily, the level energies of discrete inelastic levels lumped together should not span a range greater than 30-40%, and the angular distributions should be similar.

12. The components of a lumped reaction need not have adjacent MT-numbers.

    (a) Lumped-reaction MT-numbers must be assigned sequentially, beginning at 851. The sequence is determined by ordering the lumped reactions according to the lowest MT-number included among their respective components. Thus, the first value of MTL encountered on any component-reaction HEAD record will be 851. The next new value of MTL encountered will be 852, and so on.

    (b) Lumped reactions with only a single component are permitted. This is recommended practice when, for example, an important discrete inelastic level is treated individually, while all of its neighbors are lumped. Covariances for both the individual level and the nearby lumped levels can then be placed together in sections 851-870.

13. An LB=8 or 9 sub-subsection should be included in each (MAT,MT; 0, MT) subsection unless the cross section is known to be free from unresolved underlying structure[5]. The Doppler effect in reactor applications smooths cross sections on an energy scale too narrow to be of concern for LB=8 or 9 covariance evaluation. This sub-subsection must cover the entire energy range of the section (threshold to at least 20 MeV). Use of zero values for F_k in any part of this energy range should be avoided because such usage could induce the problem of non-physical full correlation between neighboring fine-group cross sections, the problem that the LB=8 or 9 formats was designed to solve. The LB=8 or 9 formats may not be used for cross-reaction covariances.

    Note that the law for processing LB=8 sub-subsections directly references the variance of an average cross section rather than the variance of a pointwise cross section. If

[5]For example, if covariance data for neutron scattering from hydrogen were to be represented in File 33, one would expect no component that could be properly represented by an LB=8 or 9 subsection. Covariance data in such cases may best be represented in File 30.

a fine-grid covariance matrix is developed and then collapsed to the evaluator's E_k grid with constant weighting, the resulting variance components are just the F_k. (A complete multigroup covariance matrix cannot in general be correctly "reprocessed" to a finer energy mesh; one must process the ENDF covariance files directly).

The values of F_k may be chosen by the evaluator to account for statistical fluctuations in fine-group average cross sections that are induced by the width and spacing distributions of the underlying resonances. Values may also be chosen to represent the uncertainty inherent in estimating the average cross sections for small energy intervals where little or no experimental data exist and smoothness is not certain.

The LB=8 or 9 sub-subsections help prevent mathematical difficulties when covariance matrices are generated on an energy grid finer than that used by the evaluator, but F_k values must be chosen carefully to avoid accidental significant dilution of the evaluated covariance patterns represented in the other Subsections. If no physical basis is apparent for choosing the F_k values, they may be given values about 1% as large on the evaluator's grid as the combined variance from the other sub-subsections. Such values would be small enough not to degrade the remainder of the covariance evaluation and large enough to assure that the multigroup covariance matrix will be positive definite for any energy grid if the matrix on the evaluator's energy grid is positive definite.

Since LB=8 and 9 specify absolute covariances, they should not be employed near reaction thresholds. In particular, for threshold reactions having an effective threshold above 0.1 MeV, LB=8 or 9 should not be employed for incident energies less than 1 MeV above the effective threshold.

33.3.4 Examples

We illustrate here the use of File 33 by means of two concrete examples.

33.3.4.1 Use of LTY=1 and LTY=2 NC-type Subsections

Let us consider a hypothetical evaluation of ^{239}Pu, MAT=1264. Assume that the decision is made that in File 33 only the fission cross sections and the capture cross sections shall have covariances represented. The following methods were used in performing the hypothetical evaluation:

1. Fission cross sections, MT=18
   Let X_i stand for the fission cross sections of ^{239}Pu at energies E_i.

   (a) From 10^{-5} eV to an energy E_s, X_i were evaluated in terms of "direct" or "absolute" measurements, A_i. By this we mean that in this energy range, X_i and its uncertainties are independent of any other cross sections. In this energy range $X_i \equiv A_i$.

   (b) From E_s to 20 MeV, X_i was evaluated by means of ratio measurements to Y_i, the fission cross section of ^{235}U, to which we assign the MAT number 1261. In this energy range $X_i = R_i Y_i$, where R_i is the evaluated ratio at energy E_i.

2. Capture cross sections, MT=102
   Let Z_i stand for the capture cross sections of ^{239}Pu at energies E_i. In this evaluation, Z_i were obtained by the evaluation of a_i, the ratio of capture to fission cross sections, over the complete range of the file. Therefore we have $Z_i = a_i X_i$.

In this evaluation then, only 3 quantities were evaluated: A_i from 10^{-5} eV to E_s, R_i from E_s to 20 MeV, and a_i from 10^{-5} eV to 20 MeV. The evaluation of these quantities resulted in the evaluation of three covariance matrices: $\mathrm{Cov}(A_i, A_j)$, $\mathrm{Cov}(R_i, R_j)$ and $\mathrm{Cov}(a_i, a_j)$. Let us now assume that in addition it has been determined that these three different quantities are uncorrelated, *i.e.*, covariances such as $\mathrm{Cov}(A_i, a_j)$ can be neglected.

Let us denote relative covariance matrices such as $\mathrm{Cov}(A_i A_j)/(A_i A_j)$ as $\langle dA_i\, dA_j\rangle$, and similarly for the other quantities.

From 10^{-5} to E_s (since $X_i = A_i$ and $Z_i = a_i X_i$ we have:

$$\begin{aligned}
\langle dX_i\, dX_j\rangle &= \langle dA_i\, dA_j\rangle \\
\langle dX_i\, dZ_j\rangle &= \langle dA_j\, dA_j\rangle \\
\langle dZ_i\, dZ_j\rangle &= \langle da_i\, da_j\rangle + \langle dA_i\, dA_j\rangle
\end{aligned}$$

From E_s to 20 MeV (since $X_i = R_i Y_i$ and $Z_i = a_i X_i$ we have

$$\begin{aligned}
\langle dX_i\, dX_j\rangle &= \langle dR_i\, dR_j\rangle + \langle dY_i\, dY_j\rangle \\
\langle dX_i\, dZ_j\rangle &= \langle dR_i\, dR_j\rangle + \langle dY_i\, dY_j\rangle \\
\langle dX_i\, dY_j\rangle &= \langle dY_i\, dY_j\rangle \\
\langle dZ_i\, dZ_j\rangle &= \langle da_i\, da_j\rangle + \langle dR_i\, dR_j\rangle + \langle dY_i\, dY_j\rangle \\
\langle dZ_i\, dY_j\rangle &= \langle dY_i\, dY_j\rangle
\end{aligned}$$

We note that in the above we have expressed all of the covariance matrices of the cross sections in terms of the covariance matrices of the evaluated quantities and the covariance matrix of the ^{235}U fission.

For purposes of illustrating the use of the formats we need not know the details of how the covariance matrices $\langle dA_i\, dA_j\rangle$, $\langle dR_i\, dR_j\rangle$ and $\langle da_i\, da_j\rangle$ are represented. They must be represented by one or more NI-type sub-subsections having an E_k table, or could be so represented. For our purposes, we symbolically represent each one of them in terms of a single NI-type sub-subsection with a single E_k table:

$$\begin{aligned}
\langle dA_j\, dA_j\rangle &\rightarrow \{E_k^A, F_k^A\} \\
\langle dR_j\, dR_j\rangle &\rightarrow \{E_k^R, F_k^R\} \\
\langle da_j\, da_j\rangle &\rightarrow \{E_k^a, F_k^a\}
\end{aligned}$$

Whether one or more NI-type sub-subsections are used, each one of the E-tables used in the sub-subsection can be written as:

$$\begin{aligned}
\{E_k^A, F_k^A\} &= \{10^{-5}, F_1^A; ...; E_k^A, F_k^A; ...; E_s, 0.0; 2\times 10^7, 0.0\}, \\
\{E_k^R, F_k^R\} &= \{10^{-5}, 0.0; E_s, F_k^R; ...; E_k^R, F_k^R; ...; 2\times 10^7, 0.0\}, \\
\{E_k^a, F_k^a\} &= \{10^{-5}, F_1^a; F_k^a; ...; E_k^a, F_k^a; ...; 2\times 10^7, 0.0\},
\end{aligned}$$

the E and F values explicitly shown must have the values indicated above for this example.

In the listing given in Example 33.1 for the File 33 of MAT=1264, corresponding to our example, we have shown with only one sub-subsection each of the matrices $\langle dA_i\ dA_j \rangle$, $\langle dR_i\ dR_j \rangle$ and $\langle da_i\ da_j \rangle$. E_S is taken as 2×10^5 eV.

Note: In the File 33 of MAT 1261 in the subsections (1261,18; 1264,18) and (1261, 18; 1264,102) an LTY=3 NC-type sub-subsection corresponding to the LTY=2 sub-subsections of Example 33.2 must be inserted.

Example 33.1. File 33 with NC-type LTY=1 sub-subsections

```
9.423900+4 2.369990+2          0          0          0       NL=3126433 18 HEAD
0.000000+0 0.000000+0     MAT1=0      T1=18       NC=1       NI=2126433 18 CONT
0.000000+0 0.000000+0          0      LTY=1          0          0126433 18 CONT
2.000000+5 2.000000+7  MATS=1261     MTS=18       NT=6       NE=2126433 18 LIST
0.000000+0 0.000000+0 2.000000+5  1.00000+0  2.00000+7  0.00000+0126433 18<dYi dYj>
0.000000+0 0.000000+0   LT=0LB=1      NY=14       NE=7           126433 18 LIST
1.000000-5 0.000000+0 1.000000+0  2.50000-3  3.00000+2  3.60000-3126433 18<dAi dAj>
3.000000+4 4.900000-3 1.000000+5  6.40000-3  2.00000+5  0.00000+0126433 18
2.000000+7 0.000000+0                                          126433 18
0.000000+0 0.000000+0       LT=0       LB=1       NT=6       NE=3126433 18 LIST
1.000000-5 0.000000+0 2.000000+5  4.00000-4  2.00000+7  0.00000+0126433 18<dRi dRj>
```

(1264,18; 0,102)

```
0.00000+0 0.00000+0 MAT1=1261    MT1=18      NC=1     NI=0126433 18 CONT
0.00000+0 0.00000+0         0     LTY=2         0        0126433 18 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18      NT=6     NE=2126433 18 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.0000+0126433 18<dYi dYj>
0.00000+0 0.00000+0         0         0         0        0126433  0 SEND
```

(1264,102; 0,102)

```
9.42390+4 2.36999+2         0         0         0      NL=2126433102 HEAD
0.00000+0 0.00000+0     MAT=0   MT1=102      NC=1      NI=2126433 18 CONT
0.00000+0 0.00000+0         0     LTY=1         0         0126433 18 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18      NT=6      NE=2126433 18 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433 18<dYi dYj>
0.00000+0 0.00000+0      LT=0      LB=1     NT=14      NE=7126433 18 LIST
1.00000-5 0.00000+0 1.00000+0 2.50000-3 3.00000+2 3.60000-3126433 18<dAi dAj>
3.00000+4 4.90000-3 1.00000+5 6.40000-3 2.00000+5 0.00000+0126433 18
2.00000+7 0.00000+0                                          126433 18
0.00000+0 0.00000+0      LT=0      LB=1      NT=6      NE=3126433 18 LIST
1.00000-5 0.00000+0 2.00000+5 4.00000-4 2.00000+7 0.00000+0126433 18<dRi dRj>
```

(1264,18; 1261,18)

```
0.00000+0 0.00000+0    MAT1=0   MT1=102      NC=1      NI=3126433102 CONT
0.00000+0 0.00000+0         0     LTY=1         0         0126433102 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18      NT=6      NE=2126433102 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433102<dYi dYj}>
0.00000+0 0.00000+0      LT=0      LB=1     NT=14      NE=7126433102 LIST
1.00000-5 0.00000+0 1.00000+0 2.50000-3 3.00000+2 3.60000-3126433102<dAi dAj>
3.00000+4 4.90000-3 1.00000+5 6.40000-3 2.00000+5 0.00000+0126433102
2.00000+7 0.00000+0                                          126433102
0.00000+0 0.00000+0      LT=0      LB=1      NT=6      NE=3126433102 LIST
1.00000-5 0.00000+5 2.00000+5 4.00000-4 2.00000+7 0.00000+0126433102<dRi dRj>
0.00000+0 0.00000+0      LS=1      LB=5     NT=21      NE=6125433102 LIST
1.00000-5 2.53000-2 9.00000-2 2.50000-1 1.00000+0 2.00000+7126433102<dai daj>
2.21000-3 4.84000-4 3.62000-4 3.56000-4 0.00000+0 4.84000-4126433102
3.10000-4 3.04000-4 0.00000+0 6.25000-4 2.30000-4 0.00000+0126433102
2.21000-3 0.00000+0 0.00000+0 0.00000+0 0.00000+0 0.00000+0126433102
```

(1264,102; 1261,18)

```
0.00000+0 0.00000+0 MAT1=1261    MT1=18      NL=1      NI=0126433102 CONT
0.00000+0 0.00000+0         0     LTY=2         0         0126433102 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18      NT=6      NE=2126433102 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433102<dYi dYj>
0.00000+0 0.00000+0         0         0         0         0126433  0 SEND
```

33.3.4.2 Use of LTY=0, NC-type Sub-Subsections

Let us consider a hypothetical evaluation of ^{12}C, MAT=1274. The decision is made that in File 33 the MT values 1, 2, 4, 102 and 107 shall have covariances represented. We shall use the notation developed in the previous example. The following method was used in this evaluation:

1. Total cross sections (MT=1),
   σ_i^T, were evaluated over the complete energy range, with the covariance matrix obtained, and:
   $$\langle d\sigma_i^T \; d\sigma_j^T \rangle \rightarrow \{E_k^T, F_k^T\},$$
   with $\{E_k^T,\, F_k^T\} = \{10^{-5},\, F_1^T\ ;\ ...;\ E_k^T,\, F_k^T\ ;\ ...\ ;\ 2 \times 10^7,\, 0.0\}$,

2. Elastic cross sections (MT=2),
   σ_i^E, were "derived" up to 8.5 MeV from the "evaluated" cross sections:
   $$\sigma_i^E = \sigma_i^T - \sigma_i^I - \sigma_i^C - \sigma_i^\alpha.$$
   Above 8.5 MeV the elastic cross sections were evaluated and:
   $$\langle d\sigma_i^E \; d\sigma_j^E \rangle \rightarrow \{E_k^E, F_k^E\},$$
   with $\{E_k^E,\, F_k^E\} = \{10^{-5},\, 0.0;\, 8.5 \times 10^6,\, F_k^E\ ;\ ...\ ;\ E_k^E,\, F_k^E\ ;\ ...\ ;\ 2 \times 10^7,\, 0.0\}$.

3. Inelastic cross sections (MT=4),
   σ_i^I, were evaluated from threshold at 4.8 MeV, to 8.5 MeV and:

$$\langle d\sigma_i^I \; d\sigma_j^I \rangle \rightarrow \{E_k^I, F_k^I\},$$

   with $\{E_k^I,\, F_k^I\} = \{10^{-5},\, 0.0;\, 4.8 \times 10^6,\, F_k^I\, ;\, ...\, ;\, E_k^I,\, F_k^I\, ;\, ...\, ;\, 8.5 \times 10^6,\, 0.0;\, 2 \times 10^7,\, 0.0\}$,
   Above 8.5 MeV the inelastic cross sections were "derived" and:

$$\sigma_i^I = \sigma_i^T - \sigma_i^E - \sigma_i^C - \sigma_i^\alpha.$$

4. Capture cross sections (MT=102),
   σ_i^C, were evaluated over the complete energy range and:

$$\langle d\sigma_i^C \; d\sigma_j^C \rangle \rightarrow \{E_k^C, F_k^C\},$$

   with $\{E_k^C,\, F_k^C\} = \{10^{-5},\, F_1^C\, ;\, ...\, ;\, E_k^C,\, F_k^C\, ;\, ...\, ;\, 2 \times 10^7,\, 0.0\}$,

5. The (n,α) cross sections (MT=107),
   σ_i^α, were evaluated from threshold at 6.18 MeV to 20 MeV and:

$$\langle d\sigma_i^\alpha \; d\sigma_j^\alpha \rangle \rightarrow \{E_k^\alpha, F_k^\alpha\},$$

   with $\{\; E_k^\alpha,\, F_k^\alpha \;\} = \{10^{-5},\, 0.0;\, 6.1 \times 10^6,\, F_k^\alpha\, ;\, ...\, ;\, E_k^\alpha\, ,\, F_k^\alpha\, ;\, ...\, ;\, 2 \times 10^7,\, 0.0\;\}$,

In the listing given in Example 33.2 for File 33 of MAT=1274, corresponding to our example, we have shown only one NI-type sub-subsection for each evaluated covariance matrix. Again it is assumed that there are no correlations among the directly evaluated quantities.

The above example has great similarity to the way the evaluation of ^{12}C was made, the major difference being that instead of MT=4 being evaluated, the evaluation was made for MT=51 and MT=91. Since it will illustrate some of the procedures of File 33, let us now consider adding to the above File 33 for MAT=1274 the covariance matrices for MT=51 and MT=91.

1. Discrete inelastic scattering cross section to the first excited state (MT=51)

   σ_i^{51}, up to 8.5 MeV is identical to σ_i^I. Therefore, we may consider up to 8.5 MeV that σ_i^{51} is a "derived" cross section with: $\sigma_i^{51} = \sigma_i^I$. This is permissible because MT=4 has only NI-type sub-subsections in this energy range.

   From 8.5 MeV to 20 MeV, MT=51 was evaluated and:

$$\langle d\sigma_i^{51} \; d\sigma_j^{51} \rangle \rightarrow \{E_k^{51}, F_k^{51}\},$$

   with $\{E_k^{51},\, F_k^{51}\} = \{10^{-5},\, 0.0;\, 8.5 \times 10^6,\, F_k^{51}\, ;\, ...\, ;\, E_k^{51},\, F_k^{51}\, ;\, ...\, ;\, 2 \times 10^7,\, 0.0\}$,

2. Continuum inelastic cross section (MT=91)
   From 8.5 to 20 MeV, the continuum inelastic, σ_i^{91}, was "derived" as: $\sigma_i^{91} = \sigma_i^I - \sigma_i^{51}$. However, we cannot use this relationship for the purposes of File 33 because in this energy range σ_i^I is indicated in the File as being already "derived."

   Therefore, for the purposes of File 33, we must write:

$$\sigma_i^{91} = \sigma_i^T - \sigma_i^E - \sigma_i^{51} - \sigma_i^C - \sigma_i^\alpha,$$

   which now only refers to cross sections having exclusively NI-type sub-subsections. Therefore, we may now add the sections to the File 33, MAT=1274, shown in Example 33.3, to have a more complete File 33.

Example 33.2. File 33 with NC-type LTY=0 sub-subsections.

(1274.1; 0.1)

```
 6.01200+3 1.18969+1         0         0         0         1112733  1 HEAD
 0.00000+0 0.00000+0         0         1         0         1112733  1 CONT
 0.00000+0 0.00000+0         0         1         6         3112733  1 LIST
 1.00000-5 5.00000-5 2.00000+6 2.50000-5 2.00000+7 0.00000+0112733  1
 0.00000+0 0.00000+0         0         0         0         0112733  0 SEND
```

(1274,2; 0,2)

```
 6.01200+3 1.18969+1         0         0          0        1112733  2 HEAD
 0.00000+0 0.00000+0         0         2          1        1112733  2 CONT
 0.00000+0 0.00000+0         0         0          0        0112733  2 CONT
 1.00000-5 8.50000+6         0         0          8        4112733  2 LIST
 1.00000+0 1.00000+0 1.00000+0 4.00000+0-1.000000+0 1.0200+2112733  2
-1.00000+0 1.07000+0                                         112733  2
 0.00000+0 0.00000+0         0         1          8        4112733  2 LIST
 1.00000-5 0.0000000 8.50000+6 8.00000-6  1.50000+6 2.500005112733  2
 2.00000+7 0.00000+0                                         112733  2
 0.00000+0 0.00000+0         0         0         0         0112733  0 SEND
```

(1274,4; 0,4)

```
 6.01200+3 1.18970+1         0         0         0         1112733  4 HEAD
 0.00000+0 0.00000+0         0         4         1         1112733  4 CONT
 0.00000+0 0.00000+0         0         0         0         0112733  4 CONT
 1.00000+0 1.00000+0-1.00000+0 2.00000+0-1.00000+0 1.02000+2112733  4 LIST
-1.00000+0 1.07000+2                                         112733  4
 0.00000+0 0.00000+0         0         1         8         4112733  4 LIST
 4.80000+6 1.00000-3 6.00000+6 1.00000-4 8.50000+6 0.0000000112733  4
 8.50000+6 2.00000+7         0         0         8         4112733  4
 2.00000+7 0.00000+0                                         112733  4
 0.00000+0 0.00000+0         0         0         0         0112733  0 SEND
```

(1274,102; 0,102)

```
 6.01200+3 1.18969+1         0         0         0         1112733102 HEAD
 0.00000+0 0.00000+0         0       102         0         1112733102 CONT
 0.00000+0 0.00000+0         0         1         6         3112733102 LIST
 1.00000-5 3.60000-3 1.00000+3 4.00000-2 2.00000+7 0.00000+0112733102
 0.00000+0 0.00000+0         0         0         0         0112733  0 SEND
```

(1274,107; 0,107)

```
 6.01200+3 1.18969+1         0         0         0         1112733107 HEAD
 0.00000+0 0.00000+0         0       107         0         1112733107 CONT
 0.00000+0 0.00000+0         0         0         8         4112733107 LIST
 6.18000+6 1.00000-5 6.32000+6 1.00000-4 7.36000+6 2.00000-4112733107
 2.00000+7 0.00000+0                                          112733107
 0.00000+0 0.00000+0         0         0         0         0112733  0 SEND
```

Example 33.3.
Additional sections of File 33 which could be added to File 33 are given in Example 33.3

(1274,51; 0.51)

```
 6.01200+3 1.18969+1         0         0         0         1127433 51 HEAD
 0.00000+0 0.00000+0         0        51         1         1127433 51 CONT
 0.00000+0 0.00000+0         0         0         0         0127433 51 CONT
 1.00000-5 8.50000+6         0         0         2         1127433 51 LIST
 1.00000+0 4.00000+0                                          127433 51
 0.00000+0 0.00000+0         0         1         6         3127433 51 LIST
 1.00000-5 0.00000+0 8.50000+6 2.50000-3 2.00000+7 0.00000+0127433 51
 0.00000+0 0.00000+0         0         0         0         0127433  0 SEND
```

(1274,91; 0,91)

```
 6.01200+3 1.18969+1         0         0         0         1127433 91 HEAD
 0.00000+0 0.00000+0         0        91         1         0127433 91 CONT
 0.00000+0 0.00000+0         0         0         0         0127433 51 CONT
 8.50000+6 2.00000+7         0         0        10         5127433 51 LIST
 1.00000+0 1.00000+0-1.00000+0 2.00000+0-1.00000+0 5.10000+1127433 51
-1.00000+0 1.02000+2-1.00000+0 1.07000+2                    127433 51
 0.00000+0 0.00000+0         0         0         0         0127433  0 SEND
```

Chapter 34

File 34. COVARIANCES FOR ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES

34.1 General Comments

File 34 contains covariances for angular distributions of secondary particles. It is assumed that uncertainties will not be required on all quantities in File 4.

A central question is whether quantities in File 3 may have important correlations with those in File 4, or whether one needs to be concerned only with correlations of angular distribution parameters as a function of incident energy. It is judged that covariances between the magnitude and shape are likely to be important only when theory plays a strong role in an evaluation. When such covariances occur, the idea, developed below, is that one expresses covariances with the a_0 Legendre coefficients even though $a_0 \equiv 1$ in the ENDF system.

Because of the simplicity of representing the covariances of Legendre coefficients rather than normalized probability components, only the former is considered here even for cases where File 4 has tabulated $p(\mu)$. Furthermore, the covariance matrix in File 34 may refer to Legendre coefficients in the LAB coordinate system even when the data in File 34 are given in the CM coordinate system. This is done for convenience, since transport calculations involve Legendre moments of the cross sections, which are related to the Legendre coefficients of the angular distribution expansion in the LAB system, therefore the covariance matrix in the LAB system may be more easily generated (and used).

In ENDF-6 formats there is no provision for covariance components linking the angular distribution parameters for different materials, though a MAT1 field is provided, but is normally zero.

34.2 Formats

The general structure of File 34 follows the normal pattern, with sections by increasing MT values. The LTT flag definition is modified from its meaning for File 4. The following

quantities are defined:

ZA,AWR Standard material charge and mass parameters

LTT Flag to specify the representation used, and it may have the following values in File 34.

- LTT=1 the data are given as Legendre coefficient covariances as a function of incident energy, starting with a_1 or higher order coefficients.
- LTT=2 the data are given as Legendre coefficients covariances as a function of incident energy, starting with a_0. (This information is redundant in the formats, as specified below, but is considered desirable as an alarm flag.)
- LTT=3 if *either* L or L1=0 anywhere in the Section.

NMT1 Number of subsections present in File 34 for various MT1≥ MT.

A section of File 34 for a given MT has the form:

```
[MAT,34,MT/  ZA, AWR,   0, LTT,  0, NMT1]HEAD
          <subsection for MT1 = MT>
           ----------------------------
           ----------------------------
          <NMT1-th subsection for largest MT1>
[MAT,34,0/ 0.0,  0.0,   0,   0,  0,    0]SEND
```

Each subsection begins with a control record that identifies the related MT1 and indicates how many Legendre coefficients are covered for the angular distributions for reaction types MT(NL) and MT1(NL), MT1≥MT. The following quantities are defined:

MT1 "Other" reaction type; this subsection contains data for the covariances $\mathrm{Cov}[a_L(E_1), a_{L1}(E_2)]$ between Legendre coefficients for two reaction types at incident energies E_1 and E_2 for various L and L1.

NL Number of Legendre coefficients for which covariance data are given for the reaction MT. (This value must be the same for each subsection.)
(The first coefficient is a_0 if LTT=3, $a_1 \geq 1$ if LTT=1).

NL1 Number of Legendre coefficients for which covariance data are given for reaction MT1.

L Index of the Legendre coefficient for reaction MT for this sub-subsection. Note that sub-subsections need not be given for all values of L and L1.

L1 Index of the Legendre coefficient for reaction MT1 for this sub-subsection.

LCT Flag to specify the frame of reference used

- LCT=0 the data are given in the same coordinate system as used in File 4
- LCT=l the data are given in the LAB system
- LCT=2 the data are given in the CM system.

NI Number of LIST records contained in this sub-subsection.

LS Flag, recognized when LB=5, to indicate whether the matrix is symmetric (1=yes, 0=no).

LB Flag to indicate the covariance pattern as a function of incident energy. LB values 0,1,2,5 & 6 are allowed, and are defined as for File 33 in Section 33.2.

NT Total number of items in the list,
For LB=0,1,2, NT=2*NE;
for LB=5, NT is dependent on LS as given in Section 33.2;
for LB=6, NT=1+NER*NEC.

{Data} For LB=5, sequence $\{E_k\}$ $\{F_{k,k}\}$;
for LB=6, sequence $\{E_k\}$ $\{F_{k,l}\}$ (as in File 33).

A subsection has the following form:

```
[MAT,34,MT/ 0.0, 0.0, MAT1, MT1, NL, NL1]CONT   (MAT1=0)
[MAT,34,MT/ 0.0, 0.0, L1,   L11, LCT, NI1]CONT[a]
[MAT,34,MT/ 0.0, 0.0, LS1,  LB1, NT1, NE1/ {Data1}] LIST
     ----------------------------------
     ----------------------------------
[MAT,34,MT/ 0.0, 0.0, LSNI1, LBSNI1, NTSNI1, NENI1/{DataNI1}] LIST
     ----------------------------------
     ----------------------------------
[MAT,34,MT/ 0.0, 0.0, LNSS, L1NSS, 0, NINSS ] CONT
[MAT,34,MT/ 0.0, 0.0, LS1, LB1, NT1, NE1/ {Data1} LIST
     ----------------------------------
     ----------------------------------
[MAT,34,MT/ 0.0, 0.0, LSNINSS, LBNINSS, NTNINSS, NENINSS/ {DATANINSS}]
LIST
```

[a] In this first subsection, L and L1 are the smallest values present of NL and NL1.

The number of sub-subsections NSS for a given MT1 is NL*NL1, and they are ordered as (L,L1) = (1,1),(1,2),...,(NL,NL1). (Not all L-values need be included). When MT1=MT, redundancy is avoided by giving each sub-subsection only once, when L1≥ L. In this case NSS=NL*(NL+1)/2.

34.3 Procedures

It is strongly recommended that the maximum order of the Legendre expansion for uncertainty representation be minimized.

If there are important cases (*e.g.*, n-p scattering) where the shape of the angular distribution is correlated with the magnitude of the scattering cross section, the convention is that the covariances among scattering (integrated) cross sections must be in File 33 and must not be repeated, so all sub-subsections in File 34 with L=L1=0 would contain null covariance components. This procedure would maintain the convention that covariance components are summed from various portions of the ENDF file corresponding to a particular material. (The information contained in File 34 for L *or* L1 non-zero is the motivation for the present procedure). Note that, in the case of correlation between shape and magnitude of a scattering cross section, it is possible for an absorption cross section MT-value to show up in File 34 (with L=0 only).

Chapter 35

File 35. COVARIANCES FOR ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES

35.1 General Comments

File 35 contains covariance matrices for the energy distribution of secondary particles given in File 5. The data in File 5 are normally given in the Laboratory system, and are expressed as normalized probability distributions. If the spectral distributions are correlated with angular distributions and given in File 6, the covariance information in File 35 refers to the angle-integrated distributions. At present, no formats are defined for correlated distributions; for the purpose of uncertainty estimations the separability assumption in the outgoing energy and angle is implied.

Since there is usually very fragmentary experimental information with which to construct the data given in File 5, the uncertainties in the secondary distributions are highly correlated as a function of incident particle energy. It is therefore proposed that only a few covariance matrices be used in each MT value in File 35 to cover the complete incident energy range. Each covariance matrix applies to the complete secondary energy distributions for the broad incident energy range specified, regardless of how these secondary energy distributions are specified, or broken down into various components, in File 5. No covariances between the different incident energy ranges are allowed. Also, no covariances linking different materials or reaction types are allowed. Furthermore, no covariances with information in other files, for instance File 3 and $\overline{\nu}(E)$ in File 1 are allowed in File 35.

35.2 Formats

Each subsection covers a covariance matrix for one incident particle energy range, and the complete incident energy range is covered by the NK subsections.

A new type of LB subsection is defined (LB=7). Covariances in File 35 refer to normalized probabilities, therefore it is natural to specify the covariance matrices as absolute covariances of the normalized probabilities rather than the corresponding relative covariances. The

LB=7 subsection is similar to an LB=5 subsection, but with entries that are absolute rather than relative. The following quantities are defined:

NK Number of subsections

E_1 Lowest incident neutron energy to which the covariance matrix in the subsection applies.

E_2 Highest incident neutron energy to which the covariance matrix in the subsection applies. The value of E_2 in a subsection becomes the value of E_1 in the next subsection.

LS=1 Flag indicating that the covariance data matrix $F_{k,k'}$, is symmetric.

LB=7 Flag indicating that the elements of the covariance matrix $F_{k,k'}$ are absolute.

NT Total number of entries in the list. NT=[NE*(NE+1)]/2.

NE Number of entries in the array $\{E'_k\}$

$\{E'_k\}$ Array containing outgoing particle energies, and defining NE-1 energy intervals for outgoing particles. The value of E'_1 in the array must be the lowest outgoing particle energy possible at E_1; E'_{NE} in the array must be the highest outgoing particle energy possible at E_2 and represented in File 5.

$\{F_{k,k'}\}$ covariance matrix. The $F_{k,k'}$'s are ordered by rows, starting from the diagonal term

$$\{F_{k,k'}\} \equiv F_{1,1}, F_{1,2}; F_{2,2}, F_{2,3}, ..., ...; F_{NE-1,NE-1}.$$

The structure of a section of File 35 is as follows:

```
[MAT,35,MT/ ZA, AWR, 0, 0, NK, 0] HEAD
   <subsection for k=1>
   <subsection for k=NK>
[MAT,35, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The structure of a subsection is:

[MAT,35,MT/ E_1, E_2, LS, LB, NT, NE/$\{E'_k\}$,{ $F_{k,k'}$}] LIST (LS=1,LB=7)

In terms of the dimensionless operators defined in Section 33.2, the covariance between two bin-probabilities (*i.e.* yields) in the energy-intervals E_i and E_j, respectively, of the normalised probability distribution is:

$$\mathrm{Cov}\left(p\left(E \to E'_i\right), p\left(E \to E'_j\right)\right) = \sum_{k,k'} \mathcal{P}^{i,k}_{j,k'} F_{k,k'}$$

where

$E_1 \leq E \leq E_2$, and the operator $\mathcal{P}$ is defined so that only the term in the sum for $E'_k \leq E'_i \leq E'_{k+1}$ and $E'_{k'} \leq E'_j \leq E'_{k'+1}$ is non-zero.

35.3 Procedures

Because probability distributions must remain normalized to unity, covariance matrices of the bin probabilities in File 35 must satisfy the constraint (in addition to being symmetric) that the sums of the elements in any row of the matrix (hence also in any column) must be zero. Therefore, one of the covariance matrix elements in each row (or column) is redundant, but this redundancy is kept in the file to cross-check the consistency of the covariance matrix.

The $F_{k,k'}$ are the covariance matrix elements defined above for the normalized spectral yields Y_k for the outgoing particle energy intervals on the evaluator's energy grid $\{E'_k\}$ (*i.e.* bin probabilities and not bin-averaged probability distributions). Normalization of the covariance matrix is considered adequate if for each row (or column) k the following condition is satisfied:

$$\frac{S_k}{Y_k} < 10^{-5}, \quad \text{where} \quad S_k = \sum_{k'} F_{k,k'}. \tag{35.1}$$

If the above constraint has not been applied in the evaluation process, corrected values $\widehat{F}_{k,k'}$ may be obtained from the following relation:

$$\widehat{F}_{k,k'} = F_{k,k'} - S_k Y_{k'} - S_{k'} Y_k + Y_k Y_{k'} \sum_j S_j. \tag{35.2}$$

The correction is applicable not only to the covariance matrix in the ENDF file, but also to derived covariance matrices (for example, after processing and condensation on the user's energy grid).

This correction procedure is approximate and therefore appropriate only in case of relatively small deviations of the matrix from the normalization constraint given by equation (35.1).

The secondary energy distribution uncertainty analysis using the "hot-cold" technique of Gerstl, et al., (see References 1 and 2) can be based on spectral uncertainty data stored in this form. In this case the covariance matrix is a 2×2 matrix for each incident energy range.

References for Chapter 35

1. S. A. W. Gerstl, "Uncertainty Analyses for Secondary Energy Distributions", *A Review of the Theory and Application of Sensitivity and Uncertainty Analysis: Proceedings of a SeminarWorkshop, August 22-24, 1978*, C. R. Weisbin, et al., Eds, Radiation Shielding Information Center report, Oak Ridge National Laboratory **ORNL/RSIC42** (1978) p. 219.

2. S. A. W. Gerstl, R. J. LaBauve, and P. G. Young, *A Comprehensive Neutron Cross-Section and Secondary Energy Distribution Uncertainty Analysis for a Fusion Reactor*, Los Alamos Scientific Laboratory report **LA-8333-MS** (1980).

Chapter 40

File 40. COVARIANCES FOR PRODUCTION OF RADIOACTIVE NUCLEI

40.1 General Comments

File 40 contains the covariances of neutron activation cross-section information appearing in File 10. This file is based on File 33, which should be consulted for further information, and on File 10.

40.2 Formats

The following quantities are defined:

ZA,AWR Standard material charge and mass parameters.

LIS Level number of the target.

NS Number of subsections; one for each LFS.

QM Mass-difference Q-value based on the ground state of the residual nucleus

QI Reaction Q-value (eV). (See Chapter 10.)

LFS Level number of the nuclide (ZAP) produced in the neutron reaction of type MT.

NL Number of subsections.

Sections
File 40 is divided into sections identified by the value of MT. Each section of File 40 starts with a HEAD record, ends with a SEND record, and has the following structure:

```
[MAT,40,MT/  ZA, AWR, LIS,   0, NS,  0] HEAD
       <NS subsections, one for each LFS>
[MAT,40,MT/ 0.0, 0.0,   0,   0,  0,  0] SEND
```

Subsections

Each subsection has the following structure:

```
[MAT,40, MT/  QM,  QI,   0, LFS,  0, NL]CONT
      <subsubsection for L=1>
      --------------------------
      --------------------------
      <subsubsection for L=NL>
```

Sub-subsections

Each sub-subsection is used to describe a single covariance matrix, the covariance matrix of the energy-dependent cross section given in section (MAT,10,MT.LFS) with given final state (LFS) and the energy-dependent cross sections given in section (MAT1,MF1,MT1[.LFS1]) The values of MAT1, MF1, MT1, and LSF1 (if MF1=10) are given in the CONT record that begins every sub-subsection.

Each sub-subsection may contain several sub-sub-subsections. Each sub-sub-subsection describes an independent contribution to the covariance matrix given in the sub-subsection. The total covariance matrix in the sub-subsection is made up of the sum of the contributions of the individual sub-sub-subsections. The following additional quantities are defined:

XMF1 Floating point form of MF1 (the file number for the 2nd cross section to which the covariance data relates).

XLFS1 Floating point form of LFS1 (the index of the final state for the 2nd cross section to which the covariance data relates).

MAT1 MAT for the 2nd cross section to which the covariance data relates.

MT1 MT for the 2nd cross section to which the covariance data relates.

NC Number of "NC-type" subsections which follow the CONT record.

NI Number of "NI-type" subsections which follow the "NC-type" subsections.

The structure of a sub-subsection describing the covariance matrix of the cross sections defined by (MAT,10,MT.LFS] and (MAT1,MF1,MT1[.LFS1] is:

```
[MAT,40,MT/ XMF1, XLFS1, MAT1, MT1, NC, NI] CONT
   <sub-sub-subsection for n_c = 1>
   -------------------------------
   -------------------------------
   <sub-sub-subsection for n_c = NC>
   <sub-sub-subsection for n_i = 1>
   -------------------------------
   -------------------------------
   <sub-sub-subsection for n_i = NI>
```

The formats of the sub-sub-subsection for File 40 are exactly the same as the formats for the sub-subsections for File 33.

40.3 Procedures

The procedures for File 40 are the same as for File 33 except that File 40 has one more level of indexing corresponding to the LFS and LFS1 flags and as noted below.

40.4 Ordering of Sections, Subsections, Sub-subsections, and Sub-sub-subsections

1. Sections: The sections in File 40 are ordered by increasing value of MT.
2. Subsections: Within a section, (MAT,40,MT), the subsections are ordered by increasing value of LFS.
3. Sub-subsections: A sub-subsection of File 40 is uniquely identified by the set of numbers (MAT,MT,LFS; MAT1,MT1,MF1[.LFS1]); the first two numbers indicate the section, the third indicates the subsection, while the last four indicate the sub-subsection.
   (a) The sub-subsections within a subsection are ordered by increasing value of MAT1. The value of MAT1=0 shall be used to mean MAT1=MAT.
   (b) When there are several sub-subsections with the same value of MAT1 in a subsection, these sub-subsections shall be ordered by increasing values of XMF1. When MF1=MF, the XMF1 field shall be entered as blank or zero. Therefore, within a given subsection, the sub-subsections for MF1=MF will always appear before those for other MF1 values.
   (c) When there are several sub-subsections with the same value of MAT1 and MF1 in a subsection, these sub-subsections shall be ordered by increasing values of MT1. If MAT1=MAT and MF1=MF, then only those sub-subsections for MT≥MT shall be given.
   (d) When there are several sub-subsections with the same value of (MAT1,MT1,MF1) in a subsection, these sub-subsections shall be ordered by increasing values

of LFS1. If MAT1=MAT, MF1=MF, and MT1=MT, then only those sub-subsections for LFS1≥LFS shall be given. (LFS1=0 implies the ground state of the product and does not imply LFS1=LFS).

40.5 Completeness

There are no minimum requirements on the number of sections, subsections, and sub-subsections in File 40. However, the presence of certain data blocks in File 40 implies the presence of others, either in File 33 or 40 of a referenced material. In what follows, we shall identify the sub-subsections of File 40 by

(MAT,MT,LFS; MAT1,MT1,MF1[.LFS1]).

The presence of this data block with MAT1≠MAT or MF1≠10 implies the presence of appropriate data in:

a. (MAT,MT,LFS;MAT,MF=10,MT.LFS), in File 40 of MAT;

b. (MAT1,MT1[.LFS1]; MAT1,MF1,MT1.LFS1), in File (MF1+30) of MAT1;

c. (MAT1,MT1[.LFS1]; MAT ,MF=10,MT.LFS), also in File (MF1+30) of MAT1.

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Appendix A

Glossary

Terms are given in alphabetical order with numbers preceding letters, lower-case preceding upper-case letters, and Greek Letters following.

Parameter	**Definition**	**Chapter**
a	Parameter used in the Watt spectrum.	5
a_l	l^{th} Legendre coefficient.	4,6,14
$A_{k,l}$	Probability of emission of a γ ray of energy $E_\gamma = \varepsilon_k - \varepsilon_l$ as a result of the residual nucleus having a transition from the kth to the lth level.	11
A_l	Legendre coefficients (LANG=0) or μ, p_i pairs for tabulated angular distribution (LANG¿0).	6
A_n	Mass of the nth type atom; A_0 is the mass of the principal scattering atom in a molecule.	7
ABN	Abundance (atom fraction) of an isotope in this material.	2,32
AC	Channel radius	2
AC1, AC2, AC3, AC4, BC1, BC2	Background constants for the Adler-Adler radiative capture cross section.	2
AF1, AF2, AF3, AF4, BF1, BF2	Background constants for the Adler-Adler fission cross section.	2
AG	Reduced-width amplitude.	2
AJ	Floating-point value of compound nucleus spin, J (resonance spin).	2,32
AL	Floating point value of the angular momentum, l.	2
ALAB	Mnemonic of laboratory originating evaluation.	1
ALRE1 ...ALRE4	Exit-l-value for reaction.	2
AMUF	Number of degrees of freedom used in fission-width distribution.	2
AMUG	Number of degrees of freedom used in radiation-width distribution.	2

Parameter	Definition	Chapter
AMUN	Number of degrees of freedom used in neutron-width distribution.	2
AMUX	Number of degrees of freedom used in competitive-width distribution.	2
AP	Scattering radius.	2,32
APL	l-dependent scattering radius.	2
APSX	Total mass in neutron units of the n particles being treated by LAW=6.	6
AS	Floating point value of channel-spin s.	2
AT1, AT2, AT3, AT4, BT1, BT2	Background constants for the Adler-Adler total cross section.	2
AUTH	Author of evaluation.	1
AVGG	Statistical R-matrix parameter.	2
AWD	Atomic mass (not a ratio) of the daughter nucleus (amu).	2
AWI	Projectile mass in neutron units.	1
AWP	Product mass in neutron units.	6
AWR	Ratio of mass of atom (or molecule) to that of the neutron.	all
AWRI	Ratio of mass of particular isotope to that of the neutron.	2,32
AWRIC	Mass-ratio for charged-particle exit channel (see page D.40).	2
AWT	Nuclear mass (not a ratio) of outgoing particle.	2
AZD	Atomic number of daughter nucleus.	2
AZP	Atomic number of outgoing particle.	2
b	Parameter used in Watt spectrum function definition.	5
$B_i(N)$	List of constants.	7,12
BC	Boundary-condition parameter.	2
BR	Branching ratio for production of a particular nuclide and level.	8
C_n	Coefficients of a polynomial; NC coefficients are given.	1
$C_n(E_i)$	Array of yield data for the ith energy point; contains 4 parameters per fission product.	8
CI	Channel index.	2
CI	Coefficient of the cross section for a reaction contributing to the value of a "derived" cross section (usually 1.0).	31,33
CONT	Smallest possible ENDF record, a "control" record.	all
CT	Chain indicator.	8
D	Mean level spacing for a particular J-state.	2,32
DDATE	Original distribution date of the evaluation.	1
DE^2	Variance of the resonance energy ER.	32

Parameter	Definition	Chapter
DEC_r	Resonance energy for the radiative capture cross section.	2
DEF_r	Resonance energy for the fission cross section.	2
DET_r	Adler-Adler resonance energy for the total cross section.	2
DF^2	Variance of GF.	32
DG^2	Variance of GG.	32
DGDF	Covariance of GG and GF.	32
DJ^2	Variance of AJ.	32
DJDF	Covariance of AJ and GF.	32
DJDG	Covariance of AJ and GG.	32
DJDN	Covariance of AJ and GN.	32
DN^2	Variance of GN.	32
DNDF	Covariance of GN and GF.	32
DNDG	Covariance of GN and GG.	32
DWC_r	Value of $\Gamma/2$, (ν), used for the radiative capture cross section.	2
DWF_r	Value of $\Gamma/2$, (ν), used for the fission cross section.	2
DWT_r	Value of $\Gamma/2$, (ν), used for the total cross section.	2
DYC	1-σ uncertainty in cumulative fission-product yield.	8
DYI	1-σ uncertainty in fractional independent fission-product yield.	8
$\{ E_k\}$	List of energies for a covariance file energy grid	32-40
E	Energy of the incident neutron (eV).	all
E'	Secondary neutron energy (eV).	5,6,7
E1, E2	Range of neutron energies.	31,33
E_{avail}	Available energy.	5
E_{int}	Interpolation scheme for each energy range.	all
E_{th}	Threshold energy (eV).	3
$E_{"x"}$	Average decay energy (eV) of "x" radiation for decay heat applications.	8
EB	Total energy released by delayed β's.	1
EBAR	Statistical R-matrix parameter	2
EBI	Binding energy for subshell (eV)	28
ED	Logarithmic parameter for a R-matrix element	2
EDATE	Date of evaluation.	1
EFH	Constant in energy-dependent fission spectrum	5
EFL	Constant in energy-dependent fission spectrum	5
	Fluorescence yield (eV/photo-ionization). Value is zero if not photoelectric subshell ionization cross section.	23
EFR	Kinetic energy of the fragments.	1, 5
EG_k	Photon energy or Binding Energy.	12, 13, 14
EGD	Total energy released by the emission of delayed γ rays.	1
EGP	Total energy released by the emission of "prompt" γ-rays.	1

Parameter	Definition	Chapter
EH	Upper limit for a resonance region energy range.	2, 32
EI	Energy points where the weighting of the standard cross is given.	31, 33
EL	Lower limit for a resonance region energy range.	2, 32
ELFS	Excitation energy of the reaction product.	8
ELIS	Excitation energy of the target nucleus.	1
ELN	Number of electrons in subshell when neutral.	28
EMAX	Upper limit of energy range for evaluation	1
END	Kinetic energy of the delayed fission neutrons.	1
	End-point energy of the particle or quantum emitted.	8
ENDATE	Master file entry date (yyyymmdd).	1
ENP	Kinetic energy of the "prompt" fission neutrons.	1
ENU	Energy carried away by neutrinos.	1
EPE	Sub-shell binding energy (equal to photoelectric edge energy) in eV. The value is zero if MT≠534-599.	23
ER	Total energy release due to fission minus neutrino energy.	1
	Resonance energy (in the laboratory system).	2,32
	Energy (eV) of radiation produced.	8
ERAV	Average decay energy of radiation produced.	8
ES_i	Energy of the ith level.	12
ES_k	Energy of the level from which the photon originates.	12, 13, 14
ES(N)	Energy of Nth point used to tabulate energy-dependent widths.	2
ET	Total energy release due to fission.	1
ET(E)	Energy transfer during electro-atomic excitation or bremsstrahlung	26
ETR	Energy of transition (eV)	28
EU	Logarithmic parameter for a R-matrix element	2
$f_i(\mu, E, E')$	Normalized product energy-angle distribution	6
$f_k(E \rightarrow E')$	k^{th} partial energy distribution; definition depends on LF value.	5
$F(q; Z)$	Form factor for coherent photon scattering.	27
$F_{x,k,k'}(LB)$	Covariance components correlated over the energy interval with lower edges E_k and $E_{k'}$ (exact definition depends on LB value.	31-40
FC	Continuum spectrum normalization factor.	8
FD	Discrete spectrum normalization factor.	8
FPS	Floating-point value of state designator for a fission product nuclide.	8
FTR	Fractional probability for transition.	28
$g(E_\gamma \leftarrow E)$	Particular class of the functions $g_j(E_\gamma \leftarrow E)$ tabulated in File 15; in units eV-1.	15

Parameter	Definition	Chapter
$g_j(E_\gamma \leftarrow E)$	j^{th} normalized partial distribution; in units eV-1.	15
GE	Eliminated width.	2
GF	Fission width Γ_f evaluated at resonance energy ER.	2, 32
	Average fission width - may be energy dependent.	2
GFA	First partial fission width	2
GFB	Second partial fission width	2
GG	Radiation width Γ_γ evaluated at resonance energy ER.	2, 32
	Average radiation width - energy dependent if LRU=2.	2
GIC_r	Asymmetrical capture parameter.	2
GIF_r	Asymmetrical fission parameter.	2
GIT_r	Related to the asymmetrical total cross section parameter.	2
GN	Neutron width Γ_n evaluated at resonance energy ER.	2, 32
GN0	Average reduced neutron width; energy dependent.	2
$\mathrm{GP}_{j,i} \equiv \mathrm{Gp}_i$	Conditional probability of photon emission in a direct transition from level j to level i, $i < j$.	12
GRC_r	Symmetrical capture parameter.	2
GRE1 ... GRE4	Partial widths.	2
GRF_r	Symmetrical fission parameter.	2
GRT_r	Related to symmetrical total cross section parameter.	2
GT	Resonance total width Γ evaluated at the resonance energy ER.	2, 32
GX	Competitive width Γ_x evaluated at resonance energy ER, or, average competitive reaction width.	2
$H(q;Z)$	Form factor or incoherent scattering function; either $F(q;Z)$ or $S(q;Z)$, respectively.	27
H(N)	Array containing text information that describes evaluated data set.	1
HEAD	First record in a section	all
HL	Half-life of the reaction product.	8
HSUB	Library identifier (eye-readable)	1
I	Normalizing denominator (see 5.3).	5
IDP	Resonance parameter identification number.	2, 32
INT	Statistical parameter for R-matrix element (LRU=1, LRF=5), or, interpolation scheme used for interpolating between cross sections obtained from average resonance parameters (LRU=2).	2
INT(m)	Interpolation scheme identification number used in m^{th} range.	0
IPS	Imaginary part of a non-hard-sphere phase shift.	2
IPS(e)	Real part of PS(E).	2
IR0(e)	Imaginary part of R0(E).	2
IRP	Imaginary part of background-R-matrix element.	2

Parameter	Definition	Chapter
ISG	Spin group index.	2
ISH	Shift function flag.	2
k	Boltzmann's constant.	7
L	Value of the l-state (neutron angular momentum).	
LA	Value of l (for the lth coefficient).	
LAD	Angular distribution flag	
LANG	Angular distribution indicator	
LASYM	Flag indicating whether asymmetric $S(\alpha, \beta)$ is given.	7
LAT	Flag indicating which temperature has been used to compute α and β.	7
LAW	Distinguishes between different representations of f_i, the normalized energy-distribution of a reaction product	6
LB	Flag which determines meanings of the F-numbers in the arrays $\{E_k, F_k\}\{E_l, F_l\}$.	8, 31, 33, 34, 40
LBK	Background R-matrix parameter (LRU=1, LRF=5), or, background-R-function flag (LRU=1, LRF=6).	2
LCOMP	Indicates ENDF-5 compatible format.	32
LCON	Continuum spectrum flag.	8
LCOV	Indicates whether covariance data are given.	8
LCT	Indicates which reference frame is used for both secondary angles and energies.	4,6
LDRV	Distinguishes between different evaluations with the same material keys	1
LE	Indicates whether energy-dependent fission-product yields are given.	8
LEP	Selects interpolation scheme for secondary energy.	6
LF	Specifies the energy distribution law that is used for a particular subsection (partial energy distribution).	5, 6, 12, 13, 15
LFI	Indicates whether this material is fissionable.	1
LFS	Indicator that specifies the final excited state of the residual nucleus produced by a particular reaction.	3, 8, 9, 10, 40
LFW	Indicates whether average fission widths are given in the unresolved resonance region for this isotope.	2, 32
LG	Transition probability array flag for distinguishing between doublet and triplet arrays in File 12.	12
LI	Indicates kind of Adler-Adler parameters given.	2
	Isotropy flag.	4, 14
	Temperature interpolation flag.	7
LIBF	Sub-library where some data are sensitive to the same model parameters as data in present sub-library/material.	30
LIDP	Identifies identical particles for LAW=5.	6
LIP	Product modifier flag.	8

Parameter	Definition	Chapter
LIS	State number of the target nucleus (for materials that represent nuclides).	1, 3, 8, 9, 10, 40
LISO	Isomeric state number of the target nucleus.	1, 8
LIST	Record used to list a series of numbers.	all
LLN	Indicates form for storing $S(\alpha, \beta)$.	7
LMF	File number for this MT containing multiplicity or cross section.	8
LNU	Indicates representation of $\overline{\nu}(E)$ used.	1
LO	Indicates whether multiplicities or transition probability arrays given.	12
LP	Indicates whether particular photon is a primary.	12, 13
LPS	Optical model phase shift flag	2
LR	Defines x in (n,n'x); used in the reactions MT=51, 52, 53, . . . , 90, and 91. (See Section 3.4.4)	3
LREL	Release number	1
LRF	Indicates which resonance parameter representation used for energy range; definition depends on value of LRU for range.	2, 32
LRP	Indicates whether resolved and/or unresolved resonance parameters given in File 2.	1
LRU	Indicates whether energy range contains data for resolved or unresolved resonance parameters.	2, 32
LRX	Indicates whether a competitive width is given.	2
LS	Indicates whether $F_{k,k'}$ matrix is asymmetric or symmetric (LB=5 or 7).	31, 33, 35
LSSF	Indicates how File 2 and File 3 are to be combined.	2, 32
LT	Temperature dependence (see also Appendix F.1).	0
	Specifies whether temperature-dependent data are given.	3, 4, 5, 6, 7
	Number of pairs of numbers in the array $\{E_l, F_l\}$.	31, 33
LTHR	Thermal data flag.	7
LTP	Specifies representation used for LAW=5.	6
LTT	Specifies whether Legendre or probability representation used.	4, 6, 14
	Specifies whether Legendre coefficient covariance data start with a_0 coefficient.	34
LTY	In "NC-type" sub-subsections, indicates the procedure used to obtain the covariance matrix.	31, 33
L1	Integer to be used as a flag or a test.	1
	Number of Legendre coefficients.	34
L2	Integer to be used as a flag or a test.	1
M_n	Number of atoms of the nth type in the molecule.	7
MAT	Material number.	0

Parameter	Definition	Chapter
MAT1	Referenced material for covariance data.	33
MATF	MAT in which some data are sensitive to the same parameter.	30
MATP	Material number for the reaction product.	8
MATS	MAT in which a pertinent standard cross section (MTS) exists.	31, 33
MF	File number.	0
MF_n	MF of the nth section.	1
MFSEN,MTSEN	MF,MT of a section in which data are sensitive to the indicated parameter (MP).	30
MOD_n	Modification indicator for section MF_n and MT_n.	1
MP	Model parameter index.	30
MPAR	Number of parameters for which covariance data is given.	32
MPF	Model parameter index given the same parameter (MP) in another sublibrary/material	30
MT	Reaction type number, or, covariance file section identifier.	all
MT_n	MT of the nth section.	1
MT1	Referenced reaction type for covariance data.	33
MTL	Indicates MT that is a component of the lumped reaction.	33
MTS	Reaction type number for relevant standard cross section.	31, 33
MUF	Number of degrees of freedom for fission widths.	2
MTRE1 ...TRE4	MT values for inelastic or charged particle reactions	2
N0	Identifies reaction product that has radioactive ground state.	8
N1	Number of items in a list to follow (except for MT 451).	1
N2	Number of items in a second list to follow.	1
NA	Number of angles (cosines) at which secondary distributions given.	6
NAC	Number of channel radii	2
NAPS	Controls use of channel radius a and scattering radius AP.	2, 32
NB	Total number of β value given.	7
NBC	Number of boundary-condition parameters.	2
NBK	Background-R-matrix parameter.	2
NBT(n)	Value of N separating the mth and $(m+1)^{th}$ interpolation rangers.	0
NC	Number of terms used in the polynomial expansion.	1
	Total number of decay energies (eV) given (NC = 3 or 17).	8

Parameter	Definition	Chapter
	Number of partial distributions used to represent $f(E_\gamma \leftarrow E)$.	15
	Number of "NC-type" sub-subsections.	31, 33
NC_n	Number of physical records in the nth section.	1
NCH	Number of channels using particular background R-matrix element, phase shift, penetrability, channel radius, or boundary condition (LRU=1, LRF=5).	2
NCI	Number of reactions summed to obtain the reaction of interest.	1
	For a "derived" cross section, number of reaction types for which cross sections are combined in the derivation.	31, 33
NCP	Number of channels.	2
NCRE	Number of charged-particle reactions.	2
NCS	Number of channels in a particular spin group.	2
NCT	Total number of channels.	2
NCTAB	Number of CONT records in the corresponding table.	30
ND	Number of discrete energies (File 6);	6
	Number of branches into which nuclide ZAP decays.	8
NDIGIT	Number of digits for compact resonance covariance representation	32
NDIR	Number of CONT records in the MF=30 directory.	30
NDK	Total number of decay modes given.	8
NE	Number of incident-energy points at which widths given.	2
	Number of points at which tabulated distributions given.	4
	Number of points at which $\theta(E)$ (File 5) are given.	5
	Number of energy points given in a TAB2 record.	14, 15
NEI	Number of energy points in EI,WEI list.	33
NEP	Number of secondary energy points.	6
NER	Number of energy ranges given for this isotope.	2, 32
	Total number of discrete energies for given spectra type (STYP).	8
	Number of energies corresponding to the rows of LB=6 covariance matrix.	33
NF	Number of channels not requiring a phase shift.	2
	Number of secondary energy points in tabulation.	5
NFOR	Library format.	1
NFP	Number of fission-product nuclide states to be specified at each incident-energy point.	8
NFRE	Number of fission reactions.	2
NGRE	Number of capture reactions.	2
NHS	Number of channels that require hard-sphere phase shifts.	2

Parameter	Definition	Chapter
NI	Total number of items in the B(N) list; NL=6*(NS+1).	7
	Number of isotropic angular distributions given in section (MT) for which LI=0, i.e., with at least one anisotropic distribution).	14
	Number of "NI-type" sub-subsections.	31, 33
NIRE	Number of inelastic reactions.	2
NIS	Number of isotopes in this material.	2, 32
NJS	Number of sets of resonance parameters (each having the same J state) for a specified l-state.	2, 32
NK	Number of elements in transformation matrix; NK=(NM+1)2.	4
	Number of partial energy distributions (one subsection for each partial distribution).	5, 6
	Number of partial energy distributions (LCON=5).	8
	Number of discrete photons plus the photon continuum.	12, 13, 14
	Number of subsections in this section (MT).	26
	Number of incident-neutron energy ranges for covariance representation, each with a subsection.	35
NL	Highest order Legendre polynomial given at each energy.	4, 6, 14
	Number of subsections within a section.	33
NLG	Number of logarithmically parameterized elements.	2
NL1	Number of Legendre coefficients.	34
NLIB	Library identifier.	1
NLJ	Count of the number of levels for which parameters will be given.	2
NLRS	Number of subsections containing data on long-range resonance parameter covariance.	32
NLS	Number of l-values considered; a set of resonance parameters is given for each l-value.	2, 32
NLSC	Number of l-value for convergence.	2
NLSJ	Number of resonances specified by l, s, and J.	2
NM	Maximum order Legendre polynomial required to describe the angular distributions.	4
NML	Number of entries in MT list.	2
NMOD	Modification number.	1
NMT1	Number of subsections, for MT1≥MT.	34
NMU	Number of emission cosine values for LAW=7.	6
NN	Number of elements in the LIST record	8
NNF	Number of precursor families considered.	1
NO	Decay information flag.	8
NP	Number of points in a tabulation of $y(x)$ that are contained on the same record.	all but ↓
	Number of Bragg edges.	7

Parameter	Definition	Chapter
	Total number of distinct model parameters.	30
	Total number of pairs of numbers in the arrays $\{E_k, F_k\}\{E_l, F_l\}$.	31, 33
NPE	Number of charged-particle penentrabilities.	2
NPP	Number of pairs of numbers in the $\{E_k, F_k\}$ array.	8
NPS	Number of non-hard-sphere phase shifts.	2
NPSX	Number of particles distributed by LAW=6.	6
NR	Number of different interpolation intervals in a tabulation of $y(x)$ that are contained in the same record.	all
NRB	Number of resonances in block.	32
NRM	Number of interpolation intervals for emission cosine for LAW=7.	6
NRO	Energy dependence of the scattering radius.	2, 32
NRP	Number of interpolation intervals for emission energy (LAW=7).	6
NRS	Number of resolved resonances for a given l-state.	2, 32
NRT	Total number of resonances.	2
NS	Number of non-principle scattering atom types.	7
	Number of states of the radioactive reaction product.	8, 9, 10
	Number of levels below the present one, including ground state.	12
NSG	Number of spin groups.	2
NSP	Total number of spectra radiation types (STYP) given.	8
NSRS	Number of subsections for covariances among parameters of specific resonances.	32
NSS	Number of different s-values.	2
	Number of subshells.	28
NST	Number of statistically parameterized background R-matrix elements.	2
NSUB	Sub-library number.	1
NT	Number of transitions for which data given.	2
	Number of entries for each discrete energy ER.	8
	Total number of items in LIST.	33, 34, 35
NTP	Control flag for background-R-matrix or penetrability list.	2
NTR	Number of transitions.	28
NVER	Library version number.	1
NVS	Number of covariance elements for a block of resonances.	32
NW	Number of words in LIST record.	6
NWD	Number of elements in the text section.	1
NX	Number of sets of background constants to be given.	2
NXC	Number of the sections to be found in the dictionary	1
$P_j(E)$	Probability or weight given to j^{th} partial distribution, $g_j(E_\gamma \leftarrow E)$.	15

Parameter	Definition	Chapter
$P_k(E_N)$	Fractional part of cross section that can be described by the kth partial distribution of the nth incident-energy point.	5
$p(\mu, E)$		4
PAR	Parity π of target nuclide.	8
PCP(E)	Charged-particle penetrability.	2
PMT	Floating point value for MT.	2
PS(E)	Complex phase shift.	2
Q	Reaction Q-value (eV); Q=(rest mass of initial state - rest mass of final state).	3, 9, 10
	Total decay energy (eV) available in corresponding decay process, not necessarily the same as maximum energy of emitted radiation).	8
QI	Reaction Q-value.	3, 9, 10
QM	Mass-difference Q-value.	3, 9, 10
QRE1 ... QRE4	Q-values.	2
QX	Effective Q-value for the competitive width.	2, 32
$R_{mj\alpha}$	Probability of de-excitation.	11
R0, R1, R2	Logarithmic parameters for an R-matrix element.	2
R0(E)	Complex background R-function.	2
RCOV	Relative covariance of model parameters.	30
RDATE	Date and number of last revision.	1
REF	Reference to evaluation.	1
RFS	Isomeric state flag for daughter nuclide.	8
RI	Resonance index.	2
	Intensity of radiation produced (relative units).	8
RICC	Total internal conversion coefficient.	8
RICK	K-shell internal conversion coefficient.	8
RICL	L-shell internal conversion coefficient.	8
RIN	Statistical R-matrix parameters.	2
RIS	Internal pair formation coefficient (STYP=0.0); positron intensity (STYP=2.0).	8
RNPM	Number of particular sections (MT's).	2
RNSM	Number of summed sections (MT's).	2
RP	Spectrum of the continuum component of the radiation $\int \mathrm{RP}(E)\, dE = 1$.	8
RPB	Real part of background R-matrix element.	2
RPS	Real part of a non-hard-sphere phase shift.	2
RPS(E)	Real part of PS(E).	2
RR0(E)	Real part of R0(E).	2
RTYP	Mode of decay of the nuclide in its LISO state.	8
RV_{ij}	Relative covariance quantities among average unresolved parameters.	32

Parameter	Definition	Chapter
$S(\alpha, \beta, T)$	Defined (for a moderating molecule) by equation (7.6).	7
S0, S1	Logarithmic parameters for an R-matrix element.	2
SF	Statistical R-matrix parameter.	2
SMT	Floating-point value for MT.	2
SPD	Spin and parity for the daughter nucleus.	2
SPI	Nuclear spin of the target nucleus, I (positive number).	2, 8, 32
SPP	Spin and parity.	2
STA	Target stability flag.	1
STYP	Decay radiation type (defined in Section 8.4).	8
SUBI	Subshell designator.	28
SUBJ	Secondary subshell designator	28
SUBK	Tertiary subshell designator.	28
T	Temperature (K) at which temperature dependent data given.	4, 5, 6, 7
$T_{1/2}$	Half-life of the original nuclide (seconds).	8
TAB1	Control record for one-dimensional tabulated functions.	all
TAB2	Control record for two-dimensional tabulated functions.	all
TEMP	Target temperature.	1
TM	Maximum temperature parameters.	5
TP_i	Probability of a direct transition from level NS to level I, I=0,1,2, ... (NS-1).	12
TYPE	Indicates the type of transition for beta and electron capture.	8
U	Defines the upper energy limit for the secondary neutron, so that $0 \leq E \leq E - U$ (given in the Lab system).	5
V_{mn}	Variance-covariance matrix element among resonance parameters.	32
WEI	Weight of the standard cross section at a given EI relative to the next given energy.	31, 33
x	$E'/\theta(E)$.	5
$x(n)$	n^{th} value of x.	0
XLFS1	Floating-point form of final excited state number references for covariance data.	33, 40
XLFSS	Floating-point form of LFSS, final excited state number of a reaction with a standard cross section	31, 33
XMF1	Floating-point form of file number reference for covariance data.	33, 40
XMFS	Floating-point form of MFS, file number in which pertinent standard cross section (MTS) may be found.	31, 33
XMTI	Floating-point equivalent of MT number of the reaction for which the cross section contributes to a "derived" cross section.	31, 33
$y(E)$	Yield for particle described.	26

Parameter	Definition	Chapter
$y(n)$	n^{th} value of y.	0
$y_i(E)$	Product yield or multiplicity.	6
$Y(E)$	Total multiplicity at energy E(eV); given as energy-multiplicity pairs.	9, 12
	Partial multiplicity at energy E(eV).	12
YC	Cumulative yield for a particular fission product.	8
YI	Fractional independent yield for a particular fission product.	8
ZA	(Z,A) Designation of the original nuclide. ZA=1000.$Z+A$	all
ZAI	(Z,A) designation for an isotope. ZA=1000.$Z+A$	2, 32
ZAFP	(Z,A) identifier for a particular fission product. ZA=1000.$Z+A$	8
ZAN	(Z,A) designation of the next nuclide in the chain. ZA=1000.$Z+A$	8
ZAP	(Z,A) designation of the product nuclide. ZA=1000.$Z+A$	8
ZSYMA	Text representation of material: Z-chemical symbol-A	8
ZSYMAM	Text representation of material Z-chemical symbol-A-state.	1
α	Momentum transfer, $\alpha = (E' + E - 2\mu\sqrt{EE'})/A_0kT$.	7
β	Energy transfer, $\beta = (E' - E)/kT$.	7
$\delta(E_\gamma - \varepsilon_j + \varepsilon_i)$	Delta function, with ε_j, ε_i being energy levels of the residual nucleus.	11
Δ	Uncertainty in quantity.	1, 8
λ_i	Decay constant (sec^{-1}) for the ith precursor.	1
θ	Parameter describing secondary energy distribution; definition of θ depends on the energy distribution law (LF).	5
$\overline{\nu}(E)$	Total average number of neutrons formed per fission event.	1
$\sigma(E)$	Cross section (barns) for a particular reaction type at incident energy point, E, in (eV).	3, 10, 23
σ_{bn}	Bound atom scattering cross section of nth type atom,	7
σ_{fn}	Free atom scattering cross section of nth type atom.	7
$\sigma_k^\gamma(E)$	Photon production cross section for a discrete photon or photon continuum specified by k.	13
$\sigma_{m0}(E)$	Neutron cross section for exciting moth level with neutron energy E.	11
$\sigma_s(E)$	Scattering cross sections, e.g., elastic scattering at energy E as given in File 3 for the particular reaction type (MT).	4
σ_T (background)	$(AT_1 + AT_2/E + A_3/E^2 + AT_4/E^3 + BT_1E + BT_2E^2)\,\frac{C}{\sqrt{E}}$	2

Parameter	Definition	Chapter
σ_W	Wick's limit cross section in units of barns/steradian.	4
$\frac{\sigma(\Omega E)}{d\Omega}$	Differential scattering cross section in units of barns/steradian.	4
$\frac{\sigma_k^\gamma}{d\Omega}$	Differential photon production cross section in barns/steradian.	14
μ	Cosine of scattered angle in either laboratory or center-of-mass system.	4,6,14

Appendix B

Definition of Reaction Types

Reaction types (MT) are identified by an integer number from 1 through 999. Version ENDF-6 of the ENDF format supports incident charged particles and photons in a manner consistent with the definitions of MT's used in previous versions of the ENDF format to the extent possible. Users should be aware of the few differences. In the following table, those MT numbers restricted to incident neutrons are labeled (n,xxx); those that are limited to incident charged particles and photons are labeled (y,xxx) and those that allow all particles in the entrance channel are labeled (z,xxx), where x can represent any exit particle. See Section 0 for complete descriptions of MT numbers. Refer to Sections 3.4 (incident neutrons) and 3.5 (incident charged particles and photons) for the list of MT numbers that should be included in each evaluation.

For the ENDF-6 format, all particles in the exit channel are named (within the parenthesis) except for the residual. The identity of this residual can be specified explicitly in File 6 or determined implicitly from the MT number. In cases where more than one MT might describe a reaction, the choice of MT number is then determined by the residual which is the heaviest of the particles (AZ,A) in the exit channel. For example, ^{6}Li(n,t)α is represented by MT=700, rather than my MT=800; and MT=32 represents the ^{6}Li(n,nd)α reaction rather than MT=22. Sequential reaction mechanism descriptions can be used, where necessary, for reactions such as X(n,np)Y. These are described in Sections 0.4.3.3 and 0.4.3.4.

B.1 Reaction Type Numbers MT

MT		Description	Comments
1	(n,total)	Neutron total cross sections. (See sum rules for cross sections in Section 0.5.1 Table 14).	Redundant. Undefined for incident charged particles.
2	(z,z0)	Elastic scattering cross section for incident particles.	

MT		Description	Comments
3	(z,nonelas.)	Nonelastic neutron cross section. (See sum rules for cross sections in Section 0.5.1 Table 14).	Redundant. For photon production only.
4	(z,n)	Production of one neutron in the exit channel. Sum of the MT=50-91.	Redundant. For incident neutrons, this is inelastic scattering (MT=50 is undefined).
5	(z,anything)	Sum of all reactions not given explicitly in another MT number. This is a partial reaction to be added to obtain MT=1.	Each particle can be identified and its multiplicity given in File 6. Not allowed in Files 4, 5.
6-9		Not allowed in Version 6.	^{9}Be(n,2n) in format Version 5.
10	(z,contin.)	Total continuum reaction; includes all continuum reactions and excludes all discrete reactions.	Redundant; to be used for derived files only.
11	(z,2nd)	Production of two neutrons and a deuteron, plus a residual [1].	
12-15		Unassigned.	
16	(z,2n)	Production of two neutrons and a residual1. Sum of MT=875-891, if they are present.	
17	(z,3n)	Production of three neutrons and a residual.	
18	(z,fission)	Particle-induced fission (sum of MT 19, 20, 21 and 38, if present).	
19	(n,f)	First-chance neutron-induced fission [2].	
20	(n,nf)	Second-chance neutron-induced fission[2].	
21	(n,2nf)	Third-chance neutron-induced fission[2].	
22	(z,nα)	Production of a neutron and an alpha particle, plus a residual.	
23	(n,n3α)	Production of a neutron and three alpha particles, plus a residual[1].	
24	(z,2nα)	Production of two neutrons and an alpha particle, plus a residual[1].	
25	(z,3nα)	Production of three neutrons and an alpha particle, plus a residual[1].	

[1]The "residual" is the remainder after the reaction specified by has taken place (*e.g.* isotope of the target nucleus with mass $A-1$ after an (n,2n) reaction). This residula may break up further if LR¿0.

[2]Note that the partial fission cross sections are not defined for charged particles.

MT		Description	Comments
26		Not allowed in Version 6.	Version 5: (n,2n) isomeric state; used in file 8 and 6, 9, or 10.
27	(n,abs)	Absorption; sum of MT=18 and MT=102 through MT=117	Rarely used.
28	(z,np)	Production of a neutron and a proton, plus a residual.	
29	(z,n2α)	Production of a neutron and two alpha particles, plus a residual.	
30	(z,2n2α)	Production of two neutrons and two alpha particles, plus a residual.	
31		Not allowed for Version 6.	Used only as an LR flag.
32	(z,nd)	Production of a neutron and a deuteron, plus a residual.	
33	(z,nt)	Production of a neutron and a triton, plus a residual.	
34	(z,n^{3}He)	Production of a neutron and a ^{3}He particle, plus a residual.	
35	(z,nd2α)	Production of a neutron, a deuteron, and 2 alpha particles, plus a residual.	
36	(z,nt2α)	Production of a neutron, a triton, and 2 alpha particles, plus a residual.	
37	(z,4n)	Production of 4 neutrons, plus a residual.	
38	(n,3nf)	Fourth-chance fission cross section.	
39		Not allowed for Version 6.	Used only as an LR flag.
40		Not allowed for Version 6.	Used only as an LR flag.
41	(z,2np)	Production of 2 neutrons and a proton, plus a residual.	
42	(z,3np)	Production of 3 neutrons and a proton, plus a residual.	
43		(Unassigned)	
44	(z,n2p)	Production of a neutron and 2 protons, plus a residual.	
45	(z,npα)	Production of a neutron, a proton, and an alpha particle, plus a residual.	
46-49		Not allowed in Version 6.	Version 5: description of 2nd neutron from ^{9}Be(n,2n) reactions to excited states.

MT		Description	Comments
50	(y,n_0)	Production of a neutron, leaving the residual nucleus in the ground state.	Not allowed for incident neutrons; use MT=2.
51	(z,n_1)	Production of a neutron, with residual in the 1st excited state.	
52	(z,n_2)	Production of a neutron, with residual in the 2nd excited state.	
	...		
90	(z,n_{40})	Production of a neutron, with residual in the 40th excited state.	
91	(z,n_c)	Production of a neutron in the continuum not included in the above discrete representation.	
92-100		(Unassigned)	
101	(n,disap)	Neutron disappearance; equal to sum of MT=102-117.	Rarely used.
102	(z,γ)	Radiative capture.	
103	(z,p)	Production of a proton, plus a residual. Sum of MT=600-649, if they are present.	For incident protons, this is inelastic scattering (MT=600 is undefined).
104	(z,d)	Production of a deuteron, plus a residual. Sum of MT=650-699, if they are present.	For incident deuterons, this is inelastic scattering (MT=650 is undefined).
105	(z,t)	Production of a triton, plus a residual. Sum of MT=700-749, if they are present.	For incident tritons, this is inelastic scattering (MT=700 is undefined).
106	(z,^{3}He)	Production of a ^{3}He particle plus a residual. Sum of MT=750-799, if they are present.	
107	(z,α)	Production of an alpha particle, plus a residual. Sum of MT=800-849, if they are present.	
108	(z,2α)	Production of 2 alpha particles, plus a residual.	
109	(z,3α)	Production of 3 alpha particles, plus a residual.	
110		(Unassigned)	
111	(z,2p)	Production of 2 protons, plus a residual.	

MT		Description	Comments
112	(z,pα)	Production a proton and an alpha particle, plus a residual.	
113	(z,t2α)	Production of a triton and 2 alpha particles, plus a residual.	
114	(z,d2α)	Production of a deuteron and 2 alpha particles, plus a residual.	
115	(z,pd)	Production of proton and a deuteron, plus a residual.	
116	(z,pt)	Production of proton and a triton, plus a residual.	
117	(z,dα)	Production of deuteron and an alpha particle, plus a residual.	
118-119		(Unassigned)	
120		Not allowed for Version 6.	Version 5: target destruction - nonelastic minus total (n,n'γ)
121-150		(Unassigned)	
151	(n,RES)	Resonance parameters that can be used to calculate cross sections at different temperatures in the resolved and unresolved energy regions.	Incident neutrons only.
152-200		(Unassigned)	
201	(z,Xn)	Total neutron production.	Redundant; use in derived files only.
202	(z,Xγ)	Total gamma production.	Redundant; use in derived files only.
203	(z,Xp)	Total proton production.	Redundant; use in derived files only.
204	(z,Xd)	Total deuteron production.	Redundant; use in derived files only.
205	(z,Xt)	Total triton production.	Redundant; use in derived files only.
206	(z,X^{3}He)	Total ^{3}He production.	Redundant; use in derived files only.
207	(z,Xα)	Total alpha particle production.	Redundant; use in derived files only.
208	(z,Xπ^+)	Total π^+ production.	For use in high-energy evaluations.
209	(z,Xπ^0)	Total π^0 production.	For use in high-energy evaluations.
210	(z,Xπ^-)	Total π^- production.	For use in high-energy evaluations.

MT		Description	Comments
211	(z,Xμ^+)	Total μ^+ production.	For use in high-energy evaluations.
212	(z,Xμ^-)	Total μ^- production.	For use in high-energy evaluations.
213	(z,Xκ^+)	Total κ^+ production.	For use in high-energy evaluations.
214	(z,Xκ^0_{long})	Total κ^0_{long} production.	For use in high-energy evaluations.
215	(z,Xκ^0_{short})	Total κ^0_{short} production.	For use in high-energy evaluations.
216	(z,Xκ^-)	Total κ^- production.	For use in high-energy evaluations.
217	(z,Xp$^-$)	Total anti-proton production.	For use in high-energy evaluations.
218	(z,Xn$^-$)	Total anti-neutron production.	For use in high-energy evaluations.
219-250		(Unassigned)	
251	(n,...)	$\overline{\mu}$, average cosine of the scattering angle (laboratory system) for elastic scattering of neutrons.	Derived files only.
252	(n,...)	ξ, average logarithmic energy decrement for elastic scattering of neutrons.	Derived files only.
253	(n,...)	γ, average of the square of the logarithmic energy decrement divided by twice the average logarithmic energy decrement, for elastic scattering of neutrons.	Derived files only.
254-300		(Unassigned)	
301-450	(z,...)	Energy release parameters, , for total and partial cross sections; MT= 300 plus the reaction MT number, e.g., MT=302 is the elastic scattering kerma.	Derived files only.
451	(z,...)	Heading or title information; given in File 1 only.	
452	(z,...)	$\overline{\nu}_T$, average total (prompt plus delayed) number of neutrons released per fission event.	
453		(Unassigned)	
454	(z,...)	Independent fission product yield data.	
455	(z,...)	$\overline{\nu}_d$, average number of delayed neutrons released per fission event.	
456	(z,...)	$\overline{\nu}_p$, average number of prompt neutrons released per fission event.	
457	(z,...)	Radioactive decay data.	

MT		Description	Comments
458	(n,...)	Energy release in fission for incident neutrons.	
459	(z,...)	Cumulative fission product yield data.	
460-464		(Unassigned)	
465-466		Not allowed in Version 6.	Version 5: delayed and prompt neutrons from spontaneous fission.
467-499		(Unassigned)	
500		Total charged-particle stopping power.	
501		Total photon interaction.	
502		Photon coherent scattering.	
503		(Unassigned)	
504		Photon incoherent scattering.	
505		Imaginary scattering factor.	
506		Real scattering factor.	
507-514		(Unassigned)	
515		Pair production, electron field.	
516		Pair production; sum of MT=515, 517.	Redundant.
517		Pair production, nuclear field.	
518		Not allowed in Version 6.	
519-521		(Unassigned)	
522		Photoelectric absorption.	Version 5: MT=602.
523		Photo-excitation cross section.	
524-525		(Unassigned)	
526		Electro-atomic scattering.	
527		Electro-atomic bremsstrahlung.	
528		Electro-atomic excitation cross section.	
529-531		(Unassigned)	
532		Not allowed in Version 6.	Version 5: (γ,n).
533		Atomic relaxation data.	Version 5: total photonuclear
534	K	(1s1/2) subshell photoelectric or electro-atomic cross section.	
535	L1	(2s1/2) subshell photoelectric or elctro-atomic cross section.	
536	L2	(2p1/2) subshell photoelectric or elctro-atomic cross section.	
537	L3	(2p3/2) subshell photoelectric or elctro-atomic cross section.	
538	M1	(3s1/2) subshell photoelectric or elctro-atomic cross section.	

MT		Description	Comments
539	M2	(3p1/2) subshell photoelectric or elctro-atomic cross section.	
540	M3	(3p3/2) subshell photoelectric or elctro-atomic cross section.	
541	M4	(3d3/2) subshell photoelectric or elctro-atomic cross section.	
542	M5	(3d5/2) subshell photoelectric or elctro-atomic cross section.	
543	N1	(4s1/2) subshell photoelectric or elctro-atomic cross section.	
544	N2	(4p1/2) subshell photoelectric or elctro-atomic cross section.	
545	N3	(4p3/2) subshell photoelectric or elctro-atomic cross section.	
546	N4	(4dp3/2) subshell photoelectric or elctro-atomic cross section.	
547	N5	(4d5/2) subshell photoelectric or elctro-atomic cross section.	
548	N6	(4f5/2) subshell photoelectric or elctro-atomic cross section.	
549	N7	(4f7/2) subshell photoelectric or elctro-atomic cross section.	
550	O1	(5s1/2) subshell photoelectric or elctro-atomic cross section.	
551	O2	(5p1/2) subshell photoelectric or elctro-atomic cross section.	
552	O3	(5p3/2) subshell photoelectric or elctro-atomic cross section.	
553	O4	(5d3/2) subshell photoelectric or elctro-atomic cross section.	
554	O5	(5d5/2) subshell photoelectric or elctro-atomic cross section.	
555	O6	(5f5/2) subshell photoelectric or elctro-atomic cross section.	
556	O7	(5f7/2) subshell photoelectric or elctro-atomic cross section.	
557	O8	(5g7/2) subshell photoelectric or elctro-atomic cross section.	
558	O9	(5g9/2) subshell photoelectric or elctro-atomic cross section.	
559	P1	(6s1/2) subshell photoelectric or elctro-atomic cross section.	
560	P2	(6p1/2) subshell photoelectric or elctro-atomic cross section.	

MT		Description	Comments
561	P3	(6p3/2) subshell photoelectric or elctro-atomic cross section.	
562	P4	(6d3/2) subshell photoelectric or elctro-atomic cross section.	
563	P5	(6d5/2) subshell photoelectric or elctro-atomic cross section.	
564	P6	(6f5/2) subshell photoelectric or elctro-atomic cross section.	
565	P7	(6f7/2) subshell photoelectric or elctro-atomic cross section.	
566	P8	(6g7/2) subshell photoelectric or elctro-atomic cross section.	
567	P9	(6g9/2) subshell photoelectric or elctro-atomic cross section.	
568	P10	(6h9/2) subshell photoelectric or elctro-atomic cross section.	
569	P11	(6h11/2) subshell photoelectric or elctro-atomic cross section.	
570	Q1	(7s1/2) subshell photoelectric or elctro-atomic cross section.	
571	Q2	(7p1/2) subshell photoelectric or elctro-atomic cross section.	
572	Q3	(7p3/2) subshell photoelectric or elctro-atomic cross section.	
573-599		(Unassigned)	
600	(z,p_0)	Production of a proton leaving the residual nucleus in the ground state.	Not allowed for incident protons; use MT=2.
601	(z,p_1)	Production of a proton, with residual in the 1st excited state.	
602	(z,p_2)	Production of a proton, with residual in the 2nd excited state.	Version 5: photoelectric absorption; see MT=522.
603	(z,p_3)	Production of a proton, with residual in the 3rd excited state.	
604	(z,p_4)	Production of a proton, with residual in the 4th excited state.	
	...		
649	(z,p_c)	Production of a proton in the continuum not included in the above discrete representation.	
650	(z,d_0)	Production of a deuteron leaving the residual nucleus in the ground state.	

MT		Description	Comments
651	(z,d_1)	Production of a deuteron, with the residual in the 1st excited state.	
652	(z,d_2)	Production of a deuteron, with the residual in the 2nd excited state.	
	...		
699	(z,d_c)	Production of a deuteron in the continuum not included in the above discrete representation.	
700	(z,t_0)	Production of a triton leaving the residual nucleus in the ground state.	
701	(z,t_1)	Production of a triton, with residual in the 1st excited state.	
702	(z,t_2)	Production of a triton, with residual in the 2nd excited state.	
	...		
749	(z,t_c)	Production of a triton in the continuum not included in the above discrete representation.	
750	(n,$^3He_0$)	Production of a ^{3}He particle leaving the residual nucleus in the ground state.	
751	(n,$^3He_1$)	Production of a ^{3}He, with residual in the 1st excited state.	
	...		
799	(n,^3He_c)	Production of a ^{3}He in the continuum not included in the above discrete representation.	
800	(z,α_0)	Production of an alpha particle leaving the residual nucleus in the ground state.	
801	(z,α_1)	Production of an alpha particle, with residual in the 1st excited state.	
	...		
849	(z,α_c)	Production of an alpha particle in the continuum not included in the above discrete representation.	
850		(Unassigned)	
851-870		Lumped reaction covariances.	
871-874		(Unassigned)	
875	(z,$2n_0$)	Production of 2 neutrons with residual in the ground state.	
876	(z,$2n_1$)	Production of 2 neutrons with residual in the 1st excited state.	
	...		

MT		Description	Comments
891	(z,2n$_c$)	Production of 2 neutrons in the continuum not included in the above discrete representation.	
892-999		(Unassigned)	

B.2 Residual Breakup Flags LR

Many reactions are sequential in nature. That is, a particle or gamma ray may be emitted first, then the residual nucleus decays by one or more paths. Most often, the first stage of the reaction proceeds through a well-defined discrete state of the residual nucleus and the angular dependence of the first emitted particle must be uniquely described. A simple, two-body reaction is one in which the incident particle is inelastically scattered from the target nucleus leaving the target in an excited state, which immediately decays by gamma emission. Other excited states of the same target may, however, decay by particle emission, electron-positron pair formation, or internal conversion. It is often necessary to completely specify the reaction mechanism, in particular for isotopic depletion and/or build-up calculations.

The following numbers can be used as flags to indicate the mode of decay of the residual nucleus.

LR	Description
0 or blank	Simple reaction. Identity of product is implicit in MT. Only gamma rays may be emitted additionally.
1	Complex or breakup reaction. The identity and multiplicity of all products are given explicitly in File 6.
22	α emitted (plus residual, if any).
23	3α emitted (plus residual, if any).
24	nα emitted (plus residual, if any).
25	2nα emitted (plus residual, if any).
28	p emitted (plus residual, if any).
29	2α emitted (plus residual, if any).
30	n2α emitted (plus residual, if any).
31	Residual nucleus decays only by gamma emission.
32	d emitted (plus residual, if any).
33	t emitted (plus residual, if any).
34	^{3}He emitted (plus residual, if any).
35	d2α emitted (plus residual, if any).
36	t2α emitted (plus residual, if any).
39	Internal conversion.
40	Electron-positron pair formation.

Examples

1. T(d,γ)^{5}He*(16.39 MeV) MT=102 LR=24 (^{5}He decays via n+α)
2. ^{7}Li(n,n')^{7}Li*(0.48 MeV) MT=51 LR=31 (Residual decays by γ emission)
3. ^{7}Li(n,n')^{7}Li*(4.63 MeV) MT=52 LR=33 (^{7}Li* decays via t+α).

B.3 Summary

Version ENDF-6 formats and procedures are recommended for all new evaluations; this is the only format allowed for incident charged particles. It must be taken into account, however, that many old ENDF/B-V materials for incident neutrons will be carried over without technical changes to the data.

A few files and several MT numbers are defined for the first time for ENDF-6. A few MT numbers allowed for format Version 5 have now been removed and must be replaced. Other MT numbers are allowed only in ENDF/B-V and these are not defined here - the reader is referred to the ENDF/B-V format manual. Many MT numbers above the 600 series are redefined for 6 and all Version 5 materials must be changed accordingly prior to reissue.

A few of the MT numbers are not defined for certain particles incident: for example, MT=1 is not defined for incident charged particles: MT=50 is not defined for incident neutrons: MT=600 is not defined for incident protons; etc. These exceptions are labeled but should be obvious if one follows the explicit definitions closely.

Several MT numbers cannot be used with File 4 or 5; other MT numbers must have a File 6 (File 4 and 5 are not allowed). The changes between previous format manuals are significant, therefore, much effort has been expended to explicitly define the MT numbers for ENDF-6 and, hopefully to associate them with the proper files. For explicit information on usage, see Sections 0, 3.4, and 3.5.

Appendix C

ZA Designations of Materials and MAT Numbers

A floating-point number, ZA, is used to identify materials. If Z is the charge number and A the mass number then ZA is computed from

ZA = (1000.0*Z) + A

For example, ZA for ^{238}U is 92238.0, and ZA for beryllium is 4009.0. For materials other than isotopes, the following rules apply. The MAT number is 100*Z+I where I is unique for the isotope and its isomer state.

1. If the material is an element that has more than one naturally occurring isotope, then A is set to 0.0. For example, ZA for the element tungsten is 74000.0. The MAT number is 100*Z.

2. For compounds, the ZA is arbitrary and is calculated from ZA=MAT+100.

The MAT number assignments for compounds have the following structure.

Hydrogen (except organics)	1-10
Deuterium	11-20
Lithium	21-25
Beryllium	26-30
Carbon (including organics)	31-44
Oxygen	45-50
Metals	51-70
Fuels	71-99

The presently recognized assignments are:

Compound	**MAT Number**
Water	1
Para Hydrogen	2
Ortho Hydrogen	3
H in ZrH	7
Heavy Water	11
Para Deuterium	12
Ortho Deuterium	13
Be	26
BeO	27
Be_2C	28
Be in BeO	29
Graphite	31
Liquid Methane	33
Solid methane	34
Polyethylene	37
Benzene	40
O in BeO	46
Zr in ZrH	58
UO_2	75
UC	76

Appendix D

Resonance Region Formulae

D.1 The Resolved Resonance Region (LRU=1)

The following resonance formalisms are given for a particular isotope in the laboratory system, without Doppler broadening.

D.1.1 Single-Level Breit-Wigner (SLBW, LRF=1)

D.1.1.1 Elastic Scattering Cross Sections

Processing codes should sum the cross section, as shown below from $l = 0$ to l =NLS-1, including any "empty" or "non-resonant" channels, in order to get the potential-scattering contribution. If higher l-values contribute to the scattering in the resonance region, it is the responsibility of the evaluator to provide a suitable File 3 contribution. (See Sections 2.4.19 and 2.4.20.)

$$\sigma_{n,n}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma_{n,n}^{l}(E), \tag{D.1}$$

where

$$\begin{aligned} \sigma_{n,n}^{l}(E) &= (2l+1)\,\frac{4\pi}{k^2}\sin^2\phi_l \\ &+ \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}^2 - 2\Gamma_{nr}\Gamma_r \sin^2\phi_l + 2(E-E_r')\,\Gamma_{nr}\sin(2\phi_l)}{(E-E_r')^2 + \frac{1}{4}\Gamma_r^2} \end{aligned} \tag{D.2}$$

The hard-sphere phase shifts ϕ_l, the wave number k, the primed resonance energy E_r', the neutron width Γ_{nr}, and through it the total width Γ_r, are all functions of energy, $\phi_l(E)$, $k(E)$, $E_r'(E)$, $\Gamma_{nr}(E)$, and $\Gamma_r(E)$, but this dependence is not shown explicitly. Also, each resonance parameter carries the implicit quantum numbers l and J, determined by the appropriate entries in the ENDF file. In case a given pair (l, J) is compatible with two different values of the channel spin, s, the width is a sum over the two partial channel spin widths. This allows one to omit an explicit sum over channel spin when defining the cross sections.

D.1.1.2 Radiative Capture Cross Section

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^{l}_{n,\gamma}(E) \tag{D.3}$$

where:

$$\sigma^{l}_{n,\gamma}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\,\Gamma_{\gamma r}}{(E - E'_r)^2 + \frac{1}{4}\Gamma_r^2} \tag{D.4}$$

and $\Gamma_{\gamma r}$, the radiative capture width, is constant in energy.

D.1.1.3 Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^{l}_{n,f}(E)\ , \tag{D.5}$$

where

$$\sigma^{l}_{n,f}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{fr}}{(E - E'_r)^2 + \frac{1}{4}\Gamma_r^2} \tag{D.6}$$

and Γ_{fr}, the fission width, is constant in energy.

D.1.1.4 The Competitive Reaction Cross Section

The competitive reaction cross section, $\sigma_{n,x}(E)$, is given in terms of analogous formulas involving Γ_{xr}, the competitive width. By convention, the cross section for the competitive reaction is given entirely in File 3, and is not to be computed from the resonance parameters. The reason for this is that the latter calculation can be done correctly only for a single competitive channel, since the file can define only one competitive width.

The statistical factor $g_J = (2J+1)/[2(2I+1)]$ is obtained from the target spin I and the resonance spin J given in File 2 as SPI and |AJ|, respectively.

The sum on l extends over all l-values for which resonance parameters are supplied. There will be NLS terms in the sum. NLS is given in File 2 for each isotope. In general, ENDF resonance files are limited to l=0, 1, and 2, so that the potential-scattering contribution will be represented by hard-sphere scattering up to the energy where f-wave (l=3) potential scattering starts. At that point, the evaluator may have to supply File 3 scattering to simulate the higher l-values. He or she may also require a File 3 contribution at lower energies to represent any differences between hard-sphere scattering and experiment.

The sum on J extends over all possible J-values for a particular l-value. NR_J is the number of resonances for a given pair of l and J values and may be zero. NRS is the total

number of resonances for a given l-value and is given in File 2 for each l-value.

$$\begin{aligned}
\text{NRS} &= \sum_{J=\text{JMIN}}^{J=\text{JMAX}} \text{NR}_J \text{ , where} \\
\text{JMAX} &= l + I + \frac{1}{2} \quad \text{and} \\
\text{JMIN} &= \left| l - I - \frac{1}{2} \right| \quad \text{if } l \geq I \\
&= \left| I - l - \frac{1}{2} \right| \quad \text{if } I \geq l \\
&= \left| |I - l| - \frac{1}{2} \right| \quad \text{in both cases}
\end{aligned}$$

$\Gamma_{nr}(|E_r|) \equiv \text{GN}_r$ is the neutron width, for the rth resonance for a particular value of l and J, evaluated at the resonance energy E_r. For bound levels, the absolute value $|E_r|$ is used.

$$\Gamma_{nr} = \frac{P_l(E)\, \Gamma_{nr}\left(|E_r|\right)}{P_l\left(|E_r|\right)} \tag{D.7}$$

$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr} + \Gamma_{xr}$ is the total width, a function of energy through Γ_{nr} and Γ_{xr}, since $\Gamma_{\gamma r}$ and Γ_{fr} are constant with respect to energy. The "competitive" width, Γ_{xr}, is not entered explicitly in File 2. It is calculated from the equation:

$$\Gamma_{xr} = \Gamma_r - \Gamma_{nr} - \Gamma_{\gamma r} - \Gamma_{fr} \quad \text{at} \quad E = E_r \tag{D.8}$$

The following quantities are given in File 2 for each resonance:

$$\begin{aligned}
E_r &= \text{ER, the resonance energy} \\
J &= |\text{AJ}|\text{, the angular momentum ("spin") of the resonance state} \\
I &= \text{SPI, the angular momentum ("spin") of the target nucleus} \\
g_J &= \text{statistical factor } (2J+1)/[2(2I+1)] \\
\Gamma_{nr}\left(|E_r|\right) &= \text{GN, the neutron width} \\
\Gamma_{\gamma r} &= \text{GG, the radiation width} \\
\Gamma_{fr} &= \text{GF, the fission width and} \\
\Gamma_r\left(|E_r|\right) &= \text{GT, the total width evaluated at the resonance energy.}
\end{aligned}$$

Since the competitive width Γ_{xr}, is not given, Γ_r should be obtained from File 2 directly, and ***not*** by summing partial widths.

For p-, d- and higher l-values, the primed resonance energy E_r' is energy-dependent:

$$E_r' = E_r + \frac{S_l\left(|E_r|\right) - S_l\left(|E|\right)}{2P_l\left(|E_r|\right)}\,\Gamma_{nr}\left(|E_r|\right). \tag{D.9}$$

The fact that the resonance energy shift is zero at ***each*** E_r is an artifact of the SLBW formalism, and implies a different R-matrix boundary condition for each resonance.

The neutron wave number in the center-of-mass system is given as:

$$k = \frac{\sqrt{2m_n}}{\hbar}\frac{\text{AWRI}}{\text{AWRI}+1.0}\sqrt{|E|}\,, \tag{D.10}$$

where

AWRI= ratio of the mass of a particular isotope to that of the neutron.

E= laboratory energy in eV.

The energy is written with absolute value signs so that the same formula can be used for positive incident neutron energies and for negative (bound state) resonance energies. (When inelastic scattering can occur, resonances below the level threshold are at "negative energy" in the inelastic channel.)

The shift factor S_l is defined as:

$$\begin{aligned} S_0 &= 0, \\ S_1 &= -\frac{1}{1+\rho^2}, \\ S_2 &= -\frac{18+3\rho^2}{9+3\rho^2+\rho^4}, \\ S_3 &= -\frac{675+90\rho^2+6\rho^4}{225+45\rho^2+6\rho^4+\rho^6}; \end{aligned} \tag{D.11}$$

(the quantity ρ is defined below).

For higher l-values, S_l is defined by Equation (2.9) in Reference 1. In conventional R-matrix theory, the shift factors are defined differently for negative energies (Reference 1, Equations 2.11 a-c). In ENDF, the positive-energy formulas are used, but the absolute value of E is used in SLBW and MLBW. For the R-Matrix Limited format, Section D.1.7, a flag indicates whether shifts are to be calculated or assumed to be zero for each particle-pair.

The penetration factor P_l is defined:

$$\begin{aligned} P_0 &= \rho, \\ P_1 &= \frac{\rho^3}{1+\rho^2}, \\ P_2 &= \frac{\rho^5}{9+3\rho^2+\rho^4}, \\ P_3 &= \frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6}; \end{aligned} \tag{D.12}$$

For higher l-values, the expressions for P_l are defined by Equation (2.9) in Reference 1. In conventional R-matrix theory, the penetrabilities are zero for negative energies. The theory uses the "theoretical" definition of a reduced width, $\Gamma(E) = 2P_l(E)\gamma^2$, where E is a channel energy (center-of-mass), and it suffices to say that $P_l(E) = 0$ if $E < 0$.

In ENDF, the "experimental" definition is used, $\Gamma(E) = \Gamma\left(|E_r|\right) P_l(E) \;/\; P_l\left(|E_r|\right)$, and it is necessary to make the convention that a penetrability for a negative ***resonance*** energy is evaluated at its absolute value. A negative kinetic energy can occur in an exit channel if the reaction is exothermic, and in this case $P_l(E < 0)$ is zero.

The ϕ_l is the (negative of the) hardsphere phase shift and is given by:

$$\begin{aligned}
\phi_0 &= \widehat{\rho}\,, \\
\phi_1 &= \widehat{\rho} - \tan^{-1}\widehat{\rho}\,, \\
\phi_2 &= \widehat{\rho} - \tan^{-1}\left\{\frac{3\widehat{\rho}}{3-\widehat{\rho}^2}\right\}\,, \\
\phi_3 &= \widehat{\rho} - \tan^{-1}\left\{\frac{\widehat{\rho}\,(15-\widehat{\rho})^2}{15-6\widehat{\rho}^2}\right\}\,.
\end{aligned} \tag{D.13}$$

For higher l-values, the ϕ_l are defined by Equation 2.12 in Reference 1. It is not necessary to evaluate a phase shift at negative energies.

Parameters ρ and $\widehat{\rho}$ are defined as $k\times$ *radius*, where *radius* is defined as follows:

$a =$ channel radius [1] in units of 10^{-12} cm

$$a = 0.123 \times \mathrm{AWRI}^{1/3} + 0.08 \tag{D.14}$$

AP = energy-independent scattering radius, which determines the low-energy scattering cross section. It is given in File 2 following SPI.

AP(E) = energy-dependent scattering radius, given as a TAB1 card preceding the "SPI AP....NLS..." card.

If	NRO	=0	(AP energy-independent)
	NAPS	=0	$\rho = k\,a$; $\widehat{\rho} = k$ AP
	NAPS	=1	$\rho = \widehat{\rho} = k$ AP
If	NRO	=1	(AP energy-dependent)
	NAPS	=0	$\rho = k\,a$; $\widehat{\rho} = k$ AP(E)
	NAPS	=1	$\rho = \widehat{\rho} = k$ AP(E)
	NAPS	=2	$\rho = k$ AP; $\widehat{\rho} = k$ AP(E).

[1] The channel radius, strictly speaking, involves $A^{1/3}$ (the target mass in amu), and not $(\mathrm{AWRI})^{1/3}$, but as long as the mass of the incident particle is approximately unity, as it is for neutrons, the difference is not important. AWRI= A/m_n, where m_n is the neutron mass (see Appendix H).

D.1.2 Multilevel Breit-Wigner (MLBW, LRF=2)

The equations are the same as **SLBW**, except that a resonance-resonance interference term is included in the equation for elastic scattering of l-wave neutrons, $\sigma^l_{n,n}(E)$:

$$\sigma^l_{n,n}(E) = \frac{\pi}{k^2}\sum_J g_J \sum_{r=2}^{\mathrm{NR}_J}\sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left[(E-E'_r)(E-E'_s)+\frac{1}{4}\Gamma_r\Gamma_s\right]}{\left[(E-E'_r)^2+(\Gamma_r/2)^2\right]\left[(E-E'_s)^2+(\Gamma_s/2)^2\right]}. \tag{D.15}$$

This form, which has $\approx \mathrm{NR}_J^2$ energy-dependent terms and can involve a great deal of computer time, may be written in the following form with only NR_J terms: (See Section 2.4.12):

$$\sigma^l_{n,n}(E) = \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{G_r\Gamma_r + 2H_r(E-E'_r)}{(E-E'_r)^2+(\Gamma_r/2)^2} \tag{D.16}$$

where

$$G_r = \frac{1}{2}\sum_{s=1,s\neq r}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{ns}(\Gamma_r+\Gamma_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2}, \tag{D.17}$$

$$H_r = \sum_{s=1,s\neq r}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{ns}(E'_r-E'_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2} \tag{D.18}$$

For the user who does not require ψ- and χ-broadening, the amplitude-squared form of the equations, which are mathematically identical to the conventional MLBW equations, require less computing time

$$\sigma_{n,n}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,n}(E) \tag{D.19}$$

$$\sigma^l_{n,n}(E) = \frac{\pi}{k^2}\sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \left|1-U^{lsJ}_{nn}(E)\right|^2 \tag{D.20}$$

$$U^{lsJ}_{nn}(E) = e^{-2i\phi_l}\left[1+\sum_{r=1}^{\mathrm{NR}_{sJ}} \frac{i\,\Gamma^{lsJ}_{nr}}{E'_r-E-i\,\Gamma_r/2}\right] \tag{D.21}$$

Caution: The use of this formalism is NOT recommended. Computation time is no longer a valid issue for modern computers. All new evaluations should be done with the Reich-Moore formalism (LRF=3 format for very simple cases and LRF=7 for the rest).

It is important to note that the ENDF version of the multilevel Breit-Wigner formalism does not correspond exactly to the full multilevel formalism because it allows multilevel computations only for elastic; for other types of partial cross sections the formalism is single-level.

D.1.3 Reich-Moore (R-M, LRF=3)

Evaluators should be aware that the full Reich-Moore formalism is far more general than its ENDF implementation under LRF=3, which is a severely limited subset of the Reich-Moore capabilities. For a more general treatment of the Reich-Moore formalism see the section on R-Matrix Limited format (LRF=7).

This description of the ENDF Reich-Moore formalism differs from previous versions by using notation in closer agreement with References 1 and 2. The dependence of all quantities on channel spin has been made explicit, to support a format extension which permits specifying the individual channel-spin components of the neutron width.

Partial cross sections may be obtained from a collision matrix U_{ab}, which connects entrance channels a with exit channels b. In ENDF, the formalism is applied to neutron reactions, $a = n$:

$$\sigma_{nb} = \frac{\pi}{k^2}\, g_n \left|\delta_{nb} - U_{nb}\right|^2 \tag{D.22}$$

These partial cross sections are not observable, but must be summed over the appropriate entrance and exit channels to yield observable cross sections. The statistical factor g_n is a result of prior averaging over channels with different magnetic sub-states, since the ENDF formulae apply to unpolarized particles.

In the Reich-Moore formalism as implemented in LRF=3, the only reactions requiring explicit channel definitions are elastic scattering and fission; capture is obtained by subtraction (although it is possible to obtain it directly from the collision matrix elements). Neutron channels are labeled by three quantum numbers, l, s, and J. In the ENDF format, l runs from zero to NLS-1, the highest l-value that contributes to the cross section in the energy range of interest. The channel spin s is the vector sum of the target spin I and the neutron spin i $(= 1/2)$, and takes on the range of values $|I - 1/2|$ to $I + 1/2$. The total angular momentum J is the vector sum of l and s, and runs from $|l - s|$ to $l + s$. The fission channels do not correspond to individual two-body fission product breakup, but to Bohr-channels in deformation space, which is why two are adequate for describing many neutron-induced fission cross sections. It is not necessary to specify the quantum numbers associated with the two "ENDF-allowed" fission channels, and they can simply be labeled f1 and f2.

If one sums over all incident channels n and exit channels b, and invokes unitarity, the resulting total cross section can be expressed in terms of the diagonal matrix elements as:

$$\sigma_T(E) = \frac{2\pi}{k^2} \sum_{l=0}^{\mathrm{NLS}} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \mathrm{Re}\left[1 - U_{lsJ,lsJ}\right] \tag{D.23}$$

The elastic cross section is obtained by summing the incident neutron channels over all possible lsJ values and the exit neutron channels over those quantities $l's'J'$ that have the same ranges as lsJ. Conservation of total angular momentum requires that $J' = J$; the ENDF format LRF=3 imposes additional "conservation rules", namely $l' = l$ and $s' = s$ which are actually just simplifying assumptions, with some basis in theory and experiment (these assumptions are not required in LRF=7, for example). The six-fold summation then

reduces to the familiar form:

$$\sigma_{nn}(E) = \frac{2\pi}{k^2} \sum_{l=0}^{\text{NLS}} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \left|1 - U_{lsJ,lsJ}\right|^2 . \tag{D.24}$$

The absorption (non-elastic) cross section is obtained by subtraction:

$$\sigma_{abs}(E) = \sigma_T(E) - \sigma_{nn}(E). \tag{D.25}$$

Fission is obtained from the collision matrix by summing equation (D.22) over all incident lsJ values and over the two exit fission channels, b=f1 and b=f2,

$$\sigma_f(E) = \frac{2\pi}{k^2} \sum_{l=0}^{\text{NLS}} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \left[\left|U_{nf1}^{lsJ}\right|^2 + \left|U_{nf2}^{lsJ}\right|^2\right] . \tag{D.26}$$

The Reich-Moore formalism is described in Reference 3. Here we repeat the level-matrix form of the collision matrix as given in the earlier versions of this manual:

$$U_{nb}^J = e^{-i(\phi_n+\phi_b)} \left\{2\left[(I-K)^{-1}\right]_{nb} - \delta_{nb}\right\} , \tag{D.27}$$

where:

$$(I-K)_{nb} = \delta_{nb} - \frac{i}{2} \sum_r \frac{\Gamma_{nr}^{1/2}\Gamma_{br}^{1/2}}{E_r - E - i\,\Gamma_{\gamma r}/2} . \tag{D.28}$$

Here ϕ_b is zero for fission, $\phi_n = \phi_l$ (defined previously), and the summation is over those resonances r which have partial widths in both of the channels n and b; E_r is the resonance energy; $\Gamma_{\gamma r}$ is the "eliminated" radiation width; Γ_{nr} and Γ_{br} are the partial widths for the rth resonance in channels n and b.

Caution: While the following equations are correct, they can lead to serious numerical problems if programmed in this form. For a computationally more stable form the reader is referred to Section II of the SAMMY manual [Reference 4].

If we define a matrix ρ by the equation

$$\rho_{nb} = \delta_{nb} - \left[(1-K)^{-1}\right]_{nb} \tag{D.29}$$

then the various cross sections take the following forms:

Total:

$$\sigma_T(E) = \frac{2\pi}{k^2} \sum_{lsJ} g_J \left[(1-\cos 2\phi_l) + 2\text{Re}\left(\rho_{nn} e^{-2i\,\phi_l}\right)\right] . \tag{D.30}$$

Elastic:

$$\sigma_{nn} = \frac{\pi}{k^2} \sum_{lsJ} g_J \left[2 - 2\cos 2\phi_l + 4\text{Re}(\rho_{nn} e^{-2i\phi_l}) - 4\text{Re}(\rho_{nn}) + 4|\rho_{nn}|^2\right] . \tag{D.31}$$

Absorption (fission plus capture):

$$\sigma_{n,abs}(E) = \frac{4\pi}{k^2} \sum_{lsJ} g_J \ \left[\mathrm{Re}(\rho_{nn}) - |\rho_{nn}|^2\right] \ . \tag{D.32}$$

Fission:

$$\sigma_{nf}(E) = \frac{4\pi}{k^2} \sum_{lsJ} g_J \ \left[|\rho_{nf1}|^2 + |\rho_{nf2}|^2\right] \ . \tag{D.33}$$

The phase shifts and penetrabilities are evaluated in terms of a and AP as described earlier. The shift factor has been set equal to zero in the above equations ($E_r' \rightarrow E_r$); hence they are strictly correct only for s-wave resonances. Originally, the ENDF Reich-Moore format was used for low-energy resonances in fissile materials, which **are** s-waves. However, it is believed that the "no-shift" formulae can be safely applied to higher l-values also, since the difference in shape between a shifted resonance and one that is not shifted at the same energy has no practical significance. Evaluations using the correct shift factor can be reported under the newer LRF=7 format option.

The comments in Section D.1.1 about the summation over channels applies to the Reich-Moore formalism also. Until the formats revision approved by CSEWG in 1999, the format did not permit the specification of channel spin; therefore, if an evaluation includes $l > 0$ resonances for $I > 0$ nucleus, it was necessary for the processing codes to include the potential-scattering contributions from the "missing" channels. (It is adequate to arbitrarily assume that the supplied values are for the $s = I - 1/2$ channels, and to use the same potential-scattering radius in the missing $I + 1/2$ channels. See Sections 2.4.19 and 2.4.20.) Having the ability to specify which channel spin does not solve this problem, unless the evaluator actually supplies resonances for both channels. In cases where the data can be fit with all the resonances in the same s-channel, the "other one" will still be absent from the ENDF file, since the format stipulates nothing about avoiding missing channels. This is why it is reasonable for the processing codes to run over the triple lsJ loop, inserting potential scattering in every channel, and resonances whenever they are supplied.

Note: When both positive and negative AJ values are given in the file, negative AJ implies $s = I - 1/2$ and positive AJ implies $s = I + 1/2$. When AJ=0, one and only one of $I - 1/2$ or $I + 1/2$ is possible, so the possible ambiguity of ± 0 does not arise. In this case $s = l$; parity conservation prevents the occurrence, for a given J, of two s-values differing by one unit.

D.1.4 Adler-Adler (AA, LRF=4)

The formulae, taken from References 5 and 6, are given for the total, radiative capture, and fission cross sections. They have been slightly recast to make them conform to the definitions used earlier in this Appendix. Furthermore, only the $l = 0$ terms are given, consistent with current usage of this formalism. Procedures are discussed in Section 2.4.13. Since only s-waves are considered, higher l-wave contributions to the potential scattering must be put into File 3 by the evaluator.

Total Cross Section:

$$\begin{aligned}\sigma_T(E) &= \frac{4\pi}{k^2}\sin^2\phi_0 \\ &+ \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{\mathrm{NRS}}\frac{\nu_r\left(G_r^T\cos 2\phi_0 + H_r^T\sin 2\phi_0\right) + (\mu_r - E)\left(H_r^T\cos 2\phi_0 - G_r^T\sin 2\phi_0\right)}{(\mu_r - E)^2 + \nu_r^2}\right. \\ &+ \left. AT_1 + \frac{AT_2}{E} + \frac{AT_3}{E^2} + \frac{AT_4}{E^3} + BT_1E + BT_2E^2\right].\end{aligned} \tag{D.34}$$

Radiative Capture Cross Section:

$$\begin{aligned}\sigma_{n,\gamma}(E) &= \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{\mathrm{NRS}}\frac{\nu_r G_r^\gamma + (\mu_r - E)H_r^\gamma}{(\mu_r - E)^2 + \nu_r^2}\right. \\ &+ \left. AC_1 + \frac{AC_2}{E} + \frac{AC_3}{E^2} + \frac{AC_4}{E^3} + BC_1E + BC_2E^2\right].\end{aligned} \tag{D.35}$$

Fission Cross Section:

$$\begin{aligned}\sigma_{n,f}(E) &= \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{\mathrm{NRS}}\frac{\nu_r G_r^f + (\mu_r - E)H_r^f}{(\mu_r - E)^2 + \nu_r^2}\right. \\ &+ \left. AF_1 + \frac{AF_2}{E} + \frac{AF_3}{E^2} + \frac{AF_4}{E^3} + BF_1E + BF_2E^2\right].\end{aligned} \tag{D.36}$$

Although the format uses different names for μ and ν for each reaction, they are actually equal:

$$\begin{aligned}\mathrm{DET}_r &= \mathrm{DEF}_r = \mathrm{DEC}_r = \mu_r \\ \mathrm{DWT}_r &= \mathrm{DWF}_r = \mathrm{DWC}_r = \nu_r\end{aligned}$$

D.1.5 General R-Matrix (GRM, LRF=5)

The format is no longer available in ENDF-6.

D.1.6 Hybrid R-Function (HRF, LRF=6)

The format is no longer available in ENDF-6.

D.1.7 R-Matrix Limited Format (RML, LRF=7)

In R-Matrix theory, a channel may be defined by $c = (\alpha, l, s, J)$, where

- α represents the two particles making up channel; α includes mass (m_a and m_b with subscript a indicating the incident particle for an entrance channel), charge (Z_a and Z_b), spin (i_a and i_b) and parity (π_a and π_b) and all other quantum numbers for each of the two particles, plus the Q-value.

l is the orbital angular momentum; the associated parity is $(-1)^l$.

s represents the channel spin (including the associated parity); that is, s is the vector sum of the spins of the two particles of the pair.

J is the total angular momentum (and associated parity); J is the vector sum of l and s.

Only J and its associated parity are conserved for any given interaction. The other quantum numbers may differ from channel to channel, so long as the sum rules for spin and parity are obeyed.

In the Reich-Moore approximation to R-matrix theory, the radiation width is treated separately and differently from widths for other channels (which are hereafter referred to as "particle channels"). In this LRF=7 format, there is assumed to be an "eliminated channel", which, for the strict interpretation of the Reich-Moore approximation, contains all the radiation width; in this format, it is possible for some portion of the radiation width to be treated in the same fashion as the particle widths. In the equations below, the eliminated width appears only in the denominator of the R-matrix.

In all formulae given below, spin quantum numbers (e.g., J) are implicitly assumed to include the associated parity. Vector sum rules are implicitly assumed to be obeyed; readers unfamiliar with these sum rules are referred to the paragraph on Spin and Angular Momentum Conventions for details.

Let the angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J be represented by $\sigma_{cc'}$. This cross section is given in terms of the scattering matrix $U_{cc'}$ as:

$$\sigma_{cc'} = \frac{\pi}{k_a^2}\, g_{J\alpha}\, \left| e^{iw_c}\, \delta_{cc'} - U_{cc'} \right|^2\, \delta_{JJ'} \tag{D.37}$$

where

k_α is the center-of mass momentum associated with incident particle-pair α,

$g_{J\alpha}$ is the spin statistical factor,

w_c is zero for non-Coulomb channels. (Details for the charged-particle case are presented later.)

The spin statistical factor is given by:

$$g_{J\alpha} = \frac{2J+1}{(2i_a+1)(2i_b+1)}, \tag{D.38}$$

and center-of mass momentum k_α by:

$$k_\alpha^2 = \frac{2m_a m_b^2}{(m_a+m_b)^2} E. \tag{D.39}$$

The scattering matrix U can be written in terms of the matrix W as

$$U_{cc'} = \Omega_c W_{cc'}\ \Omega_{c'}, \tag{D.40}$$

where Ω is given by:

$$\Omega_c = e^{i(w_c - \phi_c)}. \tag{D.41}$$

Here again, w_c is zero for non-Coulomb channels, and the potential scattering phase shifts for non-Coulomb interactions ϕ_c are defined in many references (e.g., Reference 1). The matrix Win equation (D.40) is related to the R-matrix (in matrix notation with indices suppressed) via:

$$W = P^{1/2}(I - RL)^{-1}(I - RL^*\ )\ P^{-1/2}. \tag{D.42}$$

The quantity I in this equation represents the identity matrix. The quantity L in equation (D.42) is given by

$$L = (S - B) + iP \tag{D.43}$$

with P the penetration factor, S the shift factor, and B the arbitrary boundary constant at the channel radius a_c. Formulae for P and S are likewise found in many references (see, e.g., equation (2.9) in Reference 1); for non-Coulomb interactions see Table D.1 for the appropriate formulae. For fission, the penetrability is unity. For non-eliminated capture channels, the penetrability is unity. For two charged particles, formulae for the penetrabilities are provided in Section II.C.4 of the SAMMY Users' Manual [Reference 4].

Table D.1: Hard sphere penetrability (penetration factor) P, level shift factor S, and potential scattering phase shift ϕ for orbital angular momentum l, center of mass momentum k, and channel radius a_c, with $\rho = ka_c$.

l	$\boldsymbol{P}_l$	$\boldsymbol{S}_l$	ϕ_l
0	ρ	0	ρ
1	$\rho^3/(1+\rho^2)$	-1 / $(1+\rho^2)$	$\rho - \tan^{-1}\rho$
2	$\rho^5/(9+3\rho^2+\rho^4)$	$-(18+3\rho^2)/(9+3\rho^2+\rho^4)$	$\rho - \tan^{-1}[3\rho/(3-\rho^2)]$
3	$\rho^7/(225+45\rho^2$ $+6\rho^4+\rho^6)$	$-(675+90\rho^2+6\rho^4)/(225+45\rho^2+6\rho^4+\rho^6)$	$\rho - \tan^{-1}[\rho(15-\rho^2)/$ $(15-6\rho^2)]$
4	$\rho^9/(11025+1575\rho^2$ $+135\rho^4+10\rho^6+\rho^8$	$-(44100+4725\rho^2+270\rho^4+10\rho^6)/$ $(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)$	$\rho - \tan^{-1}[\rho(105-10\rho^2)/$ $(105-45\rho^2+\rho^4)]$
l	$\frac{\rho^2 P_{l-1}}{(l-S_{l-1})^2+P_{l-1}^2}$	$\frac{\rho^2(l-S_{l-1})}{(l-S_{l-1})^2+P_{l-1}^2}\ -\ l$	$\phi_{l-1} - \tan^{-1}\left[\frac{(P_{l-1}}{(l-S_{l-1})}\right]$ or $B_l = \frac{(B_{l-1}+X_l)}{(1-B_{l-1}X_l)}$ with $B_l = \tan(\rho - \phi_l)$ and $X_l = \frac{P_{l-1}}{(l-S_{l-1})}$

In the eliminated-channel approximation, the R-matrix of equation (D.42) [for the spin group defined by total spin J and implicit parity π] has the form:

$$R_{cc'} = \left[\sum_\lambda \frac{\gamma_{\lambda c}\ \gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} + R_c^{\text{bkg}}\ \delta_{cc'}\right]\ \delta_{JJ'} \tag{D.44}$$

where all levels (resonances) of that spin group are included in the sum. Subscripts λ designate the particular level; subscripts c and c' designate channels (including particle-pairs and all the relevant quantum numbers). Again, the width $\Gamma_{\lambda\gamma}$ occurring in the denominator corresponds to the "eliminated" non-interfering capture channels of the Reich-Moore approximation.

The "background R-matrix" $R_c^{\rm bkg}$ of equation (D.44) will be discussed in the paragraph on Extensions to R-Matrix Theory, that follows.

The channel width $\Gamma_{\lambda c}$ is given in terms of the reduced width amplitude $\gamma_{\lambda c}$ by:

$$\Gamma_{\lambda c} = 2\,\gamma_{\lambda c}^2\,P_c(E) \tag{D.45}$$

where P_c is the penetrability, whose value is a function of the type of particles in the channel, of the orbital angular momentum l, and of the energy E. Note that the reduced width amplitude $\gamma_{\lambda c}$ is always independent of energy, but the width $\Gamma_{\lambda c}$ may depend on energy via the penetration factor.

Cross sections may be calculated by using the above expressions for R and L to calculate W, and from there calculating U and, ultimately, σ. However, while equation (D.42) for W is correct, an equivalent form which is computationally more stable is:

$$W = I + 2\,i\,X, \tag{D.46}$$

where X is given in matrix notation by:

$$X = P^{1/2} L^{-1}\,\left(L^{-1} - R\right)^{-1} R\,P^{1/2}. \tag{D.47}$$

When the suppressed indices and implied summations are inserted, the expression of X becomes

$$X_{cc'} = P_c^{1/2} L_c^{-1} \sum_{c''} \left[(L^{-1} - R)^{-1}\right]_{cc''} R_{c''c'}\,P_{c'}^{1/2}\delta_{JJ'}. \tag{D.48}$$

The various cross sections are then written in terms of X.

D.1.7.1 Energy-Differential (Angle-Integrated) Cross Sections (Non-Coulomb Channels)

The observable cross sections are found in terms of X by first substituting equations (D.40, D.41, and D.46) into equation (D.37), summing over spin groups (i.e., over J^π), and then summing over all channels corresponding to those particle pairs and spin groups. If X^r represents the real part and X^i the imaginary part of X, then the angle-integrated (but energy-differential) cross section for the interaction which leads from particle-pair α to particle-pair α' has the form:

$$\sigma_{\alpha,\alpha'}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left\{ \left[\sin^2\phi_c\,(1 - 2X_{cc}^i) \;- X_{cc}^i \sin(2\phi_c)\right]\,\delta_{\alpha,\alpha'} + \sum_{c'} \left[\left(X_{cc'}^i\right)^2 + \left(X_{cc'}^r\right)^2\right]\right\}. \tag{D.49}$$

[This formula is accurate only for cases in which one of particles in α is a neutron; however, both particles in α' may be charged.]

In equation (D.49) the summations are over those channels c and c' {of the spin group defined by J^π} for which the particle-pairs are respectively α and α'. More than one "incident channel" $c = (\alpha, l, s, J)$ can contribute to this cross section, e.g., when both $l = 0$ and $l = 2$ are possible, or when, in the case of incident neutrons and non-zero spin target nuclei, both channel spins are allowed. Similarly, there may be several "exit channels" $c' = \alpha', l', s', J')$, depending on the particular reaction being calculated (elastic, inelastic, fission, etc.).

The total cross section (for non-Coulomb initial states) is the sum of equation (D.49) over all possible final-state particle-pairs α', assuming the scattering matrix is unitary (that is, assuming that the sum over c' of $|U_{cc'}|^2 = 1$). Written in terms of the X matrix, the total cross section has the form:

$$\sigma_{\alpha,\text{total}}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\frac{1}{2}\sin^2\phi_c + X_{cc}^i \cos(2\,\phi_c) - X_{cc}^r \sin(2\phi_c)\right], \tag{D.50}$$

where again the sum over c includes only those channels of the J^π spin group for which the particle-pair is α.

The angle integrated elastic cross section is given by

$$\sigma_{\alpha,\alpha}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left\{ \sin^2\phi_c\,(1 - 2X_{cc}^i) - X_{cc}^r \sin(2\phi_c) + \sum_{c'} \left[\left(X_{cc'}^i\right)^2 + \left(X_{cc'}^r\right)^2\right] \right\}. \tag{D.51}$$

In this case, both c and c' are limited to those channels of the J^π spin group for which the particle-pair is α; again, there may be more than one such channel for a given spin group.

Similarly, the reaction cross section from particle-pair α to particle-pair α' (where α' is not equal to α) is

$$\sigma_{\alpha,\alpha'}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \sum_{c'} \left[\left(X_{cc'}^i\right)^2 + \left(X_{cc'}^r\right)^2\right] \tag{D.52}$$

Here c is restricted to those channels of the J^π spin group from which the particle-pair is α, and c' to those channels for which the particle-pair is α'.

The absorption cross section has the form

$$\sigma_{\alpha,\text{absorption}}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left\{ X_{cc}^i - \sum_{c'} \left[\left(X_{cc'}^i\right)^2 + \left(X_{cc'}^r\right)^2\right] \right\}. \tag{D.53}$$

Here both the sum over c and the sum over c' include <u>all incident</u> particle channels (*i.e.*, particle-pair α only) for the J^π spin group.

The capture cross section for the eliminated radiation channels can be calculated directly as:

$$\sigma_{\alpha\gamma}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_{\text{inc}\,c} \left\{ X_{cc}^i - \sum_{\text{all}\,c'} \left[\left(X_{cc'}^i\right)^2 + \left(X_{cc'}^r\right)^2\right] \right\}, \tag{D.54}$$

or may be found by subtracting the sum of all reaction cross sections from the absorption cross section. In equation (D.54), the sum over c includes all incident particle channels for the J^π spin group, and the sum over c' includes <u>all</u> particle channels, both incident and exit, for that spin group.

D.1.7.2 Angular Distributions

Angular distributions (elastic, inelastic, or other reaction) cross sections for incident neutrons can be calculated from Reich-Moore resonance parameters. Following Blatt and Biedenharn [Reference 7] with some notational changes, the angular distribution cross section in the center-of-mass system may be written

$$\frac{d\sigma_{alpha\alpha'}}{d\Omega_{CM}} = \sum_L C_{L\alpha\alpha'}(E)\ P_L\left(\cos\beta\right) \tag{D.55}$$

in which the subscript $\alpha\alpha'$ indicates which type of cross section is being considered, P_L is the Legendre polynomial of degree L, and β is the angle of the outgoing neutron (or other particle) relative to the incoming neutron in the center-of-mass system. The coefficients $C_{L\alpha\alpha'}(E)$ are given by

$$\begin{aligned} C_{L\alpha\alpha'}(E) &= \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{c_1=(\alpha l_1 s_1 J_1)} \sum_{c_1'=(\alpha' l_1' s_1' J_1)} \sum_{c_2=(\alpha l_2 s_2 J_2)} \sum_{c_2'=(\alpha' l_2' s_2' J_2)} \\ &\times\ B_{\{l_1 s_1 l_1' s_1', J_1\}\{l_2 s_2 l_2' s_2', J_2\}L}\ \frac{1}{(2i_a+1)(2i_b+1)}\ \mathrm{Re}\left[(\delta_{c_1c_1'} - U_{c_1c_1'})(\delta_{c_2c_2'} - U^*_{c_2c_2'})\right] \end{aligned} \tag{D.56}$$

where the various summations are to be interpreted as follows:

- J_1 sum over all spin groups defined by spin J_1 and the implicit associated parity.
- J_2 sum over all spin groups defined by spin J_2 and the implicit associated parity.
- c_1 sum over all those channels c_1 belonging to the J_1 spin group and having particle-pair α $[c_1 = \alpha, l_1, s_1, J_1]$.
- c_1' sum over those channels c_1' in J_1' spin group with particle-pair α' $[c_1' = (\alpha', l_1', s_1', J_1)]$.
- c_2 sum over those channels c_2 in J_2 spin group with particle-pair α $[c_2 = (\alpha, l_2, s_2, J_2)]$.
- c_2' sum over those channels c_2' in J_2 spin group with particle-pair α' $[c_2' = (\alpha', l_2', s_2', J_2)]$.

Also note that i_a and i_b are spins of the two particles in particle-pair α.

The geometric factor B can be exactly evaluated as a product of terms:

$$B_{\{l_1 s_1 l_1' s_1', J_1\}\{l_2 s_2 l_2' s_2', J_2\}L} = A_{l_1 s_1 l_1' s_1';J_1} A_{l_2 s_2 l_2' s_2';J_2} D_{l_1 s_1 l_1' s_1' l_2 s_2 l_2' s_2';LJ_1J_2}, \tag{D.57}$$

where the factor $A_{l_1 s_1 l_1' s_1';J_1}$ is of the form:

$$A_{l_1 s_1 l_1' s_1';J_1} = \sqrt{(2l_1+1)(2l_1'+1)}\ (2J_1+1)\,\Delta(l_1 J_1 s_1)\ \Delta(l_1' J_1 s_1') \tag{D.58}$$

and similarly for $A_{l_2 s_2 l_2' s_2';J_2}$. The expression for D is:

$$\begin{aligned} D_{l_1 s_1 l_1' s_1' l_2 s_2 l_2' s_2';LJ_1J_2} &= (2L+1)\,\Delta^2(J_1J_2L)\,\Delta^2(l_1l_2L)\,\Delta^2(l_1'l_2'L) \\ &\times\; w(l_1J_1l_2J_2,s_1L)\,w(l_1'J_1l_2'J_2,s_1'L)\,\delta_{s_1s_2}\,\delta_{s_1's_2'}\,(-1)^{s_1-s_1'} \\ &\times\; \frac{n!\quad(-1)^n}{(n-l_1)!\,(n-l_2)!\,(n-L)!}\;\frac{n'!\quad(-1)^{n'}}{(n'-l_1')!\,(n'-l_2')!\,(n'-L)!}, \end{aligned} \tag{D.59}$$

in which n is defined by

$$2\,n = l_1 + l_2 + L; \tag{D.60}$$

D is zero if $l_1 + l_2 + L$ is an odd number. A similar expression defines n'. The Δ^2 term is given by:

$$\Delta^2(abc) = \frac{(a+b-c)!\,(a-b+c)!\,(-a+b+c)!}{(a+b+c+1)!}\,, \tag{D.61}$$

for which the arguments a, b, and c are to be replaced by the appropriate values given in equations (D.58) and (D.59). The expression for $\Delta^2(abc)$ implicitly includes a selection rule for the arguments; that is, the vector sum must hold:

$$\vec{a} + \vec{b} = \vec{c} \tag{D.62}$$

The quantity w in equation (D.59) is defined as:

$$\begin{aligned} w(l_1J_1l_2J_2,s\;L) &= \sum_{k=k_{\min}}^{k_{\max}} \frac{(-1)^{k+l_1+J_1+l_2+J_2}(k+1)!}{[k-(l_1+J_1+s)]!\;[k-(l_2+J_2+s)]!} \\ &\times\; \frac{1}{[k-(l_1+l_2+L)]!\;[k-(J_1+J_2+L)]!} \\ &\times\; \frac{1}{(l_1+J_1+l_2+J_2-k)!\,(l_1+J_2+s+L-k)!\,(l_2+J_1+s+L-k)!} \end{aligned} \tag{D.63}$$

(and similarly for the primed expression), where $k_{\min}$ and $k_{\max}$ are chosen such that none of the arguments of the factorials are negative. That is,

$$\begin{aligned} k_{\min} &= \max\{(l_1+J_1+s),\;(l_2+J_2+s),\;(l_1+l_2+L),\;(J_1+J_2+L)\} \\ k_{\max} &= \min\{(l_1+J_1+l_2+J_2),\;(l_1+J_2+s+L),\;(l_2+J_1+s+L)\} \end{aligned} \tag{D.64}$$

<u>Single-channel case</u>

For the single-channel case, the coefficients $C_{L\alpha\alpha'}(E)$ reduce to:

$$\begin{aligned} C_{L\alpha\alpha}(E) &= \frac{1}{4k_\alpha^2}\sum_{J_1}\sum_{J_2}\sum_{c_1=(\alpha l_1 s_1 J_1)}\sum_{c_2=(\alpha l_2 s_2 J_2)} B_{\{l_1s_1l_1s_1J_1\}\{l_2s_2l_2s_2J_2\}\;L} \\ &\times\; \frac{1}{(2i_a+1)(2i_b+1)}\,\mathrm{Re}\left[(1-U_{c_1c_1})(1-U^*_{c_2c_2})\right] \end{aligned} \tag{D.65}$$

where the existence of only one channel requires that the primed quantities of equation (D.61) be equal to the unprimed (e.g., $\alpha = \alpha'$). The geometric factor B becomes:

$$B_{\{l_1 s_1 l_1 s_1 J_1\}\,\{l_2 s_2 l_2 s_2 J_2\}\;L} = A_{l_1 s_1 l_1 s_1;J_1} A_{l_2 s_2 l_2 s_2;J_2} D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2;\,L\,J_1\,J_2} \tag{D.66}$$

where the factor A reduces to the simple form

$$A_{l_1 s_1 l_1 s_1;J_1} = (2l_1+1)(2J_1+1)\;\Delta^2(l_1 J_1 s_1) \tag{D.67}$$

and the expression for D reduces to:

$$\begin{aligned} D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2;L\,J_1\,J_2} &= (2L+1)\;\Delta^2(J_1 J_2 L)\;\Delta^4(l_1 l_2 L)\;w^2(l_1 J_1 l_2 J_2, s_1 L)\;\delta_{s_1 s_2} \\ &\times \left[\frac{n!}{(n-l_1)!\;(n-l_2)!\;(n-L)!}\right]^2 \end{aligned} \tag{D.68}$$

in which n is again defined as in equation (D.60).

D.1.7.3 Kinematics for Angular Distributions of Elastic Scattering

If E represents the laboratory kinetic energy of the incident neutron, E' the lab kinetic energy of the outgoing particle, θ the laboratory angle of the outgoing neutron, and Q the Q-value for the reaction, the E' may be expressed in terms of E, θ, and Q as

$$E' = E\left[\frac{m_a}{m_a+m_b}\;\cos\theta + \sqrt{\left(\frac{m_b}{m_a+m_b}\right)^2 - \sin^2\theta\left(\frac{m_a}{m_a+m_b}\right)^2}\right]^2 \tag{D.69}$$

where m_a represents the mass of the incident particle (neutron) and m_b, the mass of the sample (target) nucleus. Similarly, the center-of-mass angle β between outgoing and incoming neutron is found from

$$\cos\beta = \pm\frac{m_a}{m_b}\left\{\cos\theta\sqrt{\frac{m_b^2}{m_a^2} - \sin^2\theta} \;-\; \sin^2\theta\right\} \tag{D.70}$$

and the Jacobian of transformation from center-of-mass to laboratory system is

$$\frac{d(\cos\beta)}{d(\cos\theta)} = 2\cos\theta\;\frac{m_a}{m_b} + \frac{1+(2\cos^2\theta-1)\;m_a^2/m_b^2}{\sqrt{1-\sin^2\theta\;\;m_a^2/m_b^2}} \tag{D.71}$$

The elastic angular distribution cross section in the laboratory system is then found by combining equations (D.51 or D.65) with (D.71), using the relationship in equation (D.70), to give:

$$\frac{d\,\sigma}{d\,\Omega_{lab}}(\theta) = \frac{d\sigma}{d\Omega_{CM}}\;\frac{d(\cos\beta)}{d(\cos\theta)}. \tag{D.72}$$

Note that the lowest energy into which a neutron may scatter (i.e., the energy of a neutron after 180-degree scattering) is

$$E'(\cos\theta = -1) = E\left[\frac{m_b - m_a}{m_b + m_a}\right]^2 \tag{D.73}$$

and the energy of 90-degree scattering is:

$$E'(\cos\theta = 0) = E\left[\frac{m_b - m_a}{m_b + m_a}\right] \tag{D.74}$$

D.1.7.4 Spin and Angular Momentum Conventions

The spin and angular momentum conventions used in the Reich-Moore Format are described in Table D.2. Note that the word "channel" refers to the physical configuration as well as to the quantum numbers given here. For example, for an incident neutron (intrinsic spin $i = 1/2$ impinging on a target (sample) whose spin is I, the channel spin is s, where $\vec{s} = \vec{i} + \vec{I}$. The relative orbital angular momentum of this channel (neutron + target) is l, and total spin is J, where $\vec{J} = \vec{s} + \vec{l}$. The exit channel might be the same as the entrance channel, or it might include, for example, two particles whose individual spins are i' and I' and whose channel spin is s', where $\vec{s'} = \vec{i'} + \vec{I'}$. The relative angular momentum of the two particles is l', and the total J must satisfy $\vec{J} = \vec{s'} + \vec{l'}$.

Table D.2: Spin and angular momentum conventions

Symbol	**Meaning**	**Value or range of values**
i or i'	Intrinsic spin of incident neutron or outgoing particle	1/2 for incident neutron
I or I'	Spin of target or residual nuclei	integer or half-integer
l or l'	Orbital angular momentum of incident or outgoing particle	non-negative integer
s or s'	Incident or outgoing channel spin, equal to target spin plus incident particle spin	$\vec{s} = \vec{I} + \vec{i}$ or $\vec{s'} = \vec{I'} + \vec{i'}$
J	(1) Spin of resonance (2) Spin of excited level in the compound nucleus (3) Total angular momentum quantum number	$\vec{J} = \vec{l} + \vec{s} = \vec{l'} + \vec{s'}$

For readers unfamiliar with vector summation, the rules are as follows: All quantum numbers are either integer (0, 1, 2, ...) or half-integer (1/2, 3/2, 5/2, ...). If vectors of magnitude a and b are to be added, then the sum c has magnitude in the range $|a - b| \leq c \leq a + b$; c takes on only integer values if $a + b$ is integer, and half-integer values if $a + b$ is half-integer. The parity associated with c is the product of the parities associated with a and b. Note also that parity associated with orbital angular momentum l is rarely expressed explicitly, as it is always $(-1)^l$.

D.1.7.5 Extensions to R-Matrix Theory

As stated in equation(D.44), the R-matrix has the form:

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\,\gamma_{\lambda c'}}{E_\lambda - E - i\,\Gamma_{\lambda\gamma}/2} + R_c^{\text{bkg}}\,\delta_{cc'}\right]\delta_{JJ'}. \tag{D.75}$$

The external or background R-matrix $R_c^{\rm bkg}$ can be written in many different ways; four options are available in the RML format:

Option 0. $R_c^{\rm bkg} = 0$ (in which case the background is described by "dummy" resonances whose energies lie outside the range of validity of this parameterization).

Option 1. $R_c^{\rm bkg}$ is a tabulated complex function of the energy.

Option 2. $R_c^{\rm bkg}$ is a real statistical parameterization of the form available in SAMMY [Reference 4],

$$\begin{aligned} R_c^{ext}(E) &= \overline{R}_{con,c} + \overline{R}_{lin,c}E + \overline{R}_{q,c}E^2 - s_{lin,c}(E_c^{up} - E_c^{down}) \\ &- (s_{con,c} + s_{lin,c}E) \ \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right]. \end{aligned} \tag{D.76}$$

Option 3. $R_c^{\rm bkg}$is a complex statistical parameterization of the forms described by Fröhner [References 8 and 9],

$$R_c^{ext}(E) = \overline{R}_c + 2s_c\left[\tanh^{-1}\left(\frac{E-\overline{E}}{\tilde{Q}/2}\right) + i\,\frac{\overline{\Gamma}_\gamma/\tilde{Q}}{1-\left(\frac{E-\overline{E}}{\tilde{Q}/2}\right)^2}\right] \tag{D.77}$$

with

$$\tilde{Q} = E_c^{up} - E_c^{down} \quad \text{and} \quad \overline{E} = \left(E_c^{up} + E_c^{down}\right)/2 \tag{D.78}$$

The quantity $\tilde{Q}$ is not to be confused with the Q-value for channel c.

D.1.7.6 Modifications for Charged Particles

The penetrabilities P_l, shift factors S_l, and potential-scattering phase shifts ϕ_l defined in Table D.1 apply only to non-Coulomb interactions such as those involving incident neutrons, where it is possible for the two particles in a channel to both have a positive charge; examples are the (n,α) or (n,p) interactions. In this case the expressions for penetrabilities, shift factors and phase shifts must be modified to include the long-range interactions; see for example the discussion of Lane and Thomas [Reference 8].

Expressions for P_l, S_l and ϕ_l for particle pair α involve the parameter η_α, which is defined as

$$\eta_\alpha = \frac{z_\alpha Z_\alpha e^2 \mu_\alpha}{\hbar k_\alpha} \tag{D.79}$$

where z and Z are the charge numbers for the two particles in the particle pair. The reduced mass μ_α is defined in the usual manner as

$$\mu_\alpha = \frac{m_\alpha M_\alpha}{m_\alpha + M_\alpha} \tag{D.80}$$

where m and M are the masses of the two particles in the channel α. The center-of-mass momentum $\hbar k_\alpha$ is defined as

$$\hbar^2 k_\alpha^2 = \frac{2m_\alpha M_\alpha}{m_\alpha + M_\alpha}\left(E\frac{M}{m+M} + Q\right) \tag{D.81}$$

where Q is the Q-value for the particle-pair.

If a_c is the channel radius for this channel, we again define ρ as

$$\rho = k_\alpha a_c \tag{D.82}$$

The penetrabilities $P_l(\eta,\rho)$, shift factors $S_l(\eta,\rho)$ and phase shifts $\phi_l(\eta,\rho)$ are then calculated as functions of $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$, the regular and irregular Coulomb wave functions, respectively. The equations are as follows:

$$\begin{aligned} P_l &= \frac{\rho}{A_l^2} \\ S_l &= \frac{\rho}{A_l}\frac{\partial A_l}{\partial \rho} \\ \cos\phi_l &= \frac{G_l}{A_l} \\ \text{where} \quad & A_l^2 = F_l^2 + G_l^2 \end{aligned} \tag{D.83}$$

In Equation D.41, the Coulomb phase-shift difference w_c is required for charged-particle interactions. From Lane and Thomas [Reference 8], this quantity has the value

$$W_c = \begin{cases} 0 & l = 0 \\ \sum_{n=1}^{l} \tan^{-1}\left(\frac{\eta_\alpha}{n}\right) & l \neq 0 \end{cases} \tag{D.84}$$

D.2 The Unresolved Resonance Region (LRU=2)

Average resonance parameters are provided in File 2 for the unresolved region. Parameters are given for possible l and J-values (up to d-wave, $l = 2$) and the following parameters may be energy dependent: $D_{l,J}$, $\overline{\Gamma}^0_{nlJ}$, $\overline{\Gamma}_{\gamma lJ}$, $\overline{\Gamma}_{flJ}$, and $\overline{\Gamma}_{xlJ}$. The parameters are for the single-level Breit-Wigner formalism. Each width is distributed according to a chi-squared distribution with a designated number of degrees of freedom. The number of degrees of freedom may be different for neutron and fission widths and for different (l, J) values. These formulae do not consider Doppler broadening.

D.2.1 Cross Sections in the Unresolved Region

Definitions and amplifying comments on the following are given in Section D.2.2.

a. Elastic Scattering Cross Section

$$\begin{aligned}
\sigma_{n,n}(E) &= \sum_{l=0}^{\text{NLS}-1} \sigma^l_{n,n}(E), \\
\sigma^l_{n,n}(E) &= \frac{4\pi}{k^2}(2l+1)\sin^2\phi_l \\
&+ \frac{2\pi^2}{k^2}\sum_J^{\text{NJS}} \left[\frac{g_J}{\overline{D}_{l,J}} \left\langle \frac{\Gamma_n\Gamma_n}{\Gamma} \right\rangle_{l,J} - 2\overline{\Gamma}_{nl,J}\sin^2\phi_l \right].
\end{aligned} \tag{D.85}$$

The asymmetric term in $E - E'_r$ is assumed to average to zero under the energy-averaging denoted by $\langle\rangle$.

b. Radiative Capture Cross Section

$$\begin{aligned}
\sigma_{n,\gamma}(E) &= \sum_{l=0}^{\text{NLS}-1} \sigma^l_{n,\gamma}(E), \\
\sigma^l_{n,\gamma}(E) &= \frac{2\pi^2}{k^2}\sum_J^{\text{NJS}} \frac{g_J}{\overline{D}_{l,J}} \left\langle \frac{\Gamma_n\Gamma_\gamma}{\Gamma} \right\rangle_{l,J}
\end{aligned} \tag{D.86}$$

c. Fission Cross Section

$$\begin{aligned}
\sigma_{n,f}(E) &= \sum_{l=0}^{\text{NLS}-1} \sigma^l_{n,f}(E), \\
\sigma^l_{n,f}(E) &= \frac{2\pi^2}{k^2}\sum_J^{\text{NJS}} \frac{g_J}{\overline{D}_{l,J}} \left\langle \frac{\Gamma_n\Gamma_f}{\Gamma} \right\rangle_{l,J}.
\end{aligned} \tag{D.87}$$

The sum over l in the above equations extends up to $l = 2$ or NLS-1 (the highest l-value for which data are given). For each value of l, the sum over J has NJS terms. The number

of J-states for a particular l-state will depend on the value of l. NLS and NJS are given in File 2.

The averages are rewritten as:

$$\begin{aligned}
\left\langle \frac{\Gamma_n \Gamma_n}{\Gamma} \right\rangle_{l,J} &= \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{nl,J}}{\overline{\Gamma}_{l,J}} \right) R_{n,l,J} \\
\left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{l,J} &= \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{\gamma l,J}}{\overline{\Gamma}_{l,J}} \right) R_{\gamma l,J}, \\
\left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle_{l,J} &= \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{fl,J}}{\overline{\Gamma}_{l,J}} \right) R_{fl,J}
\end{aligned} \tag{D.88}$$

where $R_{\gamma l,J}$, $R_{fl,J}$ and $R_{nl,J}$ are width-fluctuation factors for capture, fission, and elastic scattering, respectively. Associated with each factor is the number of degrees of freedom for each of the average widths, and the integrals are to be evaluated using the MC^2-II method.

Data given in File 2 for each (l, J) state

$\mu_{nl,J} =$ AMUN, the number of degrees of freedom for neutron widths

$\mu_{fl,J} =$ AMUF, the number of degrees of freedom for fission widths

$\mu_{xl,J} =$ AMUX, the number of degrees of freedom for competitive widths

$\mu_{\gamma l,J} =$ AMUG, the number of degrees of freedom for radiation widths

$\overline{\Gamma}_{x,l,J} =$ GX, the average competitive reaction width

$\overline{\Gamma}^0_{n,l,J} =$ GN0, the average reduced neutron width

$\overline{\Gamma}_{\gamma,l,J} =$ GG, the average radiation width

$\overline{\Gamma}_{f,l,J} =$ GF, the average fission width

$\overline{D}_{l,J} =$ D, the average level spacing

The average neutron widths are defined in Section D.2.2.2, equation (D.98), where $\overline{\Gamma}_{nlJ} = \langle \Gamma_n(l, J) \rangle$. Degrees of freedom are discussed in Section 2.4.16.

The average total width, at energy E, is:

$$\overline{\Gamma}_{l,J} = \overline{\Gamma}_{nl,J} + \overline{\Gamma}_{\gamma l,J} + \overline{\Gamma}_{fl,J} + \overline{\Gamma}_{xl,J}, \tag{D.89}$$

and all widths are evaluated at energy E. J =AJ, I =SPI, and l=L are given in File 2. The penetration factors and phase shifts are functions of a or AP, as described earlier.

D.2.2 Definitions for the Unresolved Resonance Region

Editions of ENDF-102 prior to ENDF/B-V have had some errors in the "Definitions" section of Appendix D (previously Section D.2.1). To clarify the points and facilitate parallel reading with Gyulassy and Perkins, Reference 10, their parenthesized indices will be used. Section D.2.3 contains a table of equivalences to the notation used in section D.2.1.

D.2.2.1 Sums and Averages

In an energy interval $\Delta\varepsilon$, let the resonances be identified by a subscript $\lambda = 1, 2, \ldots$ which goes over all the resonances. The present discussion is concerned with the ***combinatorial*** aspects of level sequences, hence λ enumerates ***all*** the resonances, whether their widths are observably large or not. One purpose of this section is to permit estimation of missed resonances by comparing observed level densities or strength functions with the theoretically-expected relations. The latter are concerned with the set of all resonances, and not just those that are observable in a particular experiment.

Let x denote a set of quantum numbers that label a subset of resonances in the interval. If there are $N(x)$ such resonances, their level density is:

$$\rho(x) = N(x)/\Delta\varepsilon, \tag{D.90}$$

and their level spacing is:

$$D(x) = 1/\rho(x) \ . \tag{D.91}$$

If y_λ is some quantity associated with each resonance, λ, the sum of the y-values over the subset x is:

$$\sum_{\lambda}^{x} y_\lambda \ . \tag{D.92}$$

In this section, the summation index λ is written as a subscript, and the range of the summation is indicated by the superscript x. The expression in (D.92) says "sum the quantity y over every resonance in the interval $\Delta\varepsilon$, which has the quantum numbers x." Usually, these resonances will possess other quantum numbers too, but it is the set x which determines whether they are included or not.

An ***average*** of the quantity y over the set x is

$$\langle y \rangle^x = \frac{1}{N(x)} \sum_{\lambda}^{x} y_\lambda \tag{D.93}$$

D.2.2.2 Reduced Widths

In this section, reduced widths follow the experimental definition rather than the theoretical usage $\Gamma = 2P\gamma^2$. A partial width for the decay of a resonance into a particular channel carries many quantum numbers, but we need only three, the total and orbital angular momenta J and l, and the channel spin s. The reduced neutron width, $\Gamma^l_{n\lambda}(J, s)$, is defined by

$$\Gamma_{n\lambda}(l, J, s) = \Gamma^l_{n\lambda}(J, s)\sqrt{E}\ \nu_l(E) \tag{D.94}$$

where: $\nu_l = P_l/\rho$,
$\nu_0 = 1$,
$\nu_1 = \rho^2/(1+\rho^2)$
$\nu_2 = \rho^4/(9+3\rho^2+\rho^4)$
and $\rho = ka$, where a is the channel radius.

Assuming additivity of partial widths,

$$\Gamma^l_{n\lambda}(J) = \sum_s \Gamma^l_{n\lambda}(J,s) \tag{D.95}$$

where Σ_s is a summation over the 1 or 2 possible channel-spin values.

If we average over resonances, and assume that the average partial width is independent of channel spin,[2]

$$\left\langle \Gamma^l_n(J) \right\rangle = \sum_s \left\langle \Gamma^l_n(J,\not{s}) \right\rangle = \mu_{l,J} \left\langle \Gamma^l_n(J,\not{s}) \right\rangle \tag{D.96}$$

Equation (D.96) introduces the multiplicity $\mu_{l,J}$, which for neutrons can have the value 1 or 2, depending on whether the channel spin has one or two values. For $l = 0$, or $I = 0$, or $J = 0$, $\mu_{l,J} = 1$. In other cases, s can take on the values $I \pm 1/2$ subject to the additional vector sum

$$\vec{s} = \vec{l} + \vec{J} \tag{D.97}$$

which may again restrict $\mu_{l,J}$ to the value one.[3]

The other new notation is the line through the quantum number s, meaning that the quantity $\left\langle \Gamma^l_n(J,\not{s}) \right\rangle$ does not depend on the value of s. This is ***not*** the same as omitting s from the parentheses, since ***that*** defines the left-hand side quantity. This is the primary source of confusion in previous discussions. Since ν_l depends only on l,

$$\begin{aligned} \langle \Gamma_n(l,J) \rangle &= \langle \Gamma^l_n(J)\sqrt{E}\ \ \nu_l \rangle \\ &= \mu_{l,J} \langle \Gamma^l_n(J,\not{s})\sqrt{E}\ \ \nu_l \rangle \\ &= \mu_{l,J} \langle \Gamma^l_n(J,\not{s}) \rangle \overline{\sqrt{E}\ \nu_l} \end{aligned} \tag{D.98}$$

where the bar over $\sqrt{E}\ \nu_l$ denotes some average value appropriate to the interval.

D.2.2.3 Strength Function

The pole-strength function was originally introduced as an average over the R-matrix reduced widths for a given channel, γ_c^2. Using the experimental convention,

$$S(l,J,s) = \frac{\left\langle \Gamma^l_n(J,s) \right\rangle^{l,J,s}}{D(l,J,s)}. \tag{D.99}$$

[2]This is not true for the individual resonances.
[3]For example, if $I = 1/2$, $\mu_{1,2} = 1$.

Since the channel spin values are uniquely determined by J and l, together with the target spin I which is common to all the resonances, s is superfluous in defining the subset over which the average is taken, and:

$$S(l,J,s) = \frac{\left\langle \Gamma_n^l(J,s) \right\rangle^{l,J}}{D(l,J)}. \tag{D.100}$$

If the parity π were used as an explicit quantum number, l could be dropped:

$$S(l,J,s) = \frac{\left\langle \Gamma_n^l(J,s) \right\rangle^{J,\pi}}{D(J,\pi)}, \tag{D.101}$$

because l and π are equivalent for labeling resonances. That is, every resonance with a given J and π will have channels labeled by the same set of l-values, whether their partial widths are observably large or not. Some authors go one step further and drop π, so that J ***means*** J,π, but that is an invitation to confusion.

Expressing $S(l,J,s)$ as a sum over reduced widths gives

$$S(l,J,\not{s}) = \sum_{\lambda}^{l,J} \Gamma_{n\lambda}^l(J,s)/\Delta\varepsilon, \tag{D.102}$$

where we use the assumed independence of $\langle \Gamma_n^l(J,\not{s}) \rangle$ on s to get the same result on the left-handside.

The strength function $S(l,J)$ is defined as

$$\begin{aligned} S(l,J) &= \sum_s S(l,J,s) \\ &= \mu_{l,J} S(l,J,s) \end{aligned} \tag{D.103}$$

The corresponding sum and average forms are

$$\begin{aligned} S(l,J) &= \sum_{\lambda}^{l,J} \Gamma_{n\lambda}^l(J)/\Delta\varepsilon \\ &= \frac{\left\langle \Gamma_n^l(J) \right\rangle^{l,J}}{D(l,J)} \end{aligned} \tag{D.104}$$

The next "natural" summation would be to collect the different l-contributions to the total width, to form $S(J)$, but this is not what is observable. Instead one defines $S(l)$ as a weighted sum of the $S(l,J,s)$:

$$S(l) = \frac{\sum_{Js} g\ S(l,J,s)}{\sum_{Js} g} \tag{D.105}$$

This equation occurs in Lynn, Reference 1, as number (6.126), with a confusing typographical error, namely the index s is missing from $S(l,J,s)$.

Actually, the strength function was introduced first in the "s-wave" form:

$$S(0) = \sum_{\lambda(l=0)} \frac{g\,\Gamma_n^0}{D} \tag{D.106}$$

and later generalized by Saplakoglu et al. (Reference 11) to the p-wave form:

$$S(1) = \frac{1}{\Delta\varepsilon(2l+1)} \sum_{\lambda(l=1)} \left(g\,\Gamma_n^1\right)_\lambda . \tag{D.107}$$

For expository purposes, it is clearer to start from equation (D.105). The sum on J and s is for fixed l:

$$\sum_{Js} \equiv \sum_{s=I-\frac{1}{2}}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} . \tag{D.108}$$

It is important to note that the outer sum on channel spin is correct as written. It goes over the values $I \pm 1/2$ if $I \geq 1/2$, and over the single value $1/2$, if $I = 0$. It is ***not*** further constrained by equation (D.97) because now ***it*** is the "independent variable." The inner sum on J enumerates some J-values once, and some twice, the latter occurring when both s-values can produce that J-value. The number of times J occurs is the same $\mu_{l,J}$ that appeared previously.

If we are summing a quantity that is independent of s, then equation (D.108) can be rewritten:

$$\sum_{Js} y(\not{s}) = \widetilde{\sum_{l,J}} \mu_{lJ}\; y(\not{s}) \tag{D.109}$$

The multiplicity $\mu_{l,J}$ takes care of the sum on s, and the tilde over the sum on J, as emphasized by Gyulassy and Perkins, Reference 10, reminds us that J goes over its full range, "once-only":[4]

$$\begin{aligned} \widetilde{\sum_J} &= \sum_{J=\left|l-I-\frac{1}{2}\right|}^{l+I+\frac{1}{2}} \quad \text{if} \;\; l \geq I \\ &= \sum_{J=\left|I-l-\frac{1}{2}\right|}^{l+I+\frac{1}{2}} \quad \text{if} \;\; I \geq l \end{aligned} \tag{D.110}$$

The denominator in Equation (D.105) can be shown to be

$$\sum_{Js} g = 2l + 1 , \tag{D.111}$$

or, since g is independent of s,

$$\widetilde{\sum_J} \mu_{l,J}\; g = 2l + 1 . \tag{D.112}$$

[4]Reference 10 has this written incorrectly.

Gyulassy and Perkin (Reference 10) assume, and later approximately justify by comparison to experiment, that $S(l, J, \not{s})$ is also independent of J. With this, Equation (D.105) becomes:

$$\begin{aligned} S(l) &= \frac{1}{(2l+1)} \sum_{Js} g\, S(l, \not{J}, \not{s}) = S(l, \not{J}, \not{s}) \\ &= \frac{S(l, J)}{\mu_{l,J}}\,, \end{aligned} \tag{D.113}$$

using Equation (D.103).

Note the peculiar fact that $S(l)$ and $S(l, J, s)$ are independent of J, but $S(l, J)$ is not. This is a consequence of the fact that more than one channel spin value can contribute to $S(l, J)$, inducing a "J-dependence" in the form of a possible factor of two.

As a sum over resonances,

$$\begin{aligned} S(l) &= \frac{1}{(2l+1)} \sum_{Js} g\, S(l, \not{J}, \not{s}) \\ &= \frac{1}{(2l+1)} \sum_{Js} \sum_{\lambda(l,J)} g\, \Gamma^l_{n\lambda}(J, s)/\Delta\varepsilon \\ &= \frac{1}{(2l+1)} \widetilde{\sum_{J}} \sum_{\lambda(l,J)} g\, \Gamma^l_{n\lambda}(J)/\Delta\varepsilon \end{aligned} \tag{D.114}$$

The right hand side of equation (D.115) says to sum $\Gamma^l_{n(J)}$ over all possible values of J, which is what is meant by Equations (D.106) and (D.107). We can suppress the explicit J's and write, as in Equation (D.107),

$$S(l) = \frac{1}{\Delta\varepsilon(2l+1)} \sum_{\lambda(l)} \left(g\, \Gamma^l_{n\lambda}\right)_\lambda \tag{D.115}$$

but we have to remember that Γ^l_n is still $\Gamma^l_n(J)$, and not a new quantity.

As an average, using the same convention,

$$S(l) = \frac{1}{(2l+1)} \frac{\left\langle g\Gamma^l_n \right\rangle^l}{D(l)}. \tag{D.116}$$

Otherwise, all the notation is correct: $D(l)$ is the spacing of l-wave resonances without regard to their J-values, and the average $\langle\ \rangle^l$ goes over all resonances possessing the quantum number l, again without regard for their J-values. It is worth noting explicitly that although $S(l, J)$ is "almost" independent of J, this is not true of $\left\langle \Gamma^l_n(J) \right\rangle$. As Equation (D.104) shows, its J-dependence is canceled by the J-dependence of $D(l, J)$, up to the factor $\mu_{l,J}$. This property is what makes strength functions useful.

D.2.2.4 Level Spacings

Gyulassy and Perkin (Reference 10) emphasize that:

$$\rho(l) = \widetilde{\sum_{J}} \rho(l, J) \tag{D.117}$$

which, together with the assumption:

$$\rho(l, J) = K(l)(2J + 1) \tag{D.118}$$

leads to

$$\rho(l) = \rho(l, J)\frac{(2l + 1)}{g}\,\omega_{I,l}, \tag{D.119}$$

where

$$\begin{aligned} \omega_{I,l} &= (l + 1)/(2l + 1) \quad \text{for} \quad l \leq I \\ &= (I + 1)/(2I + 1) \quad \text{for} \quad l \geq I \end{aligned} \tag{D.120}$$

and is unity if $l = 0$ or $I = 0$.

The reader is referred to Reference 10 for a fuller discussion but here we can point out that, for a given parity, $\rho(l, J)$ is independent of l, by definition. As noted, every resonance with a given J and π has the same set of associated l-channels, whether it has an observable width or not. Hence:

$$\begin{aligned} \rho(0, J) &= \rho(2, j) = \rho(4, j) = \ldots \quad \text{and} \\ \rho(1, J) &= \rho(3, j) = \rho(5, j) = \ldots \end{aligned}$$

The further assumption of parity-independence makes $\rho(l, J)$ totally independent of l. As a result, Gyulassy and Perkin's $K(l)$ from Equation (D.118) is independent of l, and

$$\rho(l) = C(2l + 1)\,\omega_{I,l}, \tag{D.121}$$

where C depends on the nuclear species but not on any quantum numbers.

D.2.2.5 Gamma Widths

In the limited energy range usually covered by the unresolved resonance region, the gamma width may be assumed to be constant and equal to that obtained from an analysis of the resolved resonances. If, however, the energy range is rather wide, an energy dependence as given by some of the well-known theoretical models, Reference 1, may be built in. Since the observed gamma width is the sum of a large number of primary gamma transitions, each assumed to have a chi-squared distribution of $\mu = 1$, the sum is found to have a $\mu \geq 20$. In effect this implies that the gamma width is a constant, since a chi-squared distribution with a large number of degrees of freedom approximates a δ-function.

D.2.2.6 Degrees of Freedom

For the reasons enumerated for File 2 in Section 2.4.16, the following values should be used:

1. Neutron width, $1 \leq$ AMUN ≤ 2, and specifically, AMUN=$\mu_{l,J}$.

2. Radiation width, AMUG=0.

3. Fission width, $1 \leq$ AMUF ≤ 4, to be determined by comparison with experiment. Only integer values are permitted, although non-integers occur in some analyses.

4. Competitive width, $1 \leq$ AMUX ≤ 2, because only a single inelastic level excitation is permitted as a competitive reaction. Specifically, AMUX=$\mu_{l',J}$, where J is the spin of the resonance, and l' is the orbital angular momentum of the inelastically scattered neutron. Since the daughter nucleus may have a spin $\widetilde{I}$ different from the target spin I, l' may be different from l and the number of channel spin values $\mu_{l',J}$ may be different from $\mu_{l,J}$.

D.2.3 Equivalent Quantities in Sections D.1 and D.2

Symbol in Section			Definition
D.1	D.2.1	D.2.2	
r	-	λ	This is a non-equivalence. λ enumerates all resonances; r enumerates those within a subset and hence implies a set of quantum numbers.
Γ_{nr}		$\Gamma_{n\lambda}(l,J)$	The neutron width, summed over channel spin.
$\Gamma_{\gamma r}, \Gamma_{fr}, \ldots$		-	Not used in D.2.2, but the same implication of l, J holds.
P_l		$\rho\nu_l$	Penetration factor.
	$D_{l,J}$	$D(l,J)$	Average level spacing for a subset of resonances with given l and J.
	$\overline{\Gamma}^0_{nl,J}$	$\langle\Gamma^l_n(J)\rangle^{l,J}$	The l-wave reduced width, averaged over all resonances with given l and J.
	$\overline{\Gamma}_{nl,J}$	$\langle\Gamma_n(l,J)\rangle^{l,J}$	The average neutron width. In practice, the energy-dependence of this quantity is not averaged, but extracted before averaging.

D.3 The Competitive Width

D.3.1 Penetrability Factor for the Competitive Width in the Resolved Resonance Region

A. SLBW and MLBW

For these formalisms, the only physical situation which can be handled without approximation is that in which a ***single*** inelastic competitive process is possible, because the formalism presently permits the definition of only ***one*** additional quantity. The most common case will occur when inelastic scattering to the first excited state of the target nucleus is energetically possible. Ignoring, as in the case of elastic scattering, the possibility that the partial widths depend on channel spin, the penetrability is identical to that for elastic scattering,

but the energy is reduced by the excitation energy of the first excited state, corrected for recoil, so that

$$\Gamma_{xr}(E) = \Gamma_{n'r}(E) = \frac{P_l(E - E_1^*)\Gamma_{xr}(|E_r|)}{P_l(|E_r - E_1^*|)}, \quad \text{if} \quad E \geq E_1^* \tag{D.122}$$

and

$$\Gamma_{xr} = 0 \quad \text{if} \quad E < E_1^* \tag{D.123}$$

where E_1^* is (AWRI+1)/AWRI times the excitation energy of the first excited state, ($E_1^{ex} = -$QX in File 2).

This definition involves two conventions, both taken over from the elastic case. One is the way in which an "experimental" reduced width $\Gamma_{n'}^l$ is defined in terms of the theoretical reduced width γ^2, and the other is the way in which negative energy levels are treated. Neither of these problems arises in the theory, where $\Gamma = 2P\gamma^2$ and all quantities are defined in terms of the channel energy. Note that the l-value to be used in the penetrability is not that of the incident neutron, but of the "exit" inelastically scattered neutron.

It is conceivable that an (n,α) or (n,p) reaction to the ground state of the daughter nucleus could be open, without inelastic competition, in which case the formula for Γ_{xr} would be the same, but the P_l would be a Coulomb penetrability, and the excitation energy E_l^* would be replaced by the approximate Q-value and reduced mass. The R-Matrix Limited format allows for this possibility (see Section D.1.7), as well as for accurate treatment of the inelastic channels.

If more than one competitive process is energetically possible, then the SLBW and MLBW formats are inadequate to give the correct energy dependence of the competitive width, since they supply only one number, and a partial width is required for each process. For example, when two inelastic levels can be reached,

$$\Gamma_{xr}(E) = \frac{P_{l_1}(E - E_1^*)\Gamma_{n_1'r}(|E_r|)}{P_{l_1}(|E_r - E_1^*|)} + \frac{P_{l_2}(E - E_2^*)\Gamma_{n_2'r}(|E_r|)}{P_{l_2}(|E_r - E_2^*|)}, \tag{D.124}$$

with appropriate modification below each threshold. Note that the exit l-values are independent of the incident-neutron l-value.

For codes that presently approximate Γ as a constant in the denominator, a possible procedure is to substitute a step function:

$$\begin{aligned} \Gamma_{xr}(E) &= 0 && \text{if} \quad E < E_1^* \\ &= \Gamma_{xr}(|E_r|) && \text{if} \quad E \geq E_1^* \end{aligned}$$

and then make some provision to handle the resultant discontinuity in the cross section.

Users who are unable to handle this degree of complexity, and would like to use GT_r from File 2 as the total width without regard for whether the competitive process is energetically possible or not should at least be aware of the problem.

B. When the Adler-Adler and Reich-Moore formalisms are used for low-energy fissile materials, no recommendation concerning the treatment of Γ_{xr} need be given, and users can presume that it is zero. When Reich-Moore formalism is used above the thermal region, the same comments apply as for the SLBW/MLBW formalism.

C. The R-matrix Limited format (LRF=7) allows multiple reaction channels and multiple elastic channels as needed. Detailed formulae are given in Section D.1.7.

D.3.2 Penetrability Factor for the Competitive Width in the Unresolved Resonance Region

Since many codes treat the average total width in the denominator of expressions like $\langle \Gamma_n \Gamma_\gamma / \Gamma \rangle$ as an energy-independent constant, the penetrability factor of the competitive width needs to be handled by specifying energy-dependent unresolved resonance parameters.

The formalism, which is a simple average over SBLW line shapes, takes account of the energy-dependence of the neutron widths in the numerator, by extracting their penetrability factors before the averaging is done. These then contribute to the energy-dependence of the average cross section. The energy-dependence of the neutron width in the denominator, *i.e.*, in $\overline{\Gamma}$, is neglected. No such fix is readily available for the energy-dependence of the competitive width, whose penetrability factor will involve the threshold dependence of an inelastic cross section. The evaluator can circumvent this difficulty by specifying energy-dependent parameters and setting $\langle \Gamma_x \rangle = 0$ below its threshold; then allowing it to build up according to the formulas given in Section D.3.

The degrees of freedom, AMUX, should be 1.0 or 2.0. (See Section 2.4.16).

D.3.3 Calculation of the Total Cross Section when a Competitive Reaction is Specified

When a competitive reaction is specified for SBLW or MLBW and Γ exceeds the sum of the partials $\Gamma_n + \Gamma_\gamma + \Gamma_f$, the ENDF convention is that the scattering, capture, and fission cross sections will be calculated from the sum of File 2 and File 3 contributions, but the competitive reaction will be contained entirely in File 3, and no File 2 contribution should be added to it. The reason for this is that users can avoid problems in coding up resonant competitive widths. In the File 2 calculations, the correct total width Γ must be used in order to get the correct line shape.

This puts the ***total*** cross section in a special category. If it is calculated as the sum of σ_n, σ_γ, σ_f, σ_x, then the above prescription works satisfactorily. However, if it is calculated from the SLBW formula,

$$\sigma_{n,t}(E) = \frac{\pi}{k^2} \sum_J g_J \frac{\Gamma_{nr}\Gamma_r}{(E - E_{r'})^2 + \frac{1}{4}\left(\frac{\Gamma_r}{2}\right)^2} \tag{D.125}$$

as it is in some applications, then it will include the competitive reaction, and the user should not add the File 3 contribution to it. The ENDF convention presumes that $\sigma_{n,t}$ will be calculated by summing the partial reactions.

The R-matrix Limited format does not have this problem. The "competitive" reactions are treated normally, and File 2 and File 3 are added together for all reactions. That is because the total width is always the sum of the explicitly given partial widths. If a File 3 contribution were specified for the total cross section, then it would be added to the {1-ReU} calculation, but not to the sum-of-parts calculation, as the latter would already include the File 3 contribution for each partial reaction. This assumes that the File 3 total is the sum of the File 3 partials.

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Appendix E

Kinematic Formulas

The notation used to describe two-body kinematics is shown in Fig.E-1. The scattering treatment used for neutrons can be generalized to two-particle reactions by allowing the emitted particle mass to be different from the incident particle mass (*i.e.,* $m_3 \neq m_1$). Applying conservation of mass, energy, and momentum gives the following non-relativistic kinematic equations:

$$A = \frac{m_2}{m_1} \tag{E.1}$$

$$A' = \frac{m_3}{m_1} \tag{E.2}$$

$$\beta = \left(\frac{A(A+1-A')}{A'} \left[1 + \frac{1+A}{A} \frac{Q}{E_1} \right] \right)^{1/2} , \tag{E.3}$$

$$\gamma = \frac{A'}{A+1-A'} \beta , \tag{E.4}$$

$$\frac{\varepsilon_3}{\varepsilon_1} = \frac{A'}{A^2} \beta^2 , \tag{E.5}$$

$$\varepsilon_1 = \left(\frac{A}{A+1} \right)^2 E_1 , \tag{E.6}$$

$$\mu_3 = \mu , \tag{E.7}$$

$$\frac{\varepsilon_4}{\varepsilon_1} = \frac{A'}{A+1-A'} \frac{\varepsilon_3}{\varepsilon_1} , \tag{E.8}$$

$$\mu_4 = -\mu , \tag{E.9}$$

$$\frac{E_3}{E_1} = \frac{A'}{(1+A)^2} \left(\beta^2 + 1 + 2\beta\mu \right) , \tag{E.10}$$

$$\omega_3 = \frac{1+\beta\mu}{\sqrt{\beta^2+1+2\beta\mu}} , \tag{E.11}$$

$$\frac{E_4}{E_1} = \frac{A+1-A'}{(1+A)^2} \left(\gamma^2 + 1 - 2\gamma\mu \right) , \tag{E.12}$$

$$\omega_4 = \frac{1-\gamma\mu}{\sqrt{\gamma^2+1-2\gamma\mu}} . \tag{E.13}$$

If the incident and scattered particles are the same, $A' = 1$, and these formulas reduce to the familiar set used for neutron scattering. The elastic reaction corresponds to $A' = 1$ and $Q = O$.

According to these formulas, the secondary energy distribution of the emitted particle and the complete energy-angle distribution of the recoil nucleus are completely determined by A, A', Q, and the angular distribution for the emitted particle.

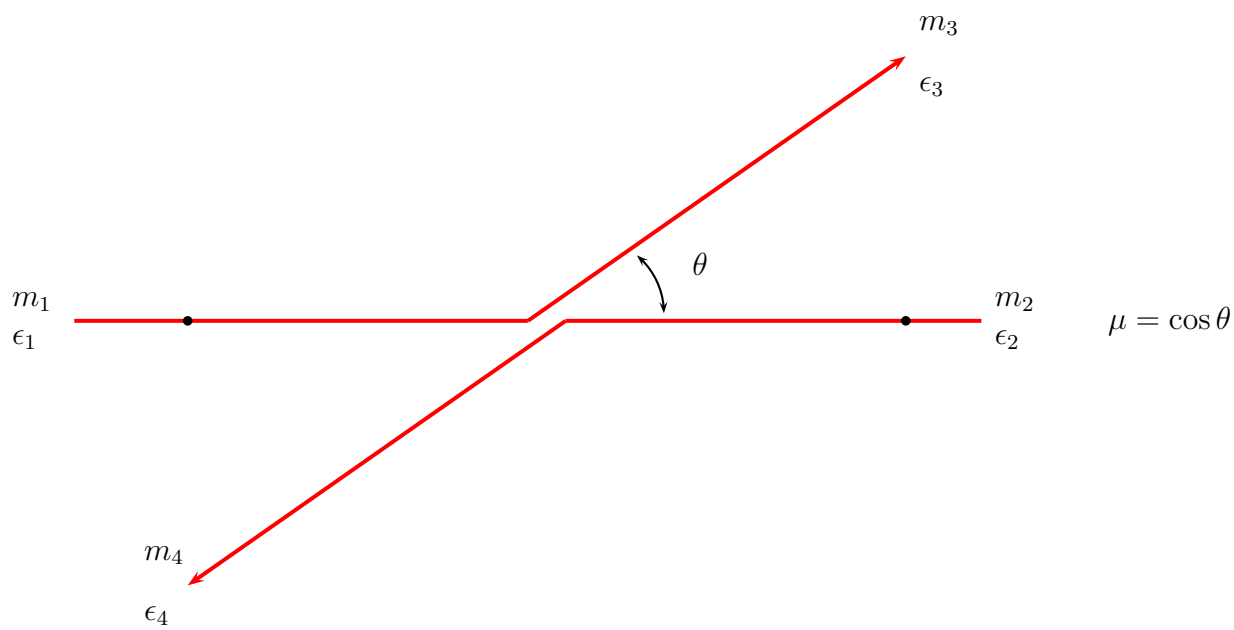

Figure E.1: Kinematics variables for two-particle reactions in the center-of-mass system.

When the masses are small and the energies large, or when either m_1 or m_2 is a photon, it is appropriate to use relativistic kinematics. A good example of the this is calculating the energy and emission angle for the photon from neutron capture on ^{1}H as the center of mass cosine μ varies over its range. Another example is the distributions for the products of the photo breakup of the deuteron. Define:

AWR	target mass ratio to the neutron,
AWRI	projectile mass ratio to the neutron,
AWRP	product mass ratio to the neutron, and
Q	reaction Q-value.

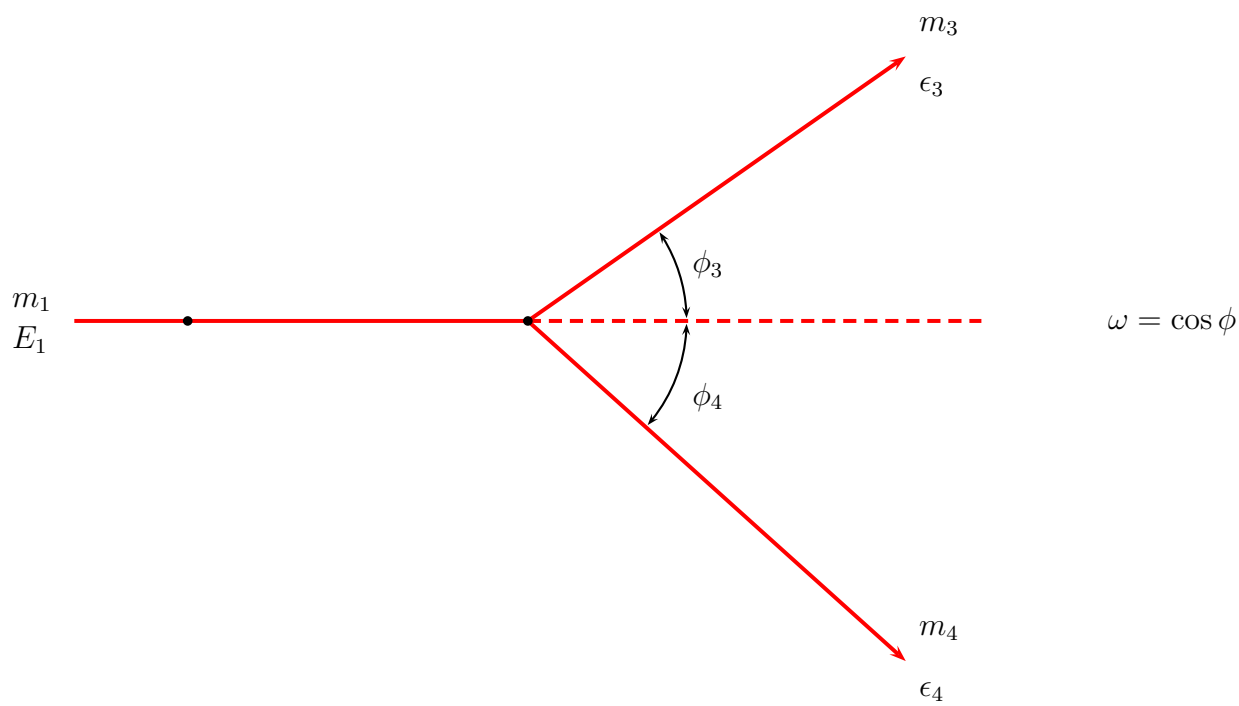

Figure E.2: Kinematics variables for two-particle reactions in the laboratory system.

The following equations can be used to compute the quantities shown in Figure E:

$$m = m_{\text{neutron}}\, c^2 \text{ in eV, see Appendix E.} \tag{E.14}$$

$$m_1 = \text{AWRI}_m \tag{E.15}$$

$$m_2 = \text{AWR}_m \tag{E.16}$$

$$m_3 = \text{AWRP}_m \tag{E.17}$$

$$m_4 = m_1 + m_2 - m_3 = Q \tag{E.18}$$

$$s_i = m_1 + m_2 \tag{E.19}$$

$$d_i = m_1 - m_2 \tag{E.20}$$

$$s_f = m_3 + m_4 \tag{E.21}$$

$$d_f = m_3 - m_4 \tag{E.22}$$

$$s = s_i^2 + 2m_2E_1 \tag{E.23}$$

$$k_i^2 = \frac{(s - s_i^2)(s - d_i^2)}{(4s)} \tag{E.24}$$

$$k_f^2 = \frac{(s - s_f^2)(s - d_f^2)}{4s} \tag{E.25}$$

$$z_2 = \sqrt{k_i^2 + m_2^2} \tag{E.26}$$

$$z_3 = \sqrt{k_f^2 + m_3^2} \tag{E.27}$$

$$z_4 = \sqrt{k_f^2 + m_4^2} \tag{E.28}$$

$$E_3 = \frac{z_2 z_3 - \sqrt{k_i^2 k_f^2 u}}{m_2} - m_3 \tag{E.29}$$

$$E_4 = \frac{z_2 z_4 - \sqrt{k_i^2 k_f^2 u}}{m_2} - m_4 \tag{E.30}$$

$$p_1^2 = E_1^2 + 2m_1 E_1 \tag{E.31}$$

$$p_1^2 = E_3^2 + 2m_3 E_3 \tag{E.32}$$

$$p_1^2 = E_4 + 2m_4 E_4 \tag{E.33}$$

$$\omega_3 = \frac{(E_1 + s_i)(E_3 + m_3) - z_3\sqrt{s}}{\sqrt{p1^2 p_3^2}} \tag{E.34}$$

$$\omega_3 = \frac{(E_1 + s_i)(E_4 + m_4) - z_4\sqrt{s}}{\sqrt{p1^2 p_4^2}} \tag{E.35}$$

where the k quantities are center-of-mass momenta, and the p quantities are lab momenta. The symbol z is used instead of the more conventional ω because of the conflict with the symbol used for laboratory cosines in Figure E.

Appendix F

Summary of Important ENDF Rules

F.1 General

1. Cross sections for all significant reactions should be included.
2. The data in an ENDF file are specified over the entire energy range 10^{-5} eV to 20 MeV. It should be possible to determine values between tabulated points with use of the interpolation schemes provided.
3. All cross sections are in barns, all energies in eV, all temperatures in degrees Kelvin, and all times in seconds.
4. Summary documentation and unusual features of the evaluation should appear in the File 1 comments.
5. Threshold energies and Q-values must be consistent for all data presented in different files for a particular reaction.

F.2 File 2 - Resonance Parameters

1. Only one energy region containing resolved resonance parameters can be used, if needed.
2. The cross sections from resonance parameters are calculated only within the energy range EL to EH, although some of the resonance parameters may lie outside the range.
3. Every ENDF Material has a File 2 even if no resonance parameters are given in order to specify the effective scattering radius.
4. In the unresolved resonance region interpolation should be done in the cross section space and not in the unresolved resonance parameter space. Any ENDF interpolation scheme is allowed.

5. The Breit-Wigner single-level or multilevel formalisms should be used in the resolved resonance region unless experimental data prove that use of the other allowed formalisms is significantly better.

F.3 File 3 - Tabulated Cross Sections

1. All File 3 data are given in the laboratory system.

2. The total cross section MT=1 is the sum of all partial cross sections and has an energy mesh that includes all energy meshes for partial cross sections.

3. The following relationships among MT numbers are expected to be satisfied if data are presented:
   1 = 2 + 3
   3 (or 1 - 2) = 4 (or 51→ 91) + (6→ 9+16) + 17 + 18
   (or 19→ 21+38) + (22→ 25) + (28→ 37)
   + (102→ 114)
   4 = sum (51→ 91)
   18 = sum (19→ 21) + 38
   101 = sum (102→ 114)
   103 = sum (700→ 718)
   104 = sum (720→ 738)
   105 = sum (740→ 758)
   106 = sum (760→ 778)
   107 = sum (780→ 798)

4. Threshold reactions begin with a zero cross sections at the threshold energy.

F.4 Relation Between Files 2 and 3

1. If there are resonance parameters in File 2, there are contributions to the total (MT=1) and scattering (MT=2) cross sections and to the fission (MT=18) and capture (MT=102) cross sections if fission and capture widths are also given. These must be added to the File 3 Sections MT=1, 2, 18, and 102 over the resonance region in order to obtain summation values for these cross sections.

2. The cross sections in File 3 for MT=1, 2, 18, and 102 in the resonance region are used to modify the cross section calculated from the resonance formalisms, if necessary. The File 3 "background" may be positive or negative or even zero if no modifications are required. <u>The summation cross section (File 2 + File 3) should be everywhere positive.</u>

3. Double-valued points (discontinuities) are allowed anywhere but are required at resonance region boundaries. A typical situation for MT=1, 2, 18, and 102 in File 3 is a tabulated cross section from 10^{-5} to 1 eV, tabulated "background" to the cross sections

calculated in the resolved resonance region between EL1 and EH1, tabulated "background" to the cross sections calculated in the unresolved region between EL2=EH1 and EH2, and tabulated cross sections from EH2 to 20 MeV. Double-value points occur at EL1, EL2, and EH2.

4. The tabulated "background" used in File 3 to modify the cross sections calculated from File 2 should not be highly structured or represent a large fraction of the cross sections calculated from File 2. It is assumed that the "background" cross section is assumed to be at 0 Kelvin. (The "background" cross section is usually obtained from room temperature comparisons, but this should be unimportant if the "background" cross section is either small or slowly varying).

5. The generalized procedure for Doppler-broadening cross sections from Files 2+3 is to generate a pointwise cross section from the resolved resonance region on an appropriate energy mesh at 0K and add it to File 3. This summation cross section can be kernel-broadened to a higher temperature.

F.5 File 4 - Angular Distributions

1. Only relative angular distributions, normalized to an integrated probability of unity, are given in File 4. The differential scattering cross section in barns per steradian is determined by multiplying File 4 values by the File 2+3 summation scattering cross section $\sigma_s/(2\pi)$.

2. Discrete channel angular distributions (*e.g.,* MT=2,51-90,701...) should be given as Legendre coefficients in the center-of-mass system, with a maximum of 64 higher order terms, the last being even, in the expansion. If the angular distribution is highly structured and cannot be represented by a Legendre expansion, a tabular angular distribution in the CM system must be given.

3. Angular distributions for continuum and other reactions must be given as tabulated distributions in the Lab system , unless they are given in File 6 .

4. The angular distribution, whether specified as a Legendre expansion or a tabulated distribution, must be everywhere positive.

5. Angular distribution data should be given at the minimum number of incident energy points that will accurately describe the energy variation of the distributions.

F.6 File 5 - Secondary Energy Distribution

1. Only relative energy spectra, normalized to an integrated probability of unity, are given in File 5. All spectra must be zero at the end points. The differential cross section in barns per eV is obtained by multiplying the File 5 values by the File 2+3 cross section times its multiplicity (2 for the (n,2n) reaction).

2. While distribution laws 1, 3, 5, 7, 9, and 10 are allowed, distribution laws 3 and 5 are discouraged but can be used if others do not apply.

3. The sum of all probabilities for all laws used for a particular reaction must be unity at each incident energy.

4. The constant U must be specified, where applicable, to limit the energy range of emitted spectra to physical limits.

Appendix G

Maximum Dimensions of ENDF Parameters

File (MF)	**Section (MT)**	**Variable**	**Max. value**	**Definition of the number represented by the variable**
1	451	NXC	350	Card images in directory
	452	NC	4	Polynomial terms in expansion of $\overline{\nu}$
	455	NCD	4	Polynomial terms in expansion of $\overline{\nu}_d$
	456	NCP	4	Polynomial terms in expansion of $\overline{\nu}_p$
2	151	NE	250	Energy mesh in unresolved region
		NER	12	Energy ranges
		NFRE	1	Fission reactions
		NGRE	1	Radiative capture reactions
		NIRE	4	Inelastic scattering reactions
		NCRE	4	Charged-particle reactions
		NIS	10	Isotopes
		NRS	5,000	Resonances for a given l-value
		NJS	6	Number of J-values
		NLS	4	Number of l-values
		NLCS	20	Number of l-values which must be given to converge reaction
3	All$\neq$4	NP	50,000	Incident energy points
4	All	NE	2,000	Incident energy points
		NL	64	Highest order Legendre polynomial
		NM	64	Maximum order Legendre polynomials required
		NP	201	Angular points
5	All	NE	200	Incident energy points
		NF	1,000	Secondary energy points
6	All	NK	2,000	Number of subsections
		NE	2,000	Incident energy points
		NL	64	Highest order Legendre polynomial
7	All	NS	3	Non-principal scattering atom types
9,10	1 $\neq 1$	NP NP	50,000 5,000	Energy points
14	All	NL	64	Highest order Legendre polynomial
All other	All	NP	10,000	Mesh size
All	All	NR	20	Interpolation ranges

Appendix H

Recommended Values of Physical Constants to be Used in ENDF

H.1 Sources for Fundamental Constants

The basic source for Fundamental Constants used by CSEWG in evaluating and processing ENDF data are the values reported in **1998 CODATA internationally recommended values of the Fundamental Physics Constants** (Source 1) as taken from the NIST Reference on Constants, Units, and Uncertainties Web site[1].

These are supplemented by the mathematical constants from **MathSoft**[2] (Source 2).

Atomic masses not given in the CODATA recommended values should be taken from the **Atomic Mass Tables** of G. Audi and A. Wapstra[3] (Source 3).

H.2 Fundamental Constants and Derived Data

Values of the Fundamental Physics Constants, as approved by CSEWG, are given in this Appendix. These values should be used until updates are approved by CSEWG.

Values for quantities which are derived from these fundamental constants, and which were previously given in the body of this manual, are also presented in this section with the expressions by which they have been replaced in the body of this Manual. These values may not appear in subsequent revisions of this Appendix.

[1] The information was prepared by P. J. Mohr and B. N. Taylor, "The 1998 CODATA Recommended Values of the Fundamental Physics Constants", Version 3.1, National Institue of Standards and Technology (December 1999). The Web site is located at http://physics.nist.gov/cuu/Constants/.

[2] The information was prepared by Steven Finch of MathSoft, Inc., for their Web site which is located at http://www.mathsoft.com/asolve/constant/constant.html.

[3] G. Audi, A. H. Wapstra and C. Thibault, The AME2003 atomic mass evaluation, Nucl. Phys. A. 729, 337 (2003). The Web site, maintained by the NNDC is located at "http://www.nndc.bnl.gov/masses/"

Table 1: Fundamental Constants

Expression	Definition	Numeric value	Source
e	natural logarithmic base	2.718 281 828 52	2
π	Archimedes' constant	3.141 592 653 59	2
e	elementary charge	1.602 176 462 $\times 10^{-19}$ C	1
$\alpha^{-1} = 10^7\hbar/(c\,e)$	inverse fine-structure constant	137.035 999 76	1
u	atomic mass unit (amu)	931.494 013 $\times 10^6$ eV / c^2	1
h	Planck's constant	4.135 667 27 $\times 10^{-15}$ eV s	1
$\hbar$	Planck's constant/2π (=$10^7\hbar$[erg.s]/e[C])	6.582 118 89 $\times 10^{-16}$ eV s	1
k	Boltzmann's constant	8.617 342 $\times 10^{-5}$ eV K^{-1}	1
c	speed of light (in vacuum)	299 792 458 m s^{-1}	1
N_A	Avogadro's number	6.022 141 99 $\times$ 10^{23} mol^{-1}	1

H.3 Use of Fundamental Constants by Code Developers

Code developers are encouraged to locate any values for fundamental physics constants that may be currently buried deep within their codes, and to replace these values by the expressions given here; the values would then be specified in only one location in the code. This ensures internal consistency, and expedites any necessary updates.

Code developers should double-check that numerical constants (e.g., π or e) are represented to a degree of accuracy consistent with the precision of the computers on which the codes are to be run.

In subsequent revisions of this manual, values for derived quantities may not be given. Instead, code developers should calculate those quantities by directly evaluating the expressions. This will ensure that values are as precise as the computer permits.

H.4 Use of Fundamental Constants by Evaluators

Evaluators should use the fundamental constants, mass numbers, Q-values, etc., as specified in this section, for evaluations submitted for acceptance by ENDF.

Evaluators are encouraged to specify values for "hidden" physical constants within the File 1 comments of the ENDF file in order to prevent future confusion in the event of changes in the accepted values.

The following table gives values which were previously given in the body of this Manual, along with the expressions which should be used in the future for these values. These expressions have been substituted for the values at the appropriate places in the Manual. **These values should not be used in any future applications; instead, please use the values for the Fundamental Constants as specified in this Appendix**. (For example for m_p/m_n, do not use 0.99862; use the value derived from the values for m_p and m_n).

Table 2. Masses

Expression	Definition	Numeric value	Source
m_n	neutron mass	1.008 664 915 78 amu	1
m_e	electron mass	5.485 799 110 $\times 10^{-4}$ amu	1
m_p	proton mass	1.007 276 466 88 amu	1
m_d	deuteron mass	2.013 553 212 71 amu	1
m_t	triton mass	3.015 500 713 amu	3
m_{3He}	^{3}He mass (hellion)	3.014 932 234 69 amu	1
m_α	α mass	4.001 506 1747 amu	1

Table 3. Energies needed to break particles into their constituent nucleons.

d	deuteron	2.22 MeV
t	triton	8.48 MeV
^{3}He	^{3}He	7.72 MeV
α	alpha	28.3 MeV

Table 5. Derived quantities whose values were formerly given in the body of the Manual

Location	Value previously given in the Manual	Units for value	Expression
page 0.18	0.998 62 1.996 26 2.989 60 2.989 03 3.967 13		m_p/m_n m_d/m_n m_t/m_n m_{3He}/m_n m_a/m_n
Page 4.7	3.0560 $\times 10^{-8}$	1 / (eV barn steradian)	$m_n u/(2h^2c^2) \times 10^{-28}$
Eq. (6.9)	4.784 53 $\times 10^{-6}$	$(10^{-12}\text{cm})^2$ eV / amu	$2u/(\hbar^2c^2)$
Eq. (6.10)	2.480 58 $\times$ 10^4	eV / amu	$u\alpha^2/2$
page D.3	2.196 771 $\times 10^{-3}$	10^{-12}cm $(\text{eV})^{-1/2}$	$\sqrt{2m_n}/\hbar$

Appendix I

A History of the ENDF System and its Formats and Procedures

Abstract

The following information provides a short historical record of the development of the data formats and procedures of the Evaluated Nuclear Data File (ENDF) from the first proposal of specifications in May 1966 to the ENDF/B-VI.8 release in 2001.

I.1 Introduction

The process of digesting experimental data, combining it with the predictions of nuclear model calculations and attempting to extract the true value of a cross section is referred to as an evaluation.

Historically, individual laboratories around the world had prepared evaluated nuclear data, e.g., neutron-cross sections, for their use in nuclear reactor calculations. These laboratories stressed their own needs for materials, cross section types and energy ranges depending upon their specific applications. Each of these laboratories developed their own methods for the storage and retrieval of these data.

In addition, it was noted that some neutron transport programs had built-in neutron cross-section libraries that could not be modified. As a result, reactor designers could not use new cross-section data, which in some cases had been available for more than half a decade [1].

There were fairly detailed nuclear data libraries available by 1963, the United Kingdom Nuclear Data Library (UKNDL) from Ken Parker at the Atomic Weapons Research Establishment, Atomic Energy Authority in Aldermaston, UK, the fast reactor data library from Joe Schmidt at the Institute for Neutron Physics and Reactor Technology, Nuclear Research Center, Karlsruhe, Germany, the NDA library from Herb Goldstein at Nuclear Development Associates, in New York, and the Evaluated Nuclear Data Library (ENDL) from Bob Howerton at the Lawrence Radiation Laboratory in Livermore, California to name just a few.

At the 1961 Vienna Conference on the Physics of Fast and Intermediate Reactors, Ken Parker [2] indicated some of the requirements for the neutron cross section libraries. They had to specify reaction processes available or else a zero value cross section would automatically be assumed. There had to be a simple presentation of the data on punched cards, which would be easy to revise. However, the data could not be revised frequently or the reactor designers would be unable to perform comparative calculations, as they made design revisions. There was a need to cross check the data for errors and the best data should provide reasonable answers for simple systems, such as bare reactor cores.

At the 1964 Geneva Conference on Peaceful Uses of Atomic Energy, John Story [3] from the Atomic Energy Establishment, Winfrith, UK, defined a data file as a complete set of evaluated cross section data for a single material and a data library as data files for a number of materials.

The various data libraries that were available often gave different answers, when the libraries were used to calculate the same reactor configuration. However, dissimilarities in the internal formats of the various libraries made it difficult to understand why these differences occurred.

There was a need for a common file between these existing systems, which would allow for an inter-comparison of these libraries. The stimulus for action came from a discussion among Henry Honeck of Brookhaven National Laboratory, Al Henry of Westinghouse and George Joanou of General Atomics at the Colony Restaurant in Washington, D.C. The Reactor Mathematics and Computation (RMC) Division of the American Nuclear Society (ANS) was requested to sponsor two meetings to discuss this common link, as a result of the above discussion. Honeck as chairman of the Division's sub-committee on Evaluated Nuclear Data Files held some meetings. A group of eighteen representatives from fifteen US laboratories met in New York City on July 19, 1963 to review cross section libraries and discuss means for interchanging these libraries. A sub-committee was appointed to meet in Hanford on September 18-20, 1963 to examine library formats in more detail.

The conclusions of these discussions were that there was a need for a standard format for evaluated nuclear data and the format should be as flexible as possible so that existing libraries could be translated into the standard format and that future needs could be easily incorporated into the file. This standard format would serve as a link between a data library and the processing codes. It was also suggested that a center should be established and charged with the development and the maintenance of the Evaluated Nuclear Data File (ENDF) and with the collection and distribution of data.

A preliminary report of the detailed formats for ENDF was sent for review and comment. Twenty-two people attended a final meeting at Brookhaven on May 4-5, 1964 to discuss changes and settle on a final version. The description of this system (which was labeled Version A and referred to as ENDF/A) was documented in the report BNL-8381 [4]. The ENDF/A file originally contained an updated version of the UKNDL library as well as evaluated data from a number of different laboratories.

The reactor designer wants evaluated data for all neutron-induced reactions covering the full range of incident neutron energies for each material in a reactor. However, evaluators usually supply "bits and pieces", which are put together to form a fully evaluated set for a given material. ENDF/A provides a storage system for these "bits and pieces" or partial

evaluations.

In addition to the need to allow all nuclear data evaluations to be placed on a common basis, there was also a need for an evaluated nuclear data file to be used for reactor design calculations. The description of this system (which was labeled Version B and referred to as ENDF/B) was documented in the report BNL-50066 [5].

Where the format of ENDF/A was highly flexible in order to accept data in almost any arrangement or representation, the format of ENDF/B had to be simple to facilitate the writing of processing programs to use the data. This new ENDF/B library format would be mathematically rigorous, with specific interpolation schemes between tabulated points, so that cross section integrals, products and ratios would yield well-defined and repeatable results. There would be codes developed for plotting, integration and other processing of cross sections that would be written in FORTRAN for computer interchangeability and distributed to assist others who wanted to use ENDF data.

A material was defined as either an isotope or a collection of isotopes with a material number designated by the symbol MAT. The data for a material is divided into files with the file number designated by the symbol MF. A file is subdivided into sections, each containing data for a particular reaction, where the reaction type is designated by the symbol MT.

File 1 was for general information. File 2 contained information on resolved and unresolved resonance parameters. File 3 contained information on smooth cross sections. File 4 contained information on secondary angular distributions. File 5 contained information on secondary energy distributions. File 6 contained information on secondary energy-angle distributions. File 7 contained information on the thermal neutron scattering law.

I.1.1 ENDF/B-I

Version I of the ENDF/B data file was released in July 1968. As mentioned above, the description of the formats and procedures are documented in BNL-500665.

File 1 had a Hollerith description in Section 1, neutron multiplicity in Section 2, radioactive decay data in Section 3 and fission product yield data in Section 4.

File 2 used two energy ranges, one for resolved and one for unresolved parameters.

File 3 limited quantities to 500 points, except for the scattering cross section where 2000 points were allowed. Temperature dependence was ignored, except for thermal cross sections.

File 4 would contain mostly data for elastic scattering. Some data may be given for inelastic or total reaction in the thermal range and may be temperature dependent.

File 5 should have data for inelastic, (n,2n), (n,3n) and fission reactions if smooth cross sections for these reactions are given in File 3.

The evaluations for ENDF/B-I were taken from the existing evaluations of neutron interactions for 58 materials and converted into the ENDF format. The emphasis in this version was to create the necessary infrastructure to support the library system.

I.1.2 ENDF/B-II

Version II of the ENDF/B data file was released in August 1970. The description of the formats and procedures for the neutron data are documented in BNL-50274 [6]. The formats

and procedures for photon production and interaction data are documented in LA-4549 [7].

The File 1 changes included the following. An index was added to MT = 451 (general information). Each record in the index contained a file number (MF), reaction type number (MT) and the number of card images required to specify the data for each section for the material. The format for specifying radioactive decay data (MT = 453) was extensively modified. The format for specifying fission product yield data (MT = 454) was modified to allow specification of yield data for meta-stable states. A new section was defined to contain data for delayed neutrons from fission (MT = 455).

The File 2 changes included the following. The test, LRF, which indicated the type of resolved resonance formula used, was expended to include, LRF = 1, single level Breit-Wigner parameters; LRF = 2, multi level Breit-Wigner parameters; LRF = 3, R-Matrix, Reich-Moore multi level parameters and LRF = 4, Adler-Adler multi level resonance parameters are given. All materials will contain a File 2. For those materials where resolved and/or unresolved resonance parameters are not given, File 2 will contain the effective scattering radius, AP. The previous test, LIS, has been removed, where LIS = 0 indicated the scattering cross section should be calculated from resonance parameters plus the smooth cross section from File 3. This meant that the elastic scattering cross section would always be calculated using the resolved and unresolved resonance parameters. The constant C (used to calculate the penetration factor) was replaced by a quantity AWRI. AWRI is defined as the ratio of the mass of a particular isotope to that of a neutron. An option, LRU=2, was added for specifying the unresolved resonance parameters, so that all average resonance parameters could be given as a function of incident neutron energy. Energy dependent parameters could be given for each l-J state.

The File 3 changes included the reaction Q-value was defined as the kinetic energy (in eV) released by a reaction (positive Q values) or required by a reaction (negative Q values). The threshold energy (negative Q only) is given by

$$E_{\text{th}} = |Q|(AWR + 1)/AWR\,, \tag{I.1}$$

where AWR is the atomic weight ratio given on the HEAD record. The maximum number of allowed energy points per section was increased from 2,000 to 5,000. An initial state indicator was added to the HEAD record. This will allow the inclusion of cross section data for meta-stable states and more than one section may be given for the same reaction type (MT number).

No changes in File 4.

File 5 changes included the following. The definition of LF=3 (discrete energy loss law) was changed to read

$$F(E \to E') = \delta[E' - E\{(A^2 + 1)/(A + 1)^2\} + A/(A + 1)]\theta\,,$$

where $A = AWR$ and θ is the level excitation energy (positive value). T and LT have been removed from the TAB1 records that contain $p(E)$ for cases in which LF = 5, 7, or 9. A value, U, replaces T. U was introduced to define the proper upper limit for the secondary neutron energy distributions so that

$$0 \leq E' \leq E - U\,,$$

Old MT Number	New MT Number
5	51
6	52
7	53
8	54
9	55
10	56
11	57
12	58
13	59
14	60
15	91
27	No longer used
29	No longer used
51	61
52	62
53	63
-	-
-	-
80	90
109 (Not assigned)	109 (n,3) cross section
455 (Not assigned)	455 delayed neutron from fission
700-799 (not assigned)	700-799 assigned (see appendix B)

where E', E, U are given in the laboratory system. Further, the normalization constants for LF = 7 and LF = 9 have been redefined to account for the use of U. LF = 2, 4, 6, and 8 have been deleted.

For all files, certain reaction type (MT) numbers have been changed:

The format for specifying temperature dependent data has been modified so that the data for the second (and higher) temperatures may be given at a lesser number of points than was given for the first temperature.

This version included evaluations for neutron reactions with fission product nuclei and data for various components of the energy release in fission.

I.1.3 ENDF/B-III

Version III of the ENDF/B data file was released in late 1972. There was no formal documentation of the formats and procedures for this version of ENDF prepared and published.

For the first time, the "standard" cross sections for neutron-induced reactions were identified. A special purpose "Standard Library" was created and sent to the IAEA for worldwide distribution. A special purpose library for Dosimetry cross sections was created. New fission product cross sections were added to improve calculations of decay heat.

I.1.4 ENDF/B-IV

Version IV of the ENDF/B data file was released in February 1975. The description of the formats and procedures are documented in BNL-NCS-50496 [8].

A general change in this version was in the energy range for general-purpose materials, where the range covered energies from 10^{-5} eV up to 20 MeV.

The File 1 changes included a change in the formats for specifying radioactive decay. Section MT = 453 was changed to include only production of radioactive nuclides and section MT = 457 was added to include radioactive decay data. Section MT = 456 was added to supply data for the number of prompt neutrons per fission (ν_p).

The File 3 changes included the energy mesh for the total cross section must include the energy meshes for partial cross sections. Time sequential (n,2n) reactions are described by using sections MT = 6-9 and MT = 46-49. An LR flag was added to designate x in the (n,n′) reactions when x is not a photon. In this case, the temperature field S (formerly T) is used to designate the Q-value or energy difference of the combined reactions. Sections MT = 718, 738, 758, 778, 798 and MT = 719, 739, 759 779 and 799 are redefined to describe continuum levels for (n, x′) reactions. MT = 718 describes the (n,p'_c) continuum cross sections as part of the (n,p) cross section and should be included in the total cross section. MT = 719 is used to describe a continuum cross section for exit protons, whose cross section is already represented in the total cross section by other types.

Until ENDF/B-IV, the only method available to evaluators to communicate uncertainty information was through the documentation [9]. Francis Perey designed the first data covariance format, which was approved by CSEWG in May 1973 and revised in December 1973.Three general-purpose evaluations for C, for ^{14}N and for ^{16}O, were released with covariance files.

I.1.5 ENDF/B-V

Version V of the ENDF/B data file was released in June 1979, which was subsequently named Version V.0. Version V.1 was released in 1983 and Version V.2 was released in January 1985. The description of the formats and procedures are documented in BNL-NCS-50496, edition 2 [10].

The File 1 changes included the following. The HEAD card of MT = 451 was changed. NXC, the number of dictionary entries, had been moved to the sixth field of the hollerith LIST record of MT = 451. Field 5 now contained NLIB, the library identifier, and field 6 now contained NMOD, the material modification number. Following the HEAD card of MT = 451 is a new CONT card, which contains information about the excitation energy, stability, state number, and isomeric state number of the target nucleus. In the LIST record of MT = 451, the LDD and LFP flags have been abolished. The number of dictionary entries, NXC, is now in the sixth field of the first card in this LIST record. The fourth field on each dictionary card in MT = 451 is now used to indicate the modification status (MOD) for the section described by the card. Radioactive decay data (MT = 453 and 457) have been removed from File 1. Entirely new formats have been devised and the radioactive decay data is given in MF = 8, MT = 457. The fission product yields section (MT = 44) has been removed from File 1. Fission product yield information is now given in File 8 using

new formats. A new section to describe energy release in fission (MF = 1, MT = 458) has been implemented.

The File 2 changes included the restriction that the Reich-Moore resonance parameter representation is no longer permitted in ENDF/B, only in ENDF/A.

The File 3 changes included the following. The total "gas production" MT's have been defined for H(203), D(204), T(205), He-3(206) and He-4(207). The non-elastic cross section (MT = 3) is now optional and no longer required since total gamma ray production must be entered in File 13 and never as multiplicities in File 12.

The file 4 changes include a simplified format using a new flag, LI, has been introduced to indicate that all angular distributions for an MT are all isotropic.

The File 5 changes include only the distribution laws for LF = 1, 5, 7, 9 and 11 are now allowed. LF = 11 is a new format for an energy dependent Watt spectrum.

The File 8 changes include the following. Information may be given for any MT specifying a reaction in which the end product is radioactive. The MT section contains information about the end product and how it decays. Files 9 and 10 may be used to give the cross section for the production of the end product. Fission product yield information is given under MT = 454 and 459. The format has been modified to include the 1 σ uncertainty of the yields. MT = 454 is for independent yields and MT = 459 is for the cumulative yields. The spontaneous radioactive decay data is given in MT = 457. This is an entirely new format.

The file 9 and 10 changes include the following. Isomer production is described in the new File 9 or File 10. In File 9, the cross sections are obtained by use of multiplicities. In File 10, the absolute cross sections are given.

The File 17 and 18 changes are the following. Formats for time dependent photon production data files have been defined. They may be used in ENDF/A only.

The Files 19, 20, 21 and 22 changes are the electron production data files have been implemented.

The Files 31, 32 and 33 changes are the formats for data co-variance files first introduced in Version IV have been extensively modified and expanded. They are now included in this document for the first time. Twenty-four materials and reactions are available in ENDF-V format containing co-variance files.

The Department of Energy put restrictions on the distribution of the library for the first time. This version was the first to have the evaluation of standards completed in advance of the evaluation of other materials.

I.1.6 ENDF/B-VI

Version VI of the ENDF/B data file was released July 1990, which was subsequently named Version VI.0. Version VI.1 was released in September 1991 and contained corrective revisions. Version VI.2 was released in June 1993 and provided new evaluations for 24 isotopes. Version VI.3 was released in May 1995 and contained new evaluations for 11 materials, with some evaluations extending in neutron energy to 40 MeV. This was the first attempt to include high-energy evaluations. Version VI.4 was released in December 1996 and was mainly a corrective revision of Version VI.3. Version VI.5 was released over 1997-1998 and

included 14 new evaluations, as well as two proton-induced files and one deuteron-induced file. Version VI.6 was released over 1998-1999 and included 33 evaluations with a neutron energy range from 20 MeV to 150 MeV, as well as 33 proton-induced evaluations up to 150 MeV. Version VI.7 was released over 1999-2000 and included 17 new evaluations of fission products, as well as general-purpose evaluations. Finally, Version VI.8 was released in 2001 and included 8 new evaluations and 33 evaluations, which were modified to include thermal neutron photon production data. The description of the formats and procedures are documented in BNL-NCS-44945 [11].

The File 3 changes include the following. The limit on the number of energy points (NP) is changed from 10,000 to 50,000 points.

The file 4 changes include the following. The highest order Legendre polynomial (NL), (given at each energy) is 64.

The File 5 changes include the following. There is a correction of the LF = 1 example, so that all secondary energy distributions start and end with zero values for the distribution function.

The File 6 changes include the addition of the reference system for secondary energy and angle, LCT = 3, for the center of mass system for both angle and energy of light particles ($A \leq 4$), laboratory system for heavy recoils ($A > 4$). This is for use in continuum energy-angle distribution when Kalbach-Mann systematics are not used, LANG$\neq$2.

I.1.7 ENDF/B-VII

The general-purpose evaluated nuclear data file, ENDF/B-VII.0, was released in December 2006 [12]. The major advances over the ENDF/B-VI.8 library are new cross sections for actinide isotopes, more precise standard cross sections, improved thermal neutron scattering, more extensive neutron fission product cross sections, photonuclear reactions, extension of evaluations to 150 MeV, new light element reactions, post-fission beta-delayed photon decay spectra, new radioactive decay data, some sample covariance evaluations and new actinide fission energy deposition. The library is in the same ENDF-6 format as the earlier ENDF/B-VI library.

I.2 Status of ENDF Versions and Formats

In order to summarize the status of the various versions of ENDF that have been released with the formats and procedures and their documentation, which have been referenced above, we have the following short list.

- ENDF/B.I was released in ENDF-1 format [5].
- ENDF/B.II and ENDF/B.III were released in ENDF-2 format [6, 7].
- ENDF/B.IV was released in ENDF-4 format [8].
- ENDF/B.V was released in ENDF-5 format [10].
- ENDF/B.VI and ENDF/B.VII were released in ENDF-6 format [11].

I.3 CSEWG

The recommendation from the original discussion on ENDF for a center to maintain the File was met by the assignment of the task to the Brookhaven National Laboratory's Nuclear Data Center. The group that would undertake to develop ENDF/B was called the Cross Section Evaluation Group (CSEWG). It was organized under the sponsorship of the Division of Reactor Development and Technology of the U. S. Atomic Energy Commission (AEC). The first meeting was held at BNL on June 9-10, 1966, where representatives of sixteen laboratories attended the meeting. A list of materials was submitted for which data were needed. Laboratories volunteered to take responsibility for complete evaluations of materials important to their own laboratory's programs.

At the following CSEWG meeting on November 14-16, 1966, material evaluations had already been submitted and progress had been made to couple ENDF format to data library preparation programs for reactor physics calculations. Several CSEWG subcommittees were started that would provide guidance for the development of ENDF/B. One of these first subcommittees created was that of Codes and Formats. Its mission was to make all necessary revisions to assure compatibility of edit and retrieval codes with the ENDF/B and provide guidance for future code development.

I.3.1 Codes and Formats Subcommittee Leadership

- Henry Honeck (SRL), from November 1966 to September 1969
- Robert Dannels (WNES), from November 1969 to December 1973
- Donald Mathews (GA), from December 1973 to May 1976
- Raphael LaBauve (LANL), from May 1976 to May 1980
- Raphael LaBauve (LANL) and Robert Roussin (ORNL), from May 1980 to October 1995.

Starting in 1995, the activity level of CSEWG had dwindled and the subcommittee structure was abandoned. Individuals were assigned the responsibilities originally given to the subcommittees.

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