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Informal Report

ENDF-102
DATA FORMATS AND PROCEDURES FOR THE EVALUATED NUCLEAR DATA FILE ENDF-7

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Written by the Members
of the

Cross Section Evaluation Working Group

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TABLE OF CONTENTS

Introduction to the ENDF System
- **0.2. Philosophy of the ENDF System**
- **0.3. General Description of the ENDF System**
- **0.4 Contents of an ENDF Evaluation**
- **0.5 Reaction Nomenclature - MT**
- **0.6 Representation of Data**
- **0.7 General Description of Data Fromats**
- **0.8 References for Chapter 0**

1. File 1. GENERAL INFORMATION
- **1.1. Descriptive Data and Dictionary (MT = 451)**
- **1.2 Number of Neutrons per Fission, $\bar{\nu}$ (MT = 452)**
- **1.3. Delayed Neutron Data, $\overline{\nu_d}$ (MT = 455)**
- **1.4. Number of Prompt Neutrons per Fission, $\overline{\nu_p}$ (MT = 456)**
- **1.5. Components of Energy Release Due to Fission (MT = 458)**

2. File 2. RESONANCE PARAMETERS
- **2.1 General Description**
- **2.2 Resolved Resonance Parameters**
- **2.3 Unresolved Resonance Parameters**
- **2.4 Procedures for the Resolved and Unresolved Resonance Regions**
- **2.5 References for Chapter 2**

3. File 3. NEUTRON CROSS SECTIONS
- **3.1 General Description**
- **3.2 Formats**
- **3.3 General Procedures**
- **3.4 Procedures for Incident Neutrons**
- **3.5 Procedures for Incident Charged Particles and Photons**

4. File 4. ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES
- **4.1 General Description**
- **4.2 Formats**
- **4.3 Procedures**
- **4.4 Procedures for Specific Regions**

5. File 5. ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES
- **5.1 General Description**
- **5.2 Formats**
- **5.3 Procedures**
- **5.4 Additional Procedures**

6. File 6. PRODUCT ENERGY-ANGLE DISTRIBUTIONS
- **6.1 General Description**
- **6.2 Formats**
- **6.3 Procedures**

7. File 7. THERMAL NEUTRON SCATTERING LAW DATA
- **7.1 General Description**
- **7.2 Coherent Elastic Scattering**
- **7.3 Incoherent Elastic Scattering**
- **7.4 Incoherent Inelastic Scattering**

8. File 8. RADIOACTIVE DECAY DATA
- **8.1 Radioactive Nuclide Production**
- **8.2 Fission Product Yield Data (MT = 454 and MT = 459)**
- **8.3 Radioactive Decay Data (MT = 457)**

9. File 9. MULTIPLICITIES FOR PRODUCTION OF RADIOACTIVE ELEMENTS
- **9.1 General Description**
- **9.2 Formats**
- **9.3 Procedures**

10. File 10. CROSS SECTIONS FOR PRODUCTION OF RADIOACTIVE NUCLIDES
- **10.1 General Description**
- **10.2 Formats**
- **10.3 Procedures**

11. GENERAL COMMENTS ON PHOTON PRODUCTION

12. File 12. PHOTON PRODUCTION MULTIPLICITIES AND TRANSITION PROBABILITY ARRAYS
- **12.1 Formats**
- **12.2 Procedures**

13. File 13. PHOTON PRODUCTION CROSS SECTIONS
- **13.1 Formats**
- **13.2 Procedures**
- **13.3 Preferred Representations**

14. FILE 14. PHOTON ANGULAR DISTRIBUTIONS
- **14.1 Formats**
- **14.2 Procedures**

15. File 15. CONTINUOUS PHOTON ENERGY SPECTRA
- **15.1 Formats**
- **15.2 Procedures**

23. File 23. "SMOOTH" PHOTON INTERACTION CROSS SECTIONS
23.1 General Comments on Photon Interaction
23.2 General Description
23.3 Formats
23.4 Procedures

26 File 26 SECONDARY DISTRIBUTIONS FOR PHOTO- AND ELECTRO-ATOMIC DATA
26.1 General Description
26.2 Formats

27. File 27. ATOMIC FORM FACTORS OR SCATTERING FUNCTIONS
27.1 Formats
27.2 Procedures

28. File 28. ATOMIC RELAXATION DATA
27.1 Atomic Relaxation
27.2 General Description
27.3 Formats
27.4 Procedures

30. INTRODUCTION TO COVARIANCE FILES
30.1 File 30. Data Covariances Obtained from Parameter Covariances and Sensitivities
30.2 Formats
30.3 Additional Procedures
30.4 Multigroup Applications of Parameter Covariances

31. File 31. COVARIANCES OF THE AVERAGE NUMBER OF NEUTRONS PER FISSION
31.1 General Description
31.2 Formats
31.3 Procedures

32. File 32. COVARIANCES OF RESONANCE PARAMETERS
32.1 General Description
32.2 Formats
32.3 Procedures

33. File 33. COVARIANCES OF NEUTRON CROSS SECTIONS
33.1 General Description
33.2 Formats
33.3 Procedures

34. File 34. COVARIANCES FOR ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES
34.1 General Description
34.2 Formats
34.3 Procedures

35. File 35. COVARIANCES FOR ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES
35.1 General Description
35.2 Formats
35.3 Procedures

40. File 40. COVARIANCES FOR PRODUCTION OF RADIOACTIVE NUCLEI
40.1 General Description
40.2 Formats
40.3 Procedures

APPENDIX

A. Glossary
B. Definition of Reaction Types
C. ZA Designations of Materials and MAT Numbers
D. Resonance Region Formulae
E. Kinematic Formulas
F. Summary of Important ENDF Parameters
G. Maximum Dimensions of Important ENDF Parameters
H. Fundamental Constants

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List of Laboratories Currently Participating in CSEWG

ANL	Argonne National Laboratory
BET	Bechtel Bettis Inc.
BNL	Brookhaven National Laboratory
CE	ABB Combustion Engineering
CRNL	Atomic Energy of Canada Ltd., Chalk River Nuclear Laboratories
DNSB	Defense Nuclear Facilities Safety Board
DOE	U. S. Dept. of Energy
GA	General Atomics
INEL	Idaho National Engineering & Environmental Laboratory
KAPL	Knolls Atomic Power Laboratory, Inc.
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
LSU	Louisiana State University
NIST	National Institute of Standards and Technology
ORNL	Oak Ridge National Laboratory
PNL	Pacific Northwest National Laboratory
RPI	Rensselaer Polytechnic Institute
SNL	Sandia National Laboratories
TSI	TSI Research Corp.
WES	Westinghouse Electric Corp.
WSRC	Westinghouse Savannah River Company

DATA FORMATS AND PROCEDURES FOR THE EVALUATED NUCLEAR DATA FILE

0. ENDF-6 PREFACE

This update to revision 4/01 of "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF" pertains to the version 6 of the ENDF formats. The seventh version of the ENDF/B library, ENDF/B-VII, uses these formats.

Below is a list of changes to the formats and procedures that appear in this edition. In addition, some typographical error corrections 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 2004

Section	Page	Update
0.	0.5	Added table of library numbers (NLIB)
	0.23-.25	Recommended two-dimensional interpolation procedures (M. Greene)
1.	1.7-.8	Energy dependent delayed-group constants added.
2.		Miscellaneous corrections and updates (C. Lubitz).
		Updates for 2 channel spins (N. Larson, C. Lubitz).
4.	4.1-.4	Removed elastic transformation matrix (C. Dunford)
		Increase to 2000, the number of energies for which angular distributions are given (JEFF)
		Increase to 201, the number of angles at which a tabular distribution can be given for an incident energy. (JEFF)
6.	6.3-.4	Allow NA=2 for Kalbach-Mann parameterization (JEFF)
	6.6	Equation 6.4 corrected (JENDL)
	6.10	Add LTP=15 interpolation for ratio to Rutherford scattering (JENDL)
	6.12	Revised equation in laboratory frame for LAW=6 (M. Greene)
7.	7.2,7.4	Corrected incoherent inelastic scattering equations (C. Lubitz)
8.	8.9	Added section for stable nucleus (JEFF)
9.	9.1-.2	Added final product identifier, IZAP (JEFF)
10.	10.1-.2	Added final product identifier, IZAP (JEFF)
Appendix D		Replaced Section D.3.1 (C. Lubitz).
Appendix F		Corrected limit on number of Legendre coefficients
Appendix G		Increased limits of number of incident energies and number of angles per incident energy in File 4, 6 and 14
		Increased the number of allowed subsections in File 6

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,1 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 (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. In addition, this rewrite represents an extensive update to the Version V manual.2

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 required data are not available for 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 cross-section data, combining them with the predictions of nuclear model calculations, and attempting to extract the true value of a cross section. 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***.

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1 See page vi for a list of present and former members of CSEWG.

2 ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF/B-V, BNL-NCS-50496 (ENDF-102), edited by R. Kinsey, 1979. (Revised by B. Magurno, November 1983).

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 may only need a minor isotope for determining 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 version.

0.2.3. Choices of Data

The data sets contained on 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 (1) new significant experimental results become available, (2) integral tests show that the data give erroneous results, or (3) user's 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

NNDC maintains a library for experimentally measured nuclear reaction data (CSISRS). In addition to the data, the CSISRS library contains bibliographic information, as well as details about the experiment (standard, 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 database via the World Wide Web or using the NNDC Online Data Service.3 Alternately, the data may be requested from the NNDC, and transmitted in the form of listings, plots, and/or files, which may be formatted to satisfy most needs.

0.2.5. Processing Codes

Once the evaluated data sets have been prepared in ENDF format, they can be converted to forms appropriate for testing and actual applications using processing codes. Processing codes that generate group-averaged cross sections for use in neutronics calculations from the ENDF library have been written. These codes4 include such functions as resonance reconstruction, Doppler broadening, multigroup averaging, and/or rearrangement into specified interface formats.

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3 C.L. Dunford, T.W. Burrows, Online Nuclear Data Service, NNDC/ONL-99/3, periodically updated.

4 D.E. Cullen, The 1996 ENDF Pre-Processing Codes (PREPRO96), report IAEA-NDS-39, Rev. 9, 1996
R. E. MacFarlane, D. W. Muir, The NJOY Nuclear Data Processing System, Version 91, report LA-12740-M, October 1994.

The basic data formats for the 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 a library. Phase 1 testing uses a set of utility codes[5] maintained by NNDC 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] 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 0.8) 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. Parameters are written in the form of FORTRAN variables (that is, integers start with 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 will be found in Appendix A (Glossary).

0.3.1. Library Organization

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.

Library	NLIB	a collection of evaluations from a specific evaluation group (*e.g.*, NLIB 0=ENDF/B).
Version	NVER	one of the periodic updates to a library in ENDF format (*e.g.*, NVER 6=ENDF/B-VI). A change of version usually implies a change in format, standards, and procedures. A revision number is appended to the library/version name for each succeeding revision of the data set; for example, ENDF/B-VI.2. There is no parameter for the revision number in the format.

5 C. L. Dunford, ENDF Utility Codes Release 6.11, April 1999. Available on the NNDC Web page.

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

Sublibrary	NSUB	set of evaluations for a particular data type, (*e.g.*, 4=radioactive decay data, 10=incident-neutron data, 12=thermal neutron scattering data). (See Table 0.1 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 = ENDF-6).
Material	MAT	the target in a reaction sub-library, or the radioactive (parent) nuclide in a decay sub-library; see Section 0.3.2.
Mod	NMOD	"modification" flag; see Section 0.3.3.
File	MF	subdivision of a material (MAT); each file contains data for a certain class of information (*e.g.*, MF=3 contains reaction cross sections, MF=4 contains angular distributions). MF runs from 1 to 99. (See Table 0.2 for a complete list of assigned MF numbers).
Section	MT	subdivision of a file (MF) ; each section describes a particular reaction or a particular type of auxiliary data (*e.g.*, MT=102 contains capture data). MT runs from 1 to 999. (See Appendix B for a complete list of assigned MT numbers).

0.3.2. Library (NLIB)

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 the table below.

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 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
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)

0.3.3. Material (MAT)

A ***material*** is defined as either an isotope or a collection of isotopes. It 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 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.[7]

The assignment of MAT numbers for ENDF/B-VI 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 (*Z*01-*Z*99) have been allocated to each element Z, through Z = 98. Natural elements have MAT numbers *Z*00. 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.[8] 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 *Z*25 so that the formulation can easily accommodate all the neutron excess nuclides.

For the special cases of elements from einsteinium to lawrencium (Z≥99) MAT numbers 99*xx* are assigned, where *xx* = 20, 25, 20, l5, and l2 for elements 99 to 103 respectively, one covers the 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).

0.3.4. Material modification (MOD)

All versions of a data set (*i.e.*, the initial release, revisions, or total re-evaluations) are indicated using the material "modification" flags. 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 235U. After checking and testing, the evaluator feels that the data set is satisfactory and 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. After the file is released, user Y retrieves MAT 9228 from the Center's files, adds it to his ENDF library as material 9228, and refers to it in later processing programs by this number. Should the evaluation of material 9228 subsequently be revised and released with CSEWG's approval, the

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7 The strategy for assigning MAT numbers for ENDF/B-VI is described here; other libraries may have different schemes.

8 This procedure leads to difficulty for the nuclides of xenon, cesium, osmium, platinum, *etc*., where more than 100 MAT numbers could be needed to include all isotopes.

material will have a 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. Contents of an ENDF Evaluation

As described above, sub-library (NSUB) and material (MAT) specify the target and projectile for a reaction evaluation or the radioactive nuclide for a decay evaluation. MF and MT indicate the type of data represented by a section and the products being defined.

The sub-library distinguishes between different 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 for ENDF-6 are listed in Table 0.1.

Table 0.1

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
...			
20040	2004	0	Incident-Alpha data

The files (MF) allowed are summarized in Table 0.2, and their use in the different sub-libraries is discussed following.

Table 0.2
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

The following MF numbers have been retired: 16, 17, 18, 19, 20, 21, 22, 24, 25.

0.4.1. Incident-Neutron Data (NSUB 10)

The procedures for describing neutron-induced reactions for ENDF/B-VI 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 can be given to describe the number of neutrons produced per fission and the energy release from fission.

A File 2 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 is always given. The required energy range is from the threshold or from 10-5eV to 20 MeV, but higher energies are allowed. There is a section for each important reaction or sum of reactions. The MT numbers for these sections are chosen based on the emitted particles as described in Section 0.5 (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 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 and 2.4.21.)

Distributions for emitted neutrons and other particles or nuclei are given using File 4, Files 4 and 5, or File 6. As described in more detail below, 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 for A(n,2n) is two and the yield of the product A-1 is one. If File 6 is used, all yields are explicit. This is convenient for computing gas production and transmutation cross sections. Explicit yields for radioactive products may be given in File 9, or 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 when strong resonances are present (*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 0.5.9.

When File 6 is used to represent neutron and charged-particle distributions for a reaction, it should also be used for the corresponding photon distribution. 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 0.5.9.

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

0.4.2. Thermal Neutron Scattering (NSUB 12)[9]

Thermal neutron scattering data 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[10] 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 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

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9 Used with IPART=0 only.

10 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).

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.

0.4.3. 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 neutron-induced fission product yields, and for yields from spontaneous fission. The format also allows for future photon- and charged-particle-induced fission. 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 8.2, the format for these two sections is identical. Covariance data for File 8 are self-contained.

0.4.4. 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 are given in File 5. The File 5 formats are the same as for 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 8.3). Finally, covariance data for the spectra in File 5 may be given in File 35; covariance data for File 8 are self-contained.

0.4.5. Photo-Nuclear (NSUB=0) and Charged-Particle (NSUB≥10010) 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 0.5. 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 will give 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 6.2.1.)

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

0.4.6. Photo-Atomic Interaction Data (NSUB 3)

Incident photon reactions with the atomic electrons11 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 a File 23 for photon interaction cross sections, and File 27 for atomic form factors.

0.4.7. 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.

0.4.8. Atomic Relaxation Data (NSUB=6)

The target atom can be left in an ionized state due to a variety of different types of interaction, 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, a File 28 is given containing the relaxation data for all the subshells defined in the photo-atomic or electro-atomic sublibraries.

0.4.9. Energy and Angular Distributions of Reaction Products (Files 4, 5, and 6)

Several different options are available in the ENDF-6 format to describe the distribution in energy and angle of reaction products. In most cases, the double differential cross section of the emitted particle in barns/(eV-sr) is represented by

$$\sigma(\mu, E, E') = \sigma(E) y(E)\ f(\mu, E, E') / 2\pi \tag{0.1}$$

where μ is the cosine of the emission angle,
E is the energy of the incident particle,
E' is the energy of the emitted particle,
$\sigma(E)$ is the reaction cross section,
$y(E)$ is the yield or multiplicity of the emitted particle, and
$f(\mu,E,E')$ is the normalized distribution function in (eV-unit cosine)-1.

For simple two-body reactions, the energy of the emitted particle can be determined from kinematics (see Appendix E); therefore,

$$f(\mu, E, E') = f(\mu, E)\ \delta(E' - \xi) \tag{0.2}$$

11 D.E. Cullen, *et al*., Tables and Graphics of Photon-Interaction Cross Sections from 10 eV to 100 GeV. Derived from the LLNL Evaluated Photon Data Library (EPDL). UCRL-50400, Vol. 6 Rev. (October 1989)

where ξ is defined by Eq. (E.5) in Appendix E.

The distribution function $f(\mu,E)$ can be given as a section of File 4 with no corresponding section in File 5, or as a section of File 6 with no corresponding sections in Files 4 or 5. For simple continuum reactions, the full distribution is sometimes given as a product of an angular distribution and an energy distribution:

$$f(\mu, E, E') = f(\mu, E)\, g(E, E') \tag{0.3}$$

The angular function is given in File 4, and $g(E,E')$ is given in File 5. This simple continuum format does not allow adequate description of energy-angle correlations, and it can only describe one emitted particle. Emitted photons can be described by this scheme also, but the files used are 14 and 15.

For the more complex reactions, the full distribution function is given in File 6. This file allows for all reaction products to be described, and it allows for energy-angle correlation of the emitted particles.

0.5. Reaction Nomenclature - MT

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

0.5.1. 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 Section 23). For incident neutrons, the elastic scattering cross section is determined from File 3 together 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).

0.5.2. 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:

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 a typical range, 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. The elastic reaction uses MT=2 as described above; 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 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 follow.

Reaction	**MT**
$^{9}Be(\alpha,n_0)^{12}C$	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.

0.5.3. 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:

MT	Emitted Particles	MT	Emitted Particles
11	2nd	36	nt2α
16	2n	37	4n
17	3n	41	2np
22	na	42	3np
23	n3a	44	n2p
24	2na	43	npα
25	3nα	108	2α
28	np	109	3α
29	n2α	111	2p
30	2n2α	112	t2α
32	nd	113	d2α
33	nt	114	pd
34	n^3He	115	pt
35	nd2α	116	dα

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 $d+t \rightarrow n+\alpha$ must be classified as the reaction $^{3}H(d,n)^{4}He$ (MT=50) rather than the reaction $^{3}H(d,n\alpha)$ (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, File 6 is preferred because it is possible to describe energy-angle correlations resulting from pre-equilibrium effects and to give distributions for more than one kind of particle. Using File 6 also makes it possible to give an energy distribution for the recoil nucleus. This distribution is 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. Similarly, if File 6 is used to describe the outgoing particle, the photons should also be given in File 6 under the same MT number, or under MT=3, if necessary. However, it often will be necessary to use the nonelastic MT=3 as described below.

For charged-particle sub-libraries, File 6 must be used for these reactions. Photons should be given in File 6 using the reaction MT number when possible. If the photons cannot be assigned to a particular reaction, the nonelastic MT=3 can be used as described below.

0.5.4. 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. This approach provides a 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

Reaction	**MT**
$^{3}H(t,n_0)^{5}He(n\alpha)$	50
$^{6}Li(d,n_3)^{7}Be(^{3}He\alpha)$	53
$^{7}Li(n,n_c)^{7}Li(t\alpha)$	91
$^{7}Li(t,2n)^{8}Be(2\alpha)$	16
$^{7}Li(p,d_1)^{6}Li(d\alpha)$	651
$^{9}Be(a,n_3)^{12}C(3\alpha)$	53
$^{16}O(n,n_6)^{16}O(\alpha)^{12}C$	56

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,

$^{12}C(n,n')^{12}C(3\alpha)$
$^{12}C(n,\alpha)^{9}Be(n2\alpha)$

or $^{7}Li(t,2n)^{8}Be(2\alpha)$
$^{7}Li(t,n)^{9}Be(n2\alpha)$
$^{7}Li(t,\alpha)^{6}He(2n\alpha)$
$^{7}Li(t,n\alpha)^{5}He(n\alpha)$

The evaluator either must 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,

$^{6}Li(d,p_4)^{7}Li(t\alpha)$ $E_x = 7.47$ MeV,
$^{6}Li(d,p_4)^{7}Li(n^{6}Li)$.

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(X).

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(t,α) Ex = 7.4700 MeV, MT=604,
^{6}Li(d,p$_5$)^{7}Li(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.

0.5.5. LR Flags

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.

LR	Meaning
0	Simple reaction. Identity of 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:

Reaction	MT	LR
$^{6}Li(n,n_1)^{6}Li(d\alpha)$	51	32
$^{7}Li(n,n_c)^{7}Li(t\alpha)$	91	33
$^{10}B(n,n_{12})^{10}B(d2\alpha)$	62	35
$^{12}C(n,n_2)^{12}C(3\alpha)$	52	23
$^{16}O(n,n_1)^{16}O(e^{+}e^{-})^{16}O$	51	40
$^{16}O(n,n_6)^{16}O(\alpha)^{12}C$	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.

0.5.6. 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, $^{6}Li(d,X)$.

0.5.7. Radiative Capture

The radiative capture reaction is identified by MT=102. For neutron sublibraries, the only product is 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 $d+t\rightarrow\gamma+n+\alpha$, which is written as a breakup reaction $^{3}H(d,\gamma)^{5}He(n\alpha)$ 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.

0.5.8. Fission

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

MT	Meaning	Description
18	fission	total
19	f	first chance fission
20	nf	second chance fission
21	2nf	third chance fission
38	3nf	fourth chance fission
452	$\bar{\nu}$T	total neutrons per fission
455	$\bar{\nu}$d	delayed neutrons per fission
456	$\bar{\nu}$p	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 is also given to contain the sum of the partial reactions.

0.5.9. 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 0.5.2, MT=4, 103, 104, 105, 106, and 107 can also be used as summation reactions for photon production in Files 12 and 13.

0.5.10. Special Production Cross Sections

A special set of production cross sections are provided, mostly for use in derived libraries.

MT	Meaning
201	neutron production
202	photon production
203	proton production
204	deuteron production
205	triton production
206	3He production
207	a 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:

$$MT207 = MT107 + 3 \times MT91.$$

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 a particle yield of 1.0. These MT numbers will ordinarily be used in File 3 of special gas production libraries.

0.5.11. 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. The following additional values are defined

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 * ξ. 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 Section 30.

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.

0.5.12. Sum Rules for ENDF

A number of ENDF reaction types can be calculated from other reactions. The rules for these summation reactions follow.

MT	Meaning: components
1	Total cross sections (incident neutrons only): 2, 4, 5, 11, 16-18, 22-26, 28-37, 41-42, 44-45, 102-117.
4	Total of neutron level cross sections: 50-91
18	Total fission: 19-21, 38.
103	Total of proton level cross sections: 600-649
104	Total of deuteron level cross sections: 650-699
105	Total of triton level cross sections: 700-749
106	Total of 3He level cross sections: 750-799
107	Total of alpha level cross sections: 800-849

The nonelastic cross section (MT=3) is only used in connection with photon production. It contains the following MT numbers: 4, 5, 11, 16-18, 22-26, 28-37, 41-42, 44-45, 102-117.

0.6. Representation of Data

0.6.1. Definitions and Conventions

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

Parameters	Units
energies	electron volts (eV)
angles	dimensionless cosines of the angle
cross sections	barns
temperatures	Kelvin
mass	in 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

$$ZA = 1000.0 * Z + A ,$$

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.12 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.

0.6.1.0. 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≤2) should be expressed in nuclear mass units. For neutrons, this ratio is 1.00000. For charged particles likely to appear in ENDF/B-VI, see Appendix H.

0.6.2. 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" 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.

12 See Appendix H for neutron mass.

0.6.2.1. One-dimensional Interpolation Schemes

Consider how a simple function *y(x)*, which might be a cross section, σ(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 Fig. 0.1 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 allowed interpolation schemes are given in Table 0.3.

Table 0.3
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 Fig. 0.1).

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

$$\sigma = \frac{A}{E}\exp\left[-\frac{B}{\sqrt{E-T}}\right] \tag{0.4}$$

where T=0 for exothermic reactions (Q>0) and T is the kinematic threshold for endothermic reactions (Q≤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

$$B = \frac{\ln \dfrac{\sigma_2 E_2}{\sigma_1 E_1}}{\dfrac{1}{\sqrt{E_1 - T}} - \dfrac{1}{\sqrt{E_2 - T}}} \tag{0.5}$$

and

$$A = \exp\left[\frac{B}{\sqrt{E_1 - T}}\right]\sigma_1 E_1 \tag{0.6}$$

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.

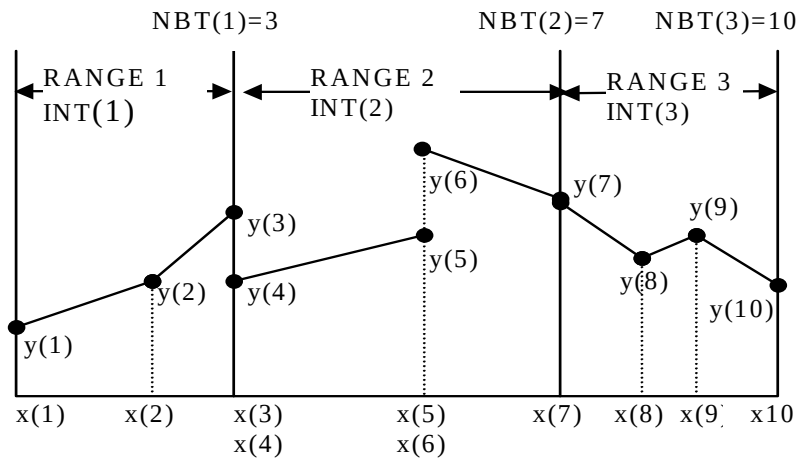
Next consider an energy distribution represented as a two-dimensional function of E and E' $f(E,E')$. Using a simple Cartesian interpolation, the function is represented by a series of tabulated functions $f(E,E')$. The simple "graph paper" rules are used for interpolating for $f(E')$ at each El. An additional interpolation table is given for interpolation between these values to get the result at E.

Distributions usually show ridges that cut diagonally across the lines of E and E'. An interpolation scheme is required that merges smoothly between adjacent distributions without generating the spurious bumps often seen when interpolation along the Cartesian axes E and E' is used.

The first non-Cartesian scheme allowed is the method of corresponding points. Given distributions for two adjacent incident energies, $f(E_i,E'_{ik})$ and $f(E_j,E'_{jk})$, the interpolation takes place along the line joining the kth points in the two functions. When the E′ grids are different and the grid points are well chosen, this interpolation scheme is analogous to following the contours on a map. Of course, if the E' grids are the same for E_i and E_j, this method is exactly equivalent to Cartesian interpolation. The method of corresponding points is selected by using INT=11-15, where the transformed values follow the interpolation laws INT=1-5, respectively.

The second non-Cartesian interpolation scheme allowed is unit-base interpolation. The spectra at E_i and E_{i+1} are transformed onto a unit energy scale by dividing each secondary energy by the respective maximum energy. The interpolation is then performed as in the Cartesian method, and the resulting intermediate spectrum is expanded using the maximum energy obtained by interpolating between the end points of the original spectra. The unit-base option is selected by using INT=21-25, where the transformed values follow the interpolation laws INT=1-5, respectively.

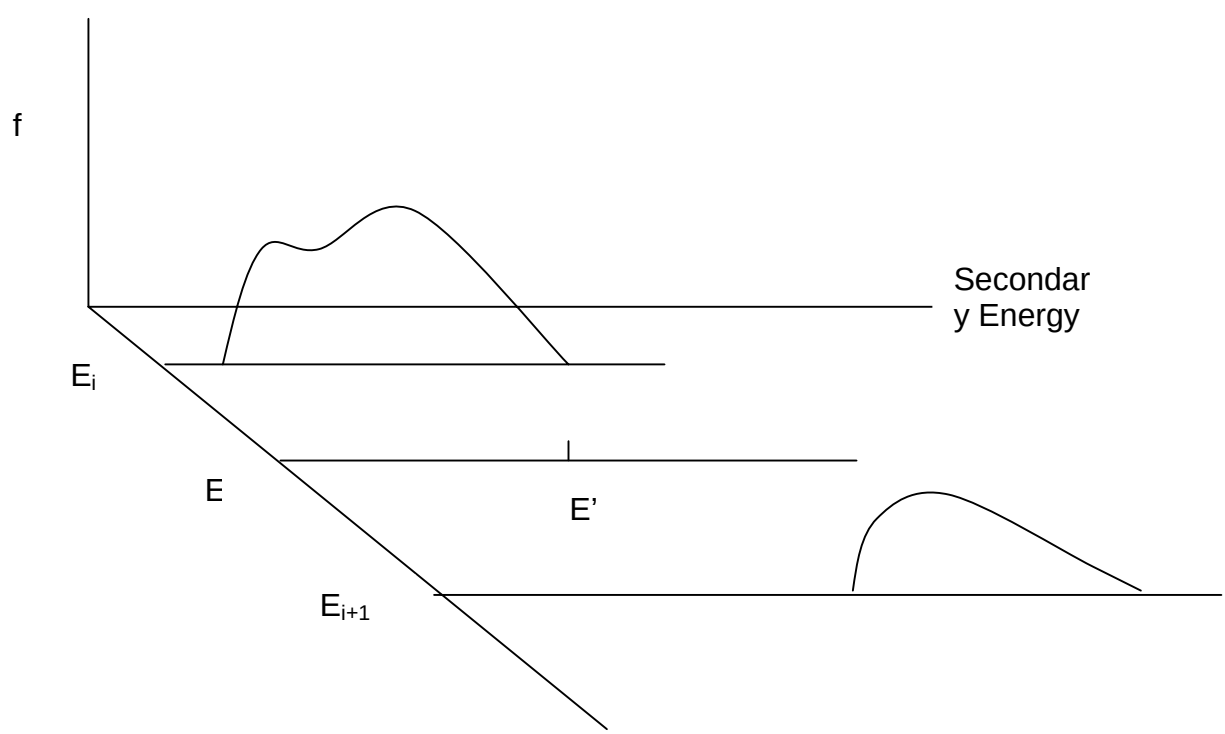
Figure 0.1
Interpolation of a Tabulated One-dimensional Function
Illustrated for the Case NP=10, NR=3



0.6.2.1 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 or corresponding energies.

Figure 0.2
Interpolation between Two-Dimensional Panels



Consider Figure 0.2. Here E is the ini **Initial** here are panels at E_i and E_{i+1}. The panels describe the probabilities of scattering from these energies to other energies; e.g., $f(E_i, E')$ and 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:

$$f(E, E') = f(E_i, E') + \frac{E - E_i}{E_{i+1} - E_i}[f(E, E') - f(E_i, E')] \tag{0.7}$$

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.

$$x \equiv \frac{E' - E_i'(1)}{E_i'(N) - E_i'(1)} \tag{0.8}$$

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 Eq. (0.7) 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.,

$$\int dE' \; f(E') = \int dx \; g(x) \tag{0.9}$$

which requires $f(E')dE' = g(x)dx$, or $g(x) = f(E')\left|\frac{dE'}{dx}\right|$. The latter radical is the Jacobian that is required for the transformation to the unit-base space and is determined from Eq. (0.8). In other words, when Eqn. (0.7) 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: 1) if the end points of two panels are the same, unit-base transform is exactly equivalent to Cartesian interpolation, and 2) 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

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

(0.10)

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.

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

(0.11)

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 Eqn (0.12) shown below.

The secondary energy at E_i that corresponds to an E' at E is calculated from

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

(0.12)

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 Eqn. (0.7) (or other 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.

0.7. General Description of Data Formats

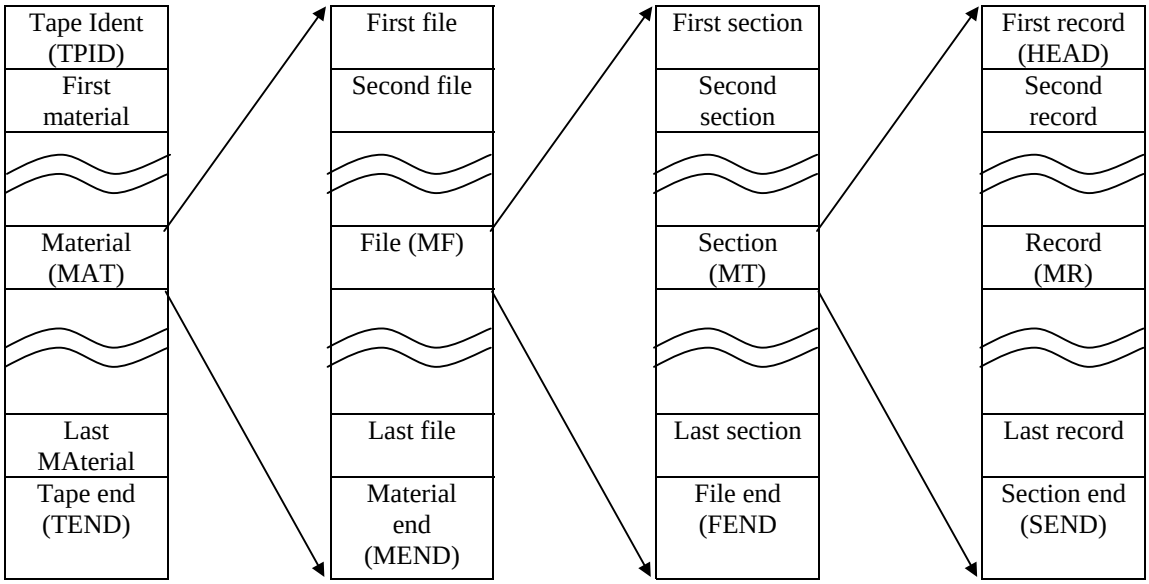
An ENDF "tape" is built up from a small number of basic structures called "records," such as TPID, TEND, CONT, TAB1, and so on. These "records" normally consist of one or more 80-character FORTRAN records. It is also possible to use binary mode, where each of the basic structures is implemented as a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

0.7.1. 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***. The data for a material is divided into ***files***, and each file (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 (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 0.3

Structure of an ENDF data tape



0.7.2. Format Nomenclature

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

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

b) The letter I or a symbol starting with I refers to an interpolation code (see Section 0.6.2).

c) Letters J, K, L, M, or N when used alone are indices.

d) A symbol starting with M is a control number. Examples are MAT, MF, MT.

e) A symbol starting with L is a test number.

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:

$\pm 1.234567 \pm n$

$\pm 1.23456 \pm nn$, where $nn \leq 38$

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 available to the NNDC must be used to output numbers in the above format. If evaluations are produced using numbers written by "1PE11.5" (that is, 1.2345E±nn), the numbers will be standardized into 6 or 7 digit form, but the real precision will remain at the 5 digit level.

0.7.3. Types of Records

All records on an ENDF tape are one of five possible types, denoted by TEXT, CONT, LIST, TAB1, and TAB2. 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 a sequence number. The definitions of the other fields in each record will depend on its usage as described below.

0.7.4. 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)
```

where NS is the sequence number.[13] For a normal TEXT record, MF = 1 and MT = 451. For a TPID record, MAT contains the tape number NTAPE, and MF and MT are both zero.

0.7.5. Control Records

0.7.5.1. 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.

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13 Records are sequentially numbered within a given MAT/MF/MT.

0.7.5.2. 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.

0.7.5.3. 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,99999/  0.0,  0.0,   0,   0,   0,   0] SEND14
[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
```

0.7.5.4. 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.

0.7.6. 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).

0.7.7. 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/xint/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

---

14 The SEND record has the sequence number 99999.

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.

0.7.8. TAB2 Records

The last 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.

0.8. 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.

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 four additional sections giving fission neutron 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 0.7.

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.

LRP Indicates 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[15] 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.

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

NLIB Library identifier: NLIB= 0 for ENDF/B.
Additional values have been assigned to identify other libraries using ENDF format. See 0.3.2

15 In the unresolved region, it is also possible to compute a self-shielding factor from File 2 and multiply it by a complete unshielded cross section in File 3.

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≥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 units. For incident photons or decay data sub-libraries, use AWI=0.0.

EMAX Upper limit of energy range for evaluation.

LREL Release number.

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

NVER Library version number; for example, NVER=6 for version VI.

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≥1, special derived evaluation (for example, a dosimetry evaluation using sections (MT) extracted from the primary evaluation).

NWD Number of records used to describe the data set for this material. Each record can contain 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).

ZSYNAM Character representation of the material charge, chemical symbol, atomic mass number, and metastable state in the form Z-cc-AM with
Z, right justified in col. 1 to 3,
- (hyphen) in col. 4,
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, 94-PU-239, 1-H - 2, *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" is the revision number IREV; IREV is computer retrievable.

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

HSUB Identifier for the library contained on three successive records.

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 0.1). 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 MF of the nth section.

MT_n MT 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, 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, $\bar{\nu}(E)$, *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 evaluation; 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 0.5.

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

If the material fissions (LFI=1), then a section specifying the average *total* number of neutrons per fission, $\bar{\nu}$ (MT=452), must be given. This format applies to both particle induced

$$\bar{\nu}(E) = \sum_{n=1}^{NC} C_n E^{n-1} \tag{0.13}$$

and spontaneous fission, each in its designated sub-library. Values of $\bar{\nu}$ may be tabulated as a function of energy or coefficients provided for the following polynomial expansion of $\bar{\nu}$(E),

where $\bar{\nu}$(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 $\bar{\nu}$ (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 $\bar{\nu}$ (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≤4).
C_n	Coefficients of the polynomial. There are NC coefficients given.
NR	Number of interpolation ranges used to tabulate values of $\bar{\nu}$(E). (See 0.6.2.)
NP	Total number of energy points used to tabulate $\bar{\nu}$(E).
E_{int}	Interpolation scheme (see 0.6.2 for details).
$\bar{\nu}$(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, 1,99999/ 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/Eint / ν̄(E)]TAB1
[MAT, 1,99999/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

1.2.2. Procedures

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

If tabulated values of $\bar{\nu}$ (E) are specified (LNU=2), then pairs of energy- $\bar{\nu}$ values are given. Values of $\bar{\nu}$ (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 $\bar{\nu}$ (E) given in this section are for the average total number of neutrons produced per fission event. When another section (MT=455) that specifies the delayed neutrons from fission is given, the average number of delayed neutrons per fission ($\bar{\nu}_d$) must be added to $\bar{\nu}_p$ given in section MT=456 and included in the value of $\bar{\nu}$(E) given in this section (MT=452). In this case, only LNU=2 is allowed for MT=452.

For spontaneous fission, the polynomial representation (LNU=1) is used with NC=1 and Cl = $\bar{\nu}_{total}$. There is no energy dependence.

1.3. Delayed Neutron Data, $\bar{\nu}_d$, (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, $\bar{\nu}_d$, is given, along with the decay constants, λ_i, for each precursor family. The fraction of $\bar{\nu}_d$ generated for each family is given in File 5 (section 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 $\bar{\nu}_d$(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= $\bar{\nu}_d$ 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,

$$\bar{\nu}_d = \sum_{i=1}^{NNF} \bar{\nu}(E),$$

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 section 5) and is defined as

$$P_i(E) = \frac{\bar{\nu}_i(E)}{\bar{\nu}_d(E)}$$

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≤4).
NR	Number of interpolation ranges used. (NR≤20).
NP	Total number of energy points used in the tabulation of $\nu(E)$
$\mathbf{E_{int}}$	Interpolation scheme (See Section 0.6.2)
$\overline{\nu_d}$ **(E)**	Total average number of delayed neutrons formed per fission event.
NNF	Number of precursor families considered.
$\boldsymbol{\lambda_i}$ **(E)**	Decay constant (sec^{-1}) for the ith precursor. (May be constant)
$\boldsymbol{\alpha_i}$ **(E)**	Delayed-group abundances.

The structure when values of $\bar{\nu}_d$ 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 $\bar{\nu}_d$ 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), λ3(E1), α3(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), λ3(ENE), α3(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
```

If LNU=1 (spontaneous fission) and the delayed-group constants are energy independent (LDG=0), the structure of the section is:

```
[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]LIST
[MAT, 1,  0/ 0.0, 0.0,   0,   0,   0,  0]SEND
```

If LNU=1 (spontaneous fission) 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), λ3(E1), α3(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), λ3(ENE), α3(ENE),
                                  ...λNNF(ENE), αNNF(ENE)]LIST
[MAT, 1,455/ 0.0, 0.0,   0,   0,   1,  0/ ν̄d]LIST
[MAT, 1,  0/ 0.0, 0.0,   0,   0,   0,  0]SEND
```

1.3.2. Procedures

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

The probability of producing the precursors for each family and the energy distributions of neutrons produced by each precursor family are given in File 5 (section 5 of this report). It is extremely important that the same precursor families be given in File 5 as are given in File 1 (MT=455) 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 ($\lambda_1<\lambda_2<\ldots<\lambda_{NNF}$).

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

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

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

If the material fissions (LFI=1), a section specifying the average number of prompt neutrons per fission, $\bar{\nu}_p$, (MT=456) can be given using formats identical to MT=452. For particle-induced fission, $\bar{\nu}_p$ is given as a function of energy. The prompt $\bar{\nu}$ 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 $\bar{\nu}_p(E)$ 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≤4)
NR	Number of interpolation ranges used to tabulate values of $\bar{\nu}_p(E)$. (See 0.7.7.)
NP	Total number of energy points used to tabulate $\bar{\nu}_p(E)$.
$\mathbf{E_{int}}$	Interpolation scheme (see section 0.6.2.)
$\bar{\nu}_p(E)$	Average number of prompt neutrons per fission.

If LNU=2, (tabulated values of $\bar{\nu}$), 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/ ν̄p(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/ ν̄p]LIST
[MAT, 1,  0/ 0.0, 0.0,  0,   0,  0,  0]SEND
```

1.4.2. Procedures

If tabulated values of $\bar{\nu}_p(E)$ are specified (LNU=2), then pairs of energy-$\bar{\nu}$ values are given. Values of $\bar{\nu}_p(E)$ 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 $\bar{\nu}_p(E)$ given in this section are for the average number of prompt neutrons produced per fission event. The energy independent $\bar{\nu}_p$ for spontaneous fission is given using LNU=1 with NC=1 and $C_1=\bar{\nu}_p$ 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 fragments, neutrons, gammas, betas (+ and –), and neutrinos and anti-neutrinos. The term fragments includes 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 with the fragments, and their prompt energies are correctly included with the fragment energies.

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

All of these energies are given for an incident energy of zero.[16]

$$E_i(0) = E_i(E_{inc}) + \delta E_i \tag{0.14}$$

where E_i is any of the energy release components;

16 Taken from R. Sher and C. Beck, Fission Energy Release for 16 Fissioning Nuclides, EPRI-NP-1771 (1981).

$E_i(0)$ is the value at $E_{inc} = 0$; $E_{inc} = 0$ is fictitious and represents an artifice by which it is possible to recover the values at any E_{inc}.
$E_i(E_{inc})$ is the value at incident energy E_{inc}.

The δE_i's are given by the following:

$$\delta\mathrm{ET} = -\left(1.057E_{inc} - 8.07\left(\bar{\nu}(E_{inc} - \bar{\nu}(0)\right)\right)$$
$$\delta\mathrm{EB} = 0.075E_{inc}$$
$$\delta\mathrm{EGD} = 0.075E_{inc}$$
$$\delta\mathrm{ENU} = 1.000E_{inc}$$
$$\delta\mathrm{EFR} = 0$$
$$\delta\mathrm{ENP} = -\left(1.307E_{inc} - 8.07\left(\bar{\nu}(E_{inc}) - \bar{\nu}(0)\right)\right)$$
$$\delta\mathrm{EGP} = 0$$

1.5.1. Formats

The structure of this section always starts with a HEAD record and end with a SEND record. The section contains no subsections and only one LIST record.

The structure of a section is:

```
[MAT, 1,458/  ZA,  AWR,   0,    0,   0,    0]HEAD
[MAT, 1,458/ 0.0,  0.0,   0,    0,  18,    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's allow the error estimates on the quantities listed above.

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 listed in File 1. Note that ER = the pseudo-Q for fission (MT=18) in File 3.

Other components are not so readily determined or checked. The procedure should be that File 5 and File 15 data take precedent, whenever available. That is, "prompt" fission neutron energy calculated from File 5 spectra from MT=18 should be used in 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 input into File 1, that is the prompt gammas due to the fission process.

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 $\bar{\nu}$ prompt (not $\bar{\nu}$ total) for the fission neutrons. MT=455 in File 5 contains the delayed fission neutron spectra.

In many reactor applications, 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 six-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, of 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, and the energy released in all other reactions.

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[17].

The File 2 resonance contributions should also be added to any lumped reactions included in File 3. For SLBW and MLBW, any other competing reactions in the resonance range must be given in their entirety in File 3 and included in the background for 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 explicitly in the unresolved resonance region, and implicitly in the resolved region. In the latter region, it is permissible

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

for the total width to exceed the sum of the neutron, radiative capture, and fission widths. The difference is interpreted as the competitive width:

For the Reich-Moore or Adler-Adler formalisms competitive reactions are not used. For the new General R-matrix and Hybrid R-function formats, the competitive cross section is calculated from the resonance parameters, like the other cross sections. In this case the resonance contribution is added to the background in File 3, for each competitive reaction just as for the other resonance reactions.

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. Used

[17] 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 2.4.21. 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.

for certain derived libraries only.

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 may contain two additional non-resonance ranges, also non-overlapping. 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 are essentially 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 2.4.6.4.

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 2.4.21). 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. If these background cross sections are nonzero, 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).

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).

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

It is possible to define partial widths $\Gamma_{l\ s_1\ J}$ and $\Gamma_{l\ s_2\ J}$ 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 ($s = l + 1/2$), and negative for the smaller channel spin ($s = l - 1/2$). (See definition of AJ in 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.

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 General R-matrix[18] (multilevel multichannel R-matrix with competitive reactions).

LRF=6 Hybrid R-function (includes level-level interference, but not channel-channel; allows competitive reactions).

Preferred formalisms for evaluation are discussed in Section 2.4.17. 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.

[18] Not for the faint of heart, but will handle anything. Really a generalized Reich-Moore formalism.

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

NIS Number of isotopes in the material (NIS≤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[19].

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 is required with this option);
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, General R-matrix (GRM);
LRF=6, Hybrid R-function (HRF).
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 (not allowed in the ENDF/B-VI library)[20].

[19] 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.

[20] Formerly used for radius expressed as a table of energy, radius pairs.

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 CONT (range) record; use *a* in the penetrabilities and shift factors, and AP in the hard-sphere phase shifts;

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.

The structure of File 2, for the *special case* in which just a scattering radius is specified (no resolved or unresolved parameters are given), is as follows: (such a material is not permitted to have multiple isotopes or an energy-dependent scattering radius)

```
[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=1.0,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
```

If resonance parameters are given, the structure of File 2 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 and 2.3.1, below. 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

Six 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 CONT (range) 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=1-4, 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=1-4, 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 2.4.23 and 2.4.24). Another cutoff, NLSC, is provided for converging the angular distributions. Currently, NLS≤4.

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 or 4;

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, $\Gamma_x = \Gamma - [\Gamma_n + \Gamma_\gamma + \Gamma_f]$

NRS Number of resolved resonances for a given *l*-value. (NRS$\leq$600.)

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 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$\neq$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. <u>SLBW and MLBW (LRU=1, LRF=1 or 2)</u>

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.

2.2.1.2. Reich-Moore (LRU=1, 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.1.6.5. (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/
              ER1,  AJ1,  GN1, GG1,  GFA1, GFB1,
              ER2,  AJ2,  GN2, GG2,  GFA2, GFB2,
            ---------------------------------
             ERNRS,AJNRS, GNNRS,GGNRS,GFANRS,GFBNRS] 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 (LRU=1,LRF=4)

For the case of (LRU=1, 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 $= \left[C/\sqrt{E}\left(AT_1 + AT_2/E + AT_3/E^2 + AT_4/E^3 + BT_1E + BT_2E^2 \right) \right]$

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

DEF_r [5]Resonance energy, (μ), for the fission cross section.

DEC_r [5]Resonance energy, (μ), for the radiative capture cross section.

DWT_r [5]Value of Γ/2, (v), for the total cross section.

DWF_r [5]Value of Γ/2, (v), for the fission cross section.

DWC_r [5]Value of Γ/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.

GIC_r Asymmetrical capture parameter, H_r^γ.

[21] Note: DET_r=DEF_r=DEC_r and DWT_r=DWF_r=DWC_r. The redundancy is an historical carryover.

The structure of a subsection for LRU=1 and 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 will be followed by NJS LIST records. Note that if NX=2 then the quantities AF_1, ---BF_2 will not be given in the first LIST record. Also, if LI≠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 A-A 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,GRM[22] (LRU=1, LRF=5)

For the case of (LRU=1, LRF=5) some additional quantities are defined. In the following, they are subdivided according to the part of the format to which they refer. These definitions should be read in conjunction with the procedures section, 2.2.1.5, and the equations, D.1.5.

2.2.1.4.1. MT-List

This is the first entry in the GRM format. The following quantities are defined.

ISH Flag to specify whether the shift function will be calculated from the usual formulas (ISH=1) or set equal to zero (ISH=0). The latter choice is recommended.

NML Total number of entries in the MT-list.

RNSM Number of summed-MT (SMT) values specified in the evaluation;

[22] This formalism is more accurately described as "expanded Reich-Moore".

floating-point number.

SMT Floating-point value of summed-MT for a reaction.

AWT Nuclear mass (not a ratio) of the outgoing particle for an SMT.

AZP Atomic number (charge) of the outgoing particle for an SMT.

±SPP Spin and parity of the outgoing particle for an SMT. A signed quantity. All allowable particles have positive parity, and all have spin 1/2 except the deuteron (spin 1), and the alpha-particle (spin 0).

AWD Atomic mass (not a ratio) of the daughter nucleus for an SMT. The influence of the PMT-dependent Q-value on the mass is ignored.

AZD Atomic number (charge) of the daughter nucleus for an SMT.

RNPM Number of particular-MT (PMT) values for a summed-MT; floating-point number.

PMT Floating-point value of particular-MT for an summed-MT.

±SPD Spin and parity of the daughter nucleus for a particular-MT; signed quantity.

±Q Q-value for a particular-MT; signed quantity.

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.

NCP Number of channels for a particular-MT; floating-point number.

CI Channel index. The floating-point value of a unique integer assigned to a channel. This integer is equivalent to the full set PMT, J, π, *l*, and s, the correspondence being made in the spin-group list.

The MT-list has the structure of a three-fold nested loop, on SMT, PMT, and CI.

```
[MAT, 2,151/  0.0,  0.0,  ISH,  LAD,   NML,    0/
            RNSM,  SMT1,  AWT,  AZP,  ±SPP,  AWD,
             AZD, RNPM,  PMT1, ±SPD,   ±Q,   NCP,
             CI1,   CI2,-------------------..CINCP,
            PMT2,  ±SPD,   ±Q,  NCP,   CI1,  CI2,
             CI3, -----------------------  CINCP,
                <repeat PMT's for SMT1>
           PMTNPM,  ±SPD,   ±Q,  NCP,   CI1,  CI2,
             CI3,  ----------------------- CINCP,
            SMT2,   AWT,  AZP, ±SPP,  AWD,  AZD,
           RNPM,   PMT1, ±SPD,   ±Q,   NCP,  CI1,
             CI2,  ----------------------- CINCP,
            PMT2,  ±SPD,   ±Q,  NCP,   CI1,  CI2,
             CI3,  ----------------------- CINCP,
                <repeat PMT's for SMT2>
          PMTNPM, ----------------------------
          <repeat SMT entries until all RNSM values have been specified>
           ------------------------------ CINCP] LIST
```

to specify the SMT-PMT-channel structure of the overall calculation.

2.2.1.4.2. Spin-Group List

The spin-group list, which follows the MT-list:

NLS Cutoff value for summations on the orbital angular momentum, *l*.
The evaluator may specify any value required to converge the calculation of the scattering cross section at the highest energy covered. If the current limitation to *l*=3 (NLS≤4) is too restrictive, a File 3 background will be required.

NSG Number of spin-groups in the evaluation.

±AJ Spin and parity of a spin-group; signed quantity, the sign specifying the parity.

ISG Spin-group index; integer assigned to a spin-group for the purpose of identification.
The spin-groups are sequenced by order of ascending J-values, negative parity first, then positive, *e.g.*, -0.5, +0.5, -1.5, +1.5, ... These would carry indices 1, 2, 3, 4, ….

NCS Number of channels in a particular spin-group.
Within a spin-group, a channel is identified by its PMT-value, its orbital angular momentum *l*, and its channel-spin s. NCS varies from group to group.

NCT Total number of channels in the evaluation; floating-point number.

AL Floating-point value of the orbital angular momentum *l*.
Enter zero for capture and fission channels.

AS Floating-point value of the channel-spin s.
Enter zero for capture and fission channels.

NRS Number of resonances in a spin-group.
NRS varies from group to group.

RI Resonance index; floating-point value of a unique integer assigned to a resonance.

NRT Total number of resonances in the evaluation.

±ER Resonance energy; signed quantity.

GG Capture width. (This value is used as the eliminated width).

±AG Reduced-width amplitude, in the laboratory system; signed quantity which is a factor of $\sqrt{(A+1)/A}$ larger than the conventional center-of-mass amplitude, γ.

The spin-group list has the following structure:

```
[MAT, 2,151/  0.0,  0.0,     0,      0,   NSG,   0] CONT
```

to specify the number of spin-groups.

```
[MAT, 2, 151/  ±AJ,  0.0, ISG=1,      0, 4*NCS1, NCS1/
  CI=1,  PMT1,   AL1,    AS1,  CI=2,  PMT2,
   AL2,   AS2,  CI=3, -------------------
 ----------- CI=NCS1, PMTNCS1,  ALNCS1, ASNCS1] LIST
```

to specify the spin and parity, spin-group index, number of channels, channel indices, and channel quantum numbers for the first spin-group (ISG=1)

```
[MAT, 2, 151/  0.0,  0.0,   0,     0, NRS1*(NCS+3),  NRS1/
   RI=1,  ER1,  GG1, ±AG1,1,        ±AG1,2,  ±AG1,3,
--------------------------------------±AG1,NCS,
   RI=2,  ER2,  GG2, ±AG2,1,        ±AG2,2,  ±AG2,3,
-------------------------------------±AG2,NCS,
                <repeat resonance parameters>
 RI=NRS1, ERNRS1, GGNRS1, ±AGNRS1,1,-----------------
  ±AGNRS1,3, ---------------------------- ±AGNRS1,NCS] LIST
```

to specify the indices, energies, capture widths, and reduced-width amplitudes for the resonances in the first spin-group.

```
[MAT, 2,151/     ±AJ,  0.0,    ISG=2,     0,    4*NCS2, NCS2/
CI=NCS1+1, PMTCI,      ALCI,  ASCI, CI=NCS1+2, PMTCI,
     ALCI,  ASCI, CI=NCS1+3,----------------------
--------------CI=NCS1+NCS2, PMTCI,      ALCI,  ASCI] LIST
```

to specify the spin and parity, spin-group index, number of channels, channel indices, and channel quantum numbers for the second spin-group (ISG=2)

```
[MAT, 2,151/    0.0,  0.0,   0,     0, NRS2*(NCS+3),  NRS2/
            RI=NRS1+1, ERRI, GGRI, ±AGRI,1,      ±AGRI,2, ----
            ------------------------------------- ±AGRI,NCS,
            RI=NRS1+2, ERRI, GGRI, ±AGRI,1,      ±AGRI,2, ----
            ------------------------------------- ±AGRI,NCS,
                    <repeat resonance parameters>
            RI=NRS1+NRS2, ERRI, GGRI, ±AGRI,1, ±AGRI,2, ---
            ------------------------------------ ±AGRI,NCS] LIST
```

to specify the indices, energies, capture widths, and reduced-width amplitudes for the resonances in the second spin-group.

Repeat the above LISTs until all NSG spin groups have been specified.

Note that the channel and resonance indices are unique and do not start over from one within a spin-group. The last entry in the spin-group list will be $\pm AG_{NRT,NCS}$. The last channel index specified will be CI=NCT.

2.2.1.4.3. Background R-Matrix List

The following quantities are defined for the background-R-matrix list, which, if present, follows the spin-group list:

NTP Flag to identify a CONTROL record for the background-R-matrix list, NTP=1.

LBK Flag to identify the type of background-R-matrix parameterization.
LBK=1 denotes a tabulated function,
LBK=2 is logarithmic,
LBK=3 is statistical.

NBK Number of tabulated background R-matrix elements supplied.

NCH Number of channels to which a particular background R-matrix element applies.

CI Channel index.

RRB Real part of a tabulated background R-matrix element.
IRB Imaginary part of a tabulated background R-matrix element.
NLG Number of logarithmically-parameterized background R-matrix elements supplied.
R0,R1, R2, S0, S1, EU, ED Logarithmic parameters for an R-matrix element.
NST Number of statistically-parameterized background R-matrix elements supplied.
RIN, SF, INT, EBAR, AVGG Statistical parameters for an R-matrix element.

The background R-matrix list has the following structure:

[MAT, 2,151/ 0.0, 0.0, NTP, LBK, NBK, 0] CONT (NPT=1,LBK=1)
to specify the number of tabulated background R-matrix elements, RBK(n).

[MAT, 2,151/ 0.0, 0.0, 0, 0, NCH, 0/ (NCH≥1)
CI_1, CI_2, ...CI_{NCH}] LIST
to specify which channels use the following tabulated background R-matrix element.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RRB(E)] TAB1
to specify the real part of a tabulated background R-matrix element.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IRB(E)] TAB1
to specify the imaginary part.

<Repeat the channel-index LIST and the two TAB1 records until all NBK functions have been specified>

[MAT, 2,151/ 0.0, 0.0, NTP, LBK, NLG, 0] CONT (NPT=1,LBK=2)
to specify the number of logarithmically-parameterized background R-matrix elements supplied.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NCH, 0/
CI_1, CI_2,---------- CI_{NCH}] LIST (NCH≥1)
to specify which channels use the following logarithmically-parameterized background R-matrix element.

[MAT 2,151/ 0.0, 0.0, 0, 0, 7, 0/
R0, R1, R2, S0, S1, EU,
ED] LIST
to specify the logarithmic parameters.

<Repeat the channel-index LIST and the parameter LIST until all NLG sets of parameters have been specified>

[MAT, 2,151/ 0.0, 0.0, NTP, LBK, NST, 0] CONT (NTP=1, LBK=3)
to specify the number of statistically-parameterized background R-matrix elements supplied.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NCH, 0/
CI_1, CI_2, ---------- CI_{NCH}] LIST (NCH≥1)
to specify which channels use the following statistically-parameterized background R-matrix element.

[MAT, 2,151/ 0.0, 0.0, 0, 0, 5, 0/
RIN, SF, INT, EBAR, AVGG] LIST
to specify the statistical parameters.

<Repeat the channel-index LIST and the parameter LIST until all NST sets of parameters have been specified>

The evaluator is not restricted to one type of background representation. If the need arises, different representations can be used in different channels.

2.2.1.4.4. Phase-Shift List

The following quantities are defined for the phase-shift list:

NTP	Flag to identify a CONTROL record for the phase-shift list, NTP=2.
NPS	Number of non-hard-sphere phase shifts specified.
NHS	Number of channels which require hard-sphere phase shifts.
NF	Number of channels not requiring a phase shift. (Fission, since capture is calculated by subtraction.)
NCH	Number of channels to which a particular phase shift applies.
CI	Channel index.
RPS	Real part of a tabulated non-hard-sphere phase shift.
IPS	Imaginary part of a tabulated non-hard-sphere phase shift.

The phase-shift list has the following structure:

[MAT, 2,151/ 0.0, 0.0, NTP, NPS, NHS, NF]CONT (NTP=2)

to specify the number of tabulated non-hard-sphere phase shifts supplied, the number of channels requiring hard-sphere phase shifts, and the number of fission channels requiring no phase shifts.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NCH, 0/ (NCH≥1)
CI_1, CI_2,---------- CI_{NCH}] LIST

to specify which channels use the following tabulated phase shift.

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

to specify the real part of the phase shift.

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

to specify the imaginary part of the phase shift. Omit these lists if NPS=0.

<Repeat the channel-index LIST and two TAB1 records until all NPS phase shifts have been specified>.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NHS, 0/
CI_1, CI_2,---------- CI_{NHS}] LIST

to specify which channels use hard-sphere phase shifts. Omit this list if NHS=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NF, 0/
CI_1, CI_2,---------- CI_{NF}] LIST

to specify which channels do not use phase shifts, Ω=1. Omit this list if NF=0.

The phase shifts are to be tabulated as functions of the incident neutron's laboratory energy. The conversion from an exit channel energy is described in Section D.3.1., paragraph C.

2.2.1.4.5. Penetrability List

The following quantities are defined for the penetrability list:

NTP	Flag to identify a CONT record for the penetrability list, NTP=3.
NPE	Number of charged-particle penetrabilities specified.
NHS	Number of channels which require hard-sphere penetrabilities.
NF	Number of (fission) channels not requiring penetrabilities, or more precisely, that have P=1.
NCH	Number of channels to which a particular penetrability applies.

CI Channel index.
P Tabulated charged-particle penetrability.

The penetrability list has the following structure:

[MAT, 2,151/ 0.0, 0.0, NTP, NPE, NHS, NF] CONT

to specify the number of charged-particle penetrabilities supplied, the number of channels requiring hard-sphere penetrabilities, and the number of (fission) channels requiring no penetrabilities.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NCH, 0/
CI_1, CI_2,---------- CI_{NCH}] LIST

to specify which channels use the following tabulated penetrability.

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

to specify the first tabulated penetrability. Omit these lists if NPE=0.

<Repeat the channel-index LIST and the TAB1 record until all NPE penetrabilities have been specified>.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NHS, 0/
CI_1, CI_2,---------- CI_{NHS}] LIST

to specify which channels use hard-sphere penetrabilities. Omit this list if NHS=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NF, 0/
CI_1, CI_2,---------- CI_{NF}] LIST

to specify which channels do not use penetrabilities, P=1. Omit this list if NF=0.

The penetrabilities are to be tabulated as functions of the incident neutron's laboratory energy. The conversion from an exit channel energy is described in Section D.3.1.C.

2.2.1.4.6. Channel-Radius List

The following quantities are defined for the channel-radius list, which follows the penetrability list:

AC Channel radius.
NTP Flag to identify a CONT record for the channel radius list, NTP=4.
NAC Number of different channel radii supplied.
NCH Number of channels using a specific channel radius.

The channel-radius list has the following structure:

[MAT, 2,151/ AC, 0.0, NTP, 0, NAC, 0] CONT

to specify an *optional* channel radius, and the number of radii supplied. If NAC=1, omit the following LIST and use the value in position 1 for all channels. If NAC>1,

[MAT, 2,151/ AC_1, 0.0, 0, 0, NCH_1, 0/
CI_1, CI_2, ... CI_{NCH1}] LIST

to specify the channels using the value AC_1.

[MAT, 2,151/ AC_2, 0.0, 0, 0, NCH_2, 0/
CI_1, CI_2,---------- CI_{NCH_2}] LIST

to specify the channels using the value AC_2.

<Repeat LIST's until all NAC values have been specified>.

2.2.1.4.7. Boundary-Condition List

The following quantities are defined for the boundary-condition list, which follows the radius list:

BC	boundary-condition parameter.
NTP	flag to identify a CONT record for the boundary-condition list, NTP=5.
NBC	number of different boundary-condition parameters supplied.
NCH	number of channels using a specific boundary-condition parameter.

The boundary-condition list has the following structure:

[MAT,2,151/ BC, 0.0, NTP, 0, NBC, 0] CONT

to specify an optional boundary-condition parameter, and the number of boundary-condition parameters supplied.

If NBC=1, omit the following LIST and use the value in position 1 of the preceding record for all channels.

If NBC>1, then

[MAT, 2,151/ BC_1, 0.0, 0, 0, NCH_1, 0/
CI_1, CI_2,---------- CI_{NCH1}] LIST

to specify the channels using the value BC_1.

[MAT, 2,151/ BC_2, 0.0, 0, 0, CH_2, 0/
CI_1, CI_2,---------- CI_{NCH_2}] LIST

to specify the channels using the value BC_2.

<Repeat LIST's until all NBC values have been specified>.

2.2.1.5. Procedures for the General R-matrix (GRM) format

2.2.1.5.1. Enumeration of channels in the MT-list

A channel is described by four quantities, α, *l*, s, and J[23]. Alpha is a composite quantity, specifying both the identity of the pair of particles in the channel and their state of excitation. The identity includes each one's mass, charge, spin, and parity. The intrinsic parities included in α, together with the *l*-value, determine the channel parity, so it is common to suppress explicit reference to π. As a label, J usually means Jπ, since both quantities are conserved.

In ENDF, certain MT-values play the same role as α. The following table lists them as "PMT's" or particular MT-values, meaning that they refer to a particular state of excitation of the channel pair:

PMT-values	Reaction type	Number of PMT's available	Summed MT values, SMT
2	elastic scattering	1	2
18	fission	1	18
51 - 90	inelastic levels	40	4
102	radiative capture	1	102
600 - 649	n,p levels	50	103

[23]This notation follows Lane and Thomas, Reference 9.

650 - 699	n,d levels	50	104
700 - 749	n,t levels	50	105
750 - 799	n,^{3}He levels	50	106
800 - 849	n,^{4}He levels	50	107

Thus the PMT-value 602 identifies the second excited state in an exit n,p reaction. This implicitly identifies all the quantities needed to specify α. The above table also lists the MT-value for the complete reaction, obtained by summing the PMT-reactions in each category. These are referred to as SMT's, for "summed MT-value." In the GRM format, there is an MT-list which enumerates all the SMT's and PMT's specified in the evaluation, and for each one gives the mass, charge, spin, and parity of each channel particle, and the Q-value. In addition, each PMT entry in this section carries a list of the channels that belong to it, thus specifying the hierarchical order of the calculation. The MT's should be given in the order they appear in the above table, and the channel indices should be given in ascending order within each PMT set.

In principle, both channel particles could be excited, requiring the specification of two energies, but in ENDF only the daughter nucleus can be excited.

Radiative capture, MT=102, is treated as an eliminated channel in Reich-Moore theory. Accordingly, it is filled out with zeroes if it is specified as a part of the evaluation. Since there is only one such PMT, its SMT is the same, (102.), and the number of channels is zero. Elastic scattering also has the same SMT as PMT, but there can be many channels for that single PMT.

Fission channels are also treated differently from real channels in that they are not assigned an orbital angular momentum, channel spin, penetrabilities, *etc*. If specified in the MT-list, they are entered with zeroes in the mass, charge, spin, and parity slots. Like capture and scattering, there is only one PMT, which has the same value as its SMT, 18. There is no need to specify fission to distinct daughter states, nor is there a need in this application for first-chance, second-chance, *etc*.

(Note: The number of reactions that can be specified according to the above table is based on the reaction numbers (MT's) defined in ENDF/B, and not on any expectation that this large number of possibilities will ever be used.)

2.2.1.5.2. Examples of the MT-list

Since SMT=102 is entered in the list only to flag the occurrence of a capture reaction, it is entered with no channels, and has the following form:

... SMT=102. 0. 0. 0. 0. 0. 1. PMT=102. 0. 0. NCP=0. (NEXT SMT) ..

The capture width introduces an imaginary component into the otherwise real R-matrix, so that the U-matrix becomes non-unitary and the total cross section, computed from the real parts of the scattering amplitudes, exceeds the sum of the reaction cross sections. The difference is interpreted as the capture cross section, and has essentially a single-level Breit-Wigner shape. This convenient aspect of the theory is exploited more fully in the hybrid R-function formalism, LRU=1, LRF=6.

The minimum possible MT-list consists of scattering only, and might have the following appearance:

```
[MAT, 2,151/    0.0,    0.0,      0,      0,     18,        0/

                1.0,    2.0,1.00866,    0.0,    0.5,59.930789,
```

```
28.0,    1.0,    2.0,    0.0,    0.0,      6.0,
 1.0,    2.0,    3.0,    4.0,    5.0,      6.0]  LIST
```

This LIST consists of 18 items: one summed-MT, SMT=2.0 for elastic scattering, the neutron mass, charge, and spin/parity, the target mass and charge, one particular MT, PMT=2.0 for elastic scattering, the target spin/parity, Q=0.0, the number of channels (6.0) and six channel indices (1.0-6.0). Assignment of the channel quantum numbers is done in the spin-group LIST.

An MT-list for six scattering channels, capture, and two fission channels might look like:

```
[MAT, 2, 151/ 0.0,    0.0,       0,      0,     42,         0/
              3.0,    2.0, 1.00866,    0.0,    0.5,235.043928,
             92.0,    1.0,     2.0,   -3.5,    0.0,       6.0,
              1.0,    2.0,     3.0,    4.0,    5.0,       6.0,
            102.0,    0.0,     0.0,    0.0,    0.0,       0.0,
              1.0,  102.0,     0.0,    0.0,    0.0,      18.0,
              0.0,    0.0,     0.0,    0.0,    0.0,       1.0,
             18.0,    0.0,     0.0,    2.0,    7.0,       8.0]   LIST
```

to specify six scattering channels, labeled 1-6, radiative capture (no channels), and two fission channels labeled 7 and 8.

The sizes of the Jπ sub-matrices that need to be inverted are specified in the spin-group list. The MT-list only specifies the hierarchical structure of the calculation.

2.2.1.5.3.Channels in the spin-group list

In addition to α, each channel is specified by *l*, s, and J. Following the usage in the computer codes MULTI (Reference 10) and SAMMY (Reference 11), the channels are grouped by J and π into spin-groups and the quantum numbers are specified in the spin-group list. Each spin-group is assigned an integer index to facilitate reference to it. The spin-group list specifies the spin and parity of the group, the number of channels in the group, the channel indices, the channel *l*- and s-values, and the resonance parameters belonging to the group -- energies, capture widths, and reduced-width amplitudes for the non-capture channels. The latter are given in 1:1 correspondence with the list of channel indices. Each resonance is assigned a unique integer index. The spin-group, channel, and resonance indices help to reduce the size of the file, since correlations can be made without repeating the channel quantum numbers or the resonance parameters.

Spin-groups are not required to contain resonances. It is usually necessary to include non-resonant channels to define phase shifts for the purpose of converging the elastic-scattering cross section, and even more "empty" channels will be required if angular distributions are to be calculated. (A common coding error is to sum only over channels which contain resonances, leading to incorrect results.)

The reduced-width amplitudes, γ, are signed real quantities. They are related to the ordinary widths by the relation $\Gamma=2P\gamma^2$. Neutron elastic penetrabilities are calculated from the usual formulas. The same formulas, shifted by the Q-value, are used for neutron inelastic scattering, as specified in Section D.3.1 and elsewhere in Appendix D. Charged-particle penetrabilities, if required, are supplied by the evaluator as part of the format. For fission channels, P=1 and *l*=s=0. The capture width is used as an eliminated width for each resonance. γ=0.0 for closed channels.

2.2.1.6. Hybrid R-Function (LRU=1, LRF=6)

The following 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.

NGRE Number of radiative capture reactions, 0≤NGRE≤1.

NFRE Number of fission reactions, 0≤NFRE≤1.

NIRE Number of inelastic scattering reactions, 0≤NIRE≤4.

NCRE Number of charged-particle reactions, 0≤NCRE≤4.

The above four quantities are defined for each energy range of each isotope. A maximum of four partial reactions is allowed: 0 ≤ NIRE+NCRE ≤ 4.

MTRE1,MTRE2, MTRE3, MTRE4 MT-value for each of the four inelastic or charged particle reactions. Nine values are allowed for these quantities and if present, they must be given in the following order:
51-54 (inelastic scattering to the first four excited states),
103 (n,p), 104 (n,d), 105 (n,t), 106 (n,^{3}He), 107 (n,α)
Since the input format is set up for four reactions, use zeros for the unspecified reaction MTRE values, if fewer than four are specified.

GG Energy-independent partial width for capture, Γ_γ. This-value should be zero if NGRE=0.

GF Energy-independent partial width for fission, Γ_f. This-value should be zero if NFRE=0.

GRE1, GRE2, GRE3, GRE4 Partial widths $\Gamma_{rE}(|E_r|)$ for each of the four specified reactions, evaluated at the resonance energy ER.
As usual in this manual, Γ_{rE}, without parentheses, denotes an energy- dependent quantity.

GE Eliminated width, GE=GG+GF+GRE1+GRE2+GRE3+GRE4, evaluated at ER.

QRE1, QRE2, QRE3, QRE4 Q-value for each of the four possible reactions, positive for an exothermic reaction. Use the negative of the level excitation energy for an inelastic reaction. Use zero for an unused channel.
This quantity is not required for a charged-particle channel, but it may be given for reference (see page D.40).

ALRE1, ALRE2, ALRE3, ALRE4 Exit-*l*-value for each of the four possible reactions.
Use zero for an unused channel. These quantities are needed for the penetrability factors of the exit reaction widths and are floating-point numbers with integer values. The format requires the specification of an exit-*l*-value for each resonance for each specified reaction.

AS Floating point value of s (the channel spin).

AC Channel radius (depends on J/s, *etc*.) in 10^{-12}cm. Note that AP and NAPS are not used for the HRF format, as the channel radius and the scattering radius are equal (AP=AC).

AWRIC Mass ratio for a charged-particle exit channel. One such value may be supplied for each of the NCRE charged-particle reactions. The user does not require this quantity, but it should be given for reference. (See page D.40).

PCP(E) Charged-particle penetrability. Four such functions will be supplied for each of the NCRE charged-particle reactions, one for each of the four possible *l*-values, 0, 1, 2, or 3. If the penetrability for a particular *l*-value is not actually required, zeroes should be supplied. They must be given as functions of the incident neutron's laboratory energy, to facilitate interpolation. The transformation from the exit channel energy to the incident channel is described in Section D.3.1, paragraph C, of Appendix D.

NLS Number of *l*-values for which resonance parameters are given, as required to converge the calculation of the scattering cross section at the highest energy covered. If the current limitation to *l*=3 (NLS≤4) is too restrictive, a File 3 background will be required.

NLSC number of *l*-values which must be used to converge the calculation of the scattering angular distribution at the highest energy covered. If the LAD flag has been set to zero, this entry will be ignored. See Section D.1.5.6.2. (NLS≥NLSC≤20).

NSS Number of different s-values (channel-spin) for a given *l*-value.

NJS Number of different J-values for a given pair of *l*- and s-values.

NLSJ Number of resonances in the channel specified by *l*, s, and J. This may be zero, signifying a non-resonant "phase-shift-only" channel. Such channels should still be included in the calculation, as they contribute to the potential scattering and the angular distribution. However, they may be omitted if the potential scattering is adjusted in file 3, and if the angular distributions are specified in a way other than by calculation from the R-matrix formulas, *e.g.*, in file 4.

LBK Flag to signal the presence of a background R-function in a particular channel, *l*sJ.

LBK=0, no background R-function will be given.

LBK=1, the real and imaginary parts of the background R-function will be given as tabulated functions

R0(E) Complex background R-function. Defined for a particular channel of a given isotope and energy range. Its real and imaginary parts are RR0(E) and IR0(E). The General R-matrix formalism allows two analytic representations of the background R-matrix, Section 2.2.1.4.3. These are applicable also to the Hybrid R-function, but must be converted to a tabulated function.

RR0(E) Real part of R0(E).

IR0(E) Imaginary part of R0(E).

LPS Flag to signal the presence of optical-model phase shifts to be used instead of the hard-sphere values.

LPS=0, no optical-model phase shifts will be given, and the hard-sphere values will be used.

LPS=1, the real and imaginary parts of the optical-model phase shifts will be given as tabulated functions, and these will be used in place of the hard-sphere values.

PS(E) Complex phase shift to be used if LPS=1. Defined for a particular channel of a given isotope and energy range. Its real and imaginary parts are RPS(E) and IPS(E).

RPS(E) Real part of PS(E).

IPS(E) Imaginary part of PS(E).

The structure of a subsection for HRF (Hybrid R-function) is the following:

`[MAT, 2,151/  SPI, 0.0,  LAD,  0,  NLS, NLSC] CONT`
to specify the number of incident *l*-values

`[MAT, 2,151/  0.0, 0.0,  NGRE, NFRE, NIRE, NCRE] CONT`
to specify the number of each kind of reaction.

`[MAT, 2,151/  0.0, 0.0, MTRE1, MTRE2, MTRE3, MTRE4] CONT`
to specify the kind of reaction.

`[MAT, 2,151/  0.0, 0.0,  0,  0,  4,  0/`
`  0.0, 0.0, QRE1,  QRE2,  QRE3, QRE4] LIST`
to specify the Q-value for each reaction.

`[MAT, 2,151/ AWRIC, 0.0,  0,  0,  NR,  NP/` E_{int} `/ PCP(E)] TAB1`
to specify a mass ratio and a charged-particle penetrability for the first charged-particle reaction, for *l*=0. Omit if NCRE=0.

`[MAT, 2,151/ AWRIC, 0.0,  0,  0,  NR,  NP/` E_{int} `/ PCP(E)] TAB1`
to specify a mass ratio and a charged-particle penetrability for the first charged-particle reaction, for *l*=1.

`[MAT, 2,151/ AWRIC, 0.0,  0,  0,  NR,  NP/` E_{int} `/ PCP(E)] TAB1`
to specify a mass ratio and a charged-particle penetrability for the first charged-particle reaction, for *l*=2.

`[MAT, 2,151/ AWRIC, 0.0,  0,  0,  NR,  NP/` E_{int} `/ PCP(E)] TAB1`
to specify a mass ratio and a charged-particle penetrability for the first charged-particle reaction, for *l*=3.

`[MAT, 2,151/ AWRIC, 0.0,  0,  0,  NR,  NP/` E_{int} `/ PCP(E)] TAB1`
to specify a mass ratio and a charged-particle penetrability for the second charged-particle reaction, for *l*=0.

`----------`
`----------`

`[MAT, 2,151/ AWRIC, 0.0,  0,  0,  NR,  NP/` E_{int} `/ PCP(E)] TAB1`
to specify a mass ratio and a charged-particle penetrability for the last charged-particle reaction, for *l*=3. A total of 4*NCRE penetrabilities will be supplied.

`[MAT, 2,151/ AWRI,  0.0,  `L_1`,  0,  NSS,  0] CONT`
to specify the first *l*-value and the number of its associated s-values.

`[MAT, 2,151/  `AS_1`,  0.0,  0,  0,  NJS,  0] CONT`
to specify the first s-value for this *l*-value, and the number of J-values associated with this *l*s pair.

Follow with a LIST to specify the first J-value for this *l*,s pair, and the number of resonances in the channel *l*,s,J, and parameters for all the resonances in this channel. LBK and LPS are flags for the background R-function and optical-model phase shifts.

[MAT, 2,151/ AJ_1, AC_1, LBK, LPS,12*NLSJ, NLSJ/
ER_1, GN_1, GG_1, GF_1, $GRE1_1$, $GRE2_1$,
$GRE3_1$, $GRE4_1$,$ALRE1_1$, $ALRE2_1$, $ALRE3_1$, $ALRE4_1$,
parameters for the first resonance in this channel
ER_2, GN_2, GG_2, GF_2, $GRE1_2$, $GRE2_2$,
$GRE3_2$, $GRE4_2$,$ALRE1_2$, $ALRE2_2$, $ALRE3_2$, $ALRE4_2$,
parameters for the second resonance in this channel.

ER_{NLSJ}, GN_{NLSJ}, GG_{NLSJ}, GF_{NLSJ}, $GRE1_{NLSJ}$, $GRE2_{NLSJ}$,
$GRE3_{NLSJ}$,$GRE4_{NLSJ}$,$ALRE1_{NLSJ}$,$ALRE2_{NLSJ}$,$ALRE3_{NLSJ}$,$ALRE4_{NLSJ}$] LIST
parameters for the last resonance in this channel.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RR0(E)] TAB1
to specify the real part of the background R-function in this channel. Omit if LBK=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IR0(E)] TAB1
to specify the imaginary part of the background R-function in this channel. Omit if LBK=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RPS(E)] TAB1
to specify the real part of the optical-model phase shift in this channel. Omit if LPS=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IPS(E)] TAB1
to specify the imaginary part of the optical-model phase shift in this channel. Omit if LPS=0.

[MAT, 2,151/ AJ_2, AC_2, LBK, LPS, 12*NLSJ, NLSJ/
second J-value for this *l*,s pair, and resonance parameters for this channel.
ER_1, GN_1, GG_1, GF_1, $GRE1_1$, $GRE2_1$,
$GRE3_1$, $GRE4_1$, $ALRE1_1$, $ALRE2_1$, $ALRE3_1$, $ALRE4_1$,
parameters for the first resonance in this channel
ER_2, GN_2, GG_2, GF_2, $GRE1_2$, $GRE2_2$,
$GRE3_2$, $GRE4_2$, $ALRE1_2$, $ALRE2_2$, $ALRE3_2$, $ALRE4_2$,
parameters for the second resonance in this channel

ER_{NLSJ}, GN_{NLSJ}, GG_{NLSJ}, GF_{NLSJ}, $GRE1_{NLSJ}$, $GRE2_{NLSJ}$,
$GRE3_{NLSJ}$, $GRE4_{NLSJ}$,$ALRE1_{NLSJ}$,$ALRE2_{NLSJ}$, $ALRE3_{NLSJ}$, $ALRE4_{NLSJ}$] LIST
parameters for the last resonance in this channel.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RR0(E)] TAB1
to specify the real part of the background R-function in this channel. Omit if LBK=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IR0(E)] TAB1
to specify the imaginary part of the background R-function in this channel. Omit if LBK=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RPS(E)] TAB1
to specify the real part of the optical-model phase shift in this channel. Omit if LPS=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IPS(E)] TAB1
to specify the imaginary part of the optical-model phase shift in this channel. Omit if LPS=0.

[MAT,2,151/ AS_2, 0.0, 0, 0, NJS, 0] CONT(s)
second s-value.

[MAT,2,151/ AJ_1, AC_1, LBK, LPS, 12*NLSJ, NLSJ/
first J-value for AS_2
ER_1, GN_1, GG_1, GF_1, $GRE1_1$, $GRE2_1$,

$GRE3_1$, $GRE4_1$, $ALRE1_1$, $ALRE2_1$, $ALRE3_1$, $ALRE4_1$,
parameters for the first resonance in this channel
ER_2, GN_2, GG_2, GF_2, $GRE1_2$, $GRE2_2$,
$GRE3_2$, $GRE4_2$, $ALRE1_2$, $ALRE2_2$, $ALRE3_2$, $ALRE4_2$,
parameters for the second resonance in this channel

ER_{NLSJ}, GN_{NLSJ}, GG_{NLSJ}, GF_{NLSJ}, $GRE1_{NLSJ}$, $GRE2_{NLSJ}$,
$GRE3_{NLSJ}$, $GRE4_{NLSJ}$, $ALRE1_{NLSJ}$, $ALRE2_{NLSJ}$, $ALRE3_{NLSJ}$, $ALRE4_{NLSJ}$] LIST
parameters for the last resonance in this channel.

[MAT,2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RR0(E)] TAB1
to specify the real part of the background R-function in this channel. Omit if LBK=0.

[MAT,2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IR0(E)] TAB1
to specify the imaginary part of the background R-function in this channel. Omit if LBK=0.

[MAT,2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RPS(E)] TAB1
to specify the real part of the optical-model phase shift in this channel. Omit if LPS=0.

[MAT,2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IPS(E)] TAB1
to specify the imaginary part of the optical-model phase shift in this channel. Omit if LPS=0.

When the last J-value is complete, start a new *l*-value:

[MAT,2,151/ AWRI, 0.0, L_2, 0, NSS, 0] CONT(*l*)
[MAT,2,151/ AS_1, 0.0, 0, 0, NJS, 0] CONT(s)
[MAT,2,151/ AJ_1, AC_1, LBK, LPS,1 2*NLSJ, NLSJ/
ER_1, GN_1, GG_1, GF_1, $GRE1_1$, $GRE2_1$,
$GRE3_1$, $GRE4_1$, $ALRE1_1$, $ALRE2_1$, $ALRE3_1$, $ALRE4_1$,
parameters for the first resonance in this channel for the new *l*-value.
ER_2, GN_2, GG_2, GF_2, $GRE1_2$, $GRE2_2$,
$GRE3_2$, $GRE4_2$, $ALRE1_2$, $ALRE2_2$, $ALRE3_2$, $ALRE4_2$,
parameters for the second resonance in this channel

ER_{NLSJ}, GN_{NLSJ}, GG_{NLSJ}, GF_{NLSJ}, $GRE1_{NLSJ}$, $GRE2_{NLSJ}$,
$GRE3_{NLSJ}$, $GRE4_{NLSJ}$, $ALRE1_{NLSJ}$, $ALRE2_{NLSJ}$, $ALRE3_{NLSJ}$, $ALRE4_{NLSJ}$] LIST

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RR0(E)] TAB1
to specify the real part of the background R-function in this channel. Omit if LBK=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IR0(E)] TAB1
to specify the imaginary part of the background R-function in this channel. Omit if LBK=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / RPS(E)] TAB1
to specify the real part of the optical-model phase shift in this channel. Omit if LPS=0.

[MAT, 2,151/ 0.0, 0.0, 0, 0, NR, NP/ E_{int} / IPS(E)] TAB1
to specify the imaginary part of the optical-model phase shift in this channel. Omit if LPS=0.

Continue until all the *l*-values are exhausted.

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 2.4.21.

NE Number of energy points at which energy-dependent widths are tabulated. (NE≤250).

NLS Number of *l*-values (NLS≤3).

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. (NJS≤6).

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.)[24]

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

[24] See Appendix D. Section D.2.2.6.

present AMUG = 0.0. This implies a constant value of Γ_γ.)

AMUF Number of degrees of freedom in the fission width distribution. ($1.0 \le AMUF \le 4.0$)

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

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***[25] 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).

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

```
[MAT, 2,151/ SPI,    AP,  LSSF,    0,   NLS,   0] CONT
[MAT, 2,151/ AWRI,  0.0,     L,    0, 6*NJS, NJS/
               D1,   AJ1, AMUN1,  GN01,   GG1, 0.0,
               D2,   AJ2, AMUN2,  GN02,   GG2, 0.0,
            -------------------------------------
              DNJS, AJNJS, AMUNNJS, GN0NJS, 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.

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, GN0,   GG, 0.0,
              GF1,  GF2,  GF3,--------------
            ---------------------------- GFNE] LIST
```

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

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 lin-lin. AMUG is assumed to be zero, AMUF equals MUF, and there is no competitive width.

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,  GN01,      GG1,  GF1,
             ES2,   D2,  GX2,  GN02,      GG2,  GF2,
             ----------------------------
             ESNE,  DNE,  GXNE, GN0NE,     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

CONTENTS OF THIS SECTION

2.4.1 Abbreviations
2.4.2 Interpolation in the Unresolved Resonance Region
2.4.3 Unresolved Resonances in the Resolved Resonance Range
2.4.4 Energy Range Boundary Problems
2.4.5 Numerical Integration Procedures in the Unresolved Resonance Region
2.4.6 Doppler-Broadening of File 3 Background Cross Sections
2.4.7 Assignment of Unknown J-values
2.4.8 Equivalent Single-Level Representations
2.4.9 Use of the Reich-Moore Formalism
2.4.10 Competitive Width in the Resonance Region
2.4.11 Negative Cross Sections in the Resolved Resonance Region
2.4.12 Negative Cross Sections in the Unresolved Resonance Region
2.4.13 Use of Two Nuclear Radii
2.4.14 The Multilevel Adler-Gauss Formula for MLBW
2.4.15 Notes on the Adler Formalism
2.4.16 Multilevel Versus Single-level Formalisms in the Resolved and Unresolved Resonance Regions
2.4.17 Preferred Formalisms for Evaluating Data
2.4.18 Computer Time for Generating MLBW Cross Sections
2.4.19 Amplitude-Squared Form of the MLBW Formulas
2.4.20 Degrees of Freedom for Unresolved Resonance Parameters
2.4.21 Procedures for the Unresolved Resonance Region
2.4.22 Procedures for Computing Angular Distributions in the Resolved Resonance Range
2.4.23 Completeness and Convergence of Channel Sums
2.4.24 Channel Spin and Other Considerations

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	multi-level Breit-Wigner
MLAG	multi-level 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 not correct 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 2.4.21) 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.

<u>Problem I</u>: 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 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 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 #3 is unavoidable, because the basic representation has changed. However if the RRR cross sections are group-averaged or otherwise smoothed, the discontinuity[26] 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

[26] 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.

double energy point will normally occur at this boundary, but will not eliminate the discontinuity.

Discontinuity at #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 $0.2\ E=100\times1$. 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.

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/B recommendation for doing the complicated multi-dimensional integrations was the Greebler-Hutchins 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 G-H. The MC^2-II

subroutine[27], is the recommended procedure.

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

The M. Beer [Ref.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/B make 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 2.4.14). 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 [Ref.12] to broaden File 2 to the temperature of File 3, since the latter may be based on room-temperature or other non-zero ^{0}K data.

   b.) Add File 2 and File 3.

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

   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

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

is 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±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,

$$\sigma_{nn} = \sum_{lsJ} g_J \left| A_{pot}^{lsJ} + A_{resonance}^{lsJ} \right|^2 \qquad (0.15)$$

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 *l*sJ 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. Equivalent Single-Level Representations

The single-level Breit-Wigner formalism is incorporated into the basic structure of many engineering codes used for reactor design. Its use is so widespread, that despite any shortcomings in the calculational procedures, such codes must be supplied with SLBW parameters. For ENDF/B evaluations employing other representations, one requires an "equivalent" set of SLBW parameters. This is not to minimize the importance of using improved methods, but such improved methods ***do not eliminate*** the need for SLBW parameters in reactor design. For example, the Adler formalism provides a multilevel, multichannel fission cross section in pseudo-SLBW format, permitting ψ,χ-broadening. This is very useful, but not to a code that does not recognize asymmetric fission or capture.

The following equivalences are recommended:

1. MLBW. Use the parameters "as is".
2. Reich-Moore. Use the parameters "as is", except that the absolute values of the partial fission widths are added together to form Γ_f. (Alternatively, convert Reich-Moore to Adler-Adler, and use the equivalence for that formalism).
3. Adler-Adler. Reasonable success in converting A-A parameters for ^{241}Pu and ^{233}U was

obtained using a method described in Reference 4.

4. Hybrid R-function. Use the parameters "as is".

2.4.9. Use of the Reich-Moore Formalism

If the evaluation of fissionable, low energy, s-wave-only, materials is carried out with a Reich-Moore formalism, then the parameters may be transformed to the Adler-Adler representation. R-M has some advantages in evaluating data, mainly that it uses resonance spins, is more closely tied to familiar resonance parameters, and is more "physical", but the Adler format is more convenient for the user since it permits ψ- and χ-functions for Doppler broadening.

The computer code POLLA [Ref.5], as well as some others, will convert a set of Reich-Moore multilevel s-wave resonance parameters to Adler format. If the conversion causes differences between the Adler and R-M cross sections which exceed 0.l%, these should be put into File 3, since it is not the intent of the procedure to in any way alter the original cross sections. Such differences can possibly be reduced by feeding the POLLA output parameters to a least-squares search code based on the Adler formalism, and "fitting" the original R-M values.

According to the discussion in BNL-50296[28], the Reich-Moore code RAMPl, incorporated in RESEND, sets the shift factor equal to zero. This is correct for s-waves, and should pose no problem for p- and d-waves, provided that the evaluator has included this shift factor when the calculation was performed.

2.4.10. Competitive Width in the Resonance Region

2.4.10.1. Resolved Region

Procedures for the Resolved Resonance Region are contained in Section D.3.l of Appendix D.

2.4.10.2. 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.

2.4.11. Negative Cross Sections in the Resolved Resonance Region

2.4.11.1. 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, 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

[28] M.R. Bhat, **BNL-50296** (ENDF l48) *ENDF/B Processing Codes for the Resonance Region*, June, l97l,

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 6).

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 rarely 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.

2.4.11.2. 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.

2.4.11.3. 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.

2.4.11.4. In the 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.

2.4.12. 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.l3. 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.0).

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/B 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±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/B 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 $\varphi_l(ka)$.

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.

For ENDF/B-VI, 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 HRF and GRM formalisms.

2.4.14. The Multilevel Adler-Gauss Formula for MLBW

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

$$\begin{aligned}
&\sigma_{n,\gamma}^{MLBW}(E) \equiv \sigma_{n,\gamma}^{SLBW}(E)\,, \\
&\sigma_{n,f}^{MLBW}(E) \equiv \sigma_{n,f}^{SLBW}(E)\,, \\
&\sigma_{n,n}^{MLBW}(E) \equiv \sigma_{n,n}^{SLBW}(E) + \sum_{l=0}^{NLS-1} \sigma_{n,n,RRI}^{l}(E)\,,
\end{aligned} \tag{0.16}$$

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

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=2}^{NR_J}\sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left[(E-E'_r)(E-E'_s)+\Gamma_r\Gamma_s/4\right]}{\left[(E-E'_r)^2+(\Gamma_r/2)^2\right]\left[(E-E'_s)^2+(\Gamma_s/2)^2\right]} \tag{0.17}$$

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 ~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. Most recently, DeSaussure, Olsen, and Perez (Reference 6) have written it compactly as

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{G_r\Gamma_r + 2H_r(E-E'_r)}{(E-E'_r)^2+(\Gamma_r/2)^2}\,, \quad \text{where}$$

$$G_r = \frac{1}{2}\sum_{s=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{ns}(\Gamma_r+\Gamma_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2}\,, \quad s \neq r \tag{0.18}$$

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

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, Section 2.4.19, also reduces computing time.

2.4.l5. Notes on the Adler Formalism

Questions concerning the ENDF/B treatment of the Adler formalism are enumerated below[29], 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 D-7, and the format descriptions of pages 7.9 and N-l2 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 $DET_N = DEF_N = DEC_N$ and $DWT_N = DWF_N = DWC_N$. 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/B 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/B 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:**

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

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

and then the combination:

$$vG_t + (\mu - E)\, H_t\ .$$

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

$$vG_c + (\mu - E)\, H_c \quad \text{(capture);}$$
$$vG_f + (\mu - E)\, H_f \quad \text{(fission);}$$

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

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

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 7.

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.

2.4.16. Multilevel Versus Single-Level Formalisms in the Resolved and Unresolved Resonance Regions

2.4.16.1. In the Resolved Resonance Region

The SLBW formalism is 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 should 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 low-energy fissionable s-wave evaluations. All of its cross sections are non-negative, and its only significant drawbacks, apart from the effort required for its application, are 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 makes a very 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, R-matrix, or the hybrid R-function can be used. The latter two provide more detail in describing competitive reactions, plus angular distributions, and allow treating resonances with both $l>0$ and $I>0$.

Multi-channel 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 are presented in ENDF/B as file 3 pointwise cross sections, although the new general R-matrix format can handle this case.

2.4.16.2. 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/B, for the reason that no significant multilevel effect can be 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 [Ref.8].

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.

2.4.17. Preferred Formalisms for Evaluating Data

1. <u>Light nuclei</u>: Use multilevel, multichannel R-matrix. Present as pointwise cross sections in file 3.

2. <u>Materials with negligible or moderate multilevel effects, and no multichannel interference</u>: Hybrid R-function, 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 2.4.14. For ENDF/B-VI, the Hybrid R-function is restricted to the structural materials (see next paragraph). However, it may still be a useful evaluation tool for other materials, because it treats level-level interference exactly, whereas MLBW still requires some separation between interfering resonances. In addition, HRF and RM provide the angular distribution of elastically-scattered neutrons, which MLBW does not. It can thus improve the quality of evaluations that are ultimately presented in ENDF as MLBW- plus-background. Note that the Reich-Moore and Hybrid R-Function formalisms are essentially equivalent when the fission widths are

zero. The differences are related to the treatment of competitive reactions and channel dependent radii. Therefore, evaluators can use existing RM codes for calculating HRF parameters, apart from the case where both *l*>0 and I>0.

3.

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

4. Materials with observable channel-channel interference: Reich-Moore or General R-matrix. 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/B. 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).
5. Materials with channel-channel interference and one or more competitive reactions: R-matrix, using the format LRF=5 to present the parameters.

2.4.18. Computer Time for Generating MLBW Cross Sections

Previous solutions to the problem of evaluating the double-sum form of the MLBW resonance-resonance interference term in a reasonable amount of time have been to use the amplitude-squared form from which it was derived, and kernel-broaden it, or to optimize the calculation of inner and outer loop quantities.

A third solution is to use the Multilevel Adler-Gauss formulas discussed in Section 2.4.14 and possibly approximate the energy-dependence of the G_r- and H_r-coefficients.

The amplitude-squared form of MLBW is discussed in Section 2.4.l9.

2.4.19. Amplitude-Squared Form of the MLBW Formulas

The form of the MLBW scattering cross section given in Appendix D and in Section 2.4.l4, is mathematically identical to the more fundamental "amplitude-squared" form given in Appendix D, as Equations (5) - (7) of Section D.l.2.

Those equations can be coded in complex Fortran, or broken up into their real and imaginary parts before coding. The essential point is that they sum the resonances before squaring. This avoids turning two "linear" sums into one "quadratic" one. If an isotope has 200 resonances, the above formulas have two sums with 200 terms each, whereas the ENDF form has a sum with 40000 cross terms. A discussion of points to consider in coding the above equations is given in Sections 2.4.23 and 2.4.24.

The main drawback to the above equations is that they do not admit Doppler-broadening with ψ- and χ-functions, but require kernel methods instead.

2.4.20. 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 $\vec{J} = \vec{s} + \vec{l}$, 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:

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

The penentrabilities 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 (αIiJ*l*s) is denoted by c, then the total width for the level is $\Gamma = \Sigma_c\Gamma_c$. [$\Sigma_c$ 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/B.

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±1/2. If I = 0, there is only one channel, s = i = ½; hence the restriction, 1.0≤AMUN≤ 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

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

   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→∞. 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, $\vec{l}$ and is the orbital angular momentum of the inelastically scattered neutron. Since the daughter nucleus may have a spin $\vec{I}$ different from the target spin I, $\vec{l}$ may be different from *l*, and the number of channel spin values μ_{lJ} may be different from μ_{lJ} .

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.

2.4.21. Procedures for the Unresolved Resonance Region

Up to 250 energy points are permitted for specifying energy-dependent average parameters. This number is presumed to be sufficient to reproduce the gross structure in the unresolved cross sections. 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 10000-point limitation. Under this option, File 3 represents the entire dilute unresolved cross section, 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 250-point limitation 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.

2.4.22 Procedures for Computing Angular Distributions in the Resolved Resonance Range

2.4.22.1. 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), the GRM format (Section D.1.5.2), or the HRF format (Section D.1.6.1), 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 [Ref. 7] 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 GRM and HRF formats, is given in Sections D.1.5.9 and D.1.6.5. If the Reich-Moore format is used without its fission channels, then it reduces to an R-function and the HRF angular distribution applies to it as well. 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 formulas define a center-of-mass distribution, even the isotropic case generally defines an anisotropic

laboratory distribution.

In principle, similar angular distribution formulas 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 thirty-five 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/B 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.

2.4.22.2 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 anti-resonances ("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 to 1200 angular distributions, which is usually not enough to represent a fully-detailed Blatt and Biedenharn representation. The recommended ENDF/B procedure is for the evaluator to provide an under-1200-energy-point 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, or μ. As always, the word ***significant*** is difficult to define exactly but the File 4 representation should be adequate 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.

2.4.22.3. Summary of Recommendations for Evaluation

1. **Supply an under-1200-point representation of the elastic scattering angular distribution in File 4. 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.

2.4.23. 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, A-A, and R-M formalisms, since the formats do not allow the evaluator to specify empty channels explicitly. For the HRF and GRM formalisms, 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:

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

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 $l > 0$ and $l > 0$, the same *J*-value may occur for each of the two channel spins, $s = l \pm 1/2$, and ***each*** of these *J*-values must be ***separately*** summed over. A width Γ_{lJ} is a sum of the two components, $\Gamma_{l\,s_1\,J}$ and $\Gamma_{l\,s_2\,J}$; and in the SLBW, MLBW, and A-A formalisms, only the sum is used. In the other formalisms the components must be specified separately; the specification is explicit for the HRF and GRM formats, and implicit (via the use of a signed AJ value) in Reich- Moore.

There is rarely enough information on channel-spin widths to guide the evaluator in apportioning the total width between the two sub-channels, 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,

$$\sum_{l=0}^{\infty} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \chi_{lsJ}$$

so the question of convergence arises. The simplest case is where the summand is an SLBW ***reaction*** term, as in Section D.1.6.2, 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, as in Section D.1.6.1, 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.

The Hybrid R-function and General R-matrix formalisms share the current restriction, NLS≤4 (*l*=0-3), so that if g-waves (*l*=4) are needed at high energy, their effect will have to be simulated in File 3. However, both of these formalisms admit (tabulated) optical model phase shifts, which provide more flexibility than the hard-sphere ones.

For the two R-formalisms, 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, as in Sections D.1.5.9 and D.1.6.5, 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.

2.4.24. Channel Spin and Other Considerations

For the General R-Matrix and Hybrid R-Function formalisms, channel spin is explicit and the evaluator must in general provide partial widths which depend on s as well as *l* and J. In two special cases, I=0 and *l*=0, no information is required beyond the Γ_{lJ} which are usually provided. If I=0, s is uniquely equal to 1/2 and may simply be dropped from the formalism. If *l*=0, s is the same as J and will therefore present no more difficulty for the evaluator than the usual problem of specifying J for each resonance. In the other cases, some division of the "total" width between the two s-values will be needed. Occasionally, experimental guidance will be available, but if not, the division will be rather arbitrary. The two simplest choices are "all or nothing" and "50/50". The cross section is expected to be insensitive to the division, while the angular distributions may show an effect. More

CSEWG experience is needed in this area.

For the Adler-Adler formalism, the usual area of application is to low-energy fissile nuclides, with l = 0, so that 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.

MLBW is essentially the same as the Hybrid R-Function, except that 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.

$$\Gamma_{lJ} = \Gamma_{ls_1J} + \Gamma_{ls_2J}$$

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**

$$\frac{4\pi}{k^2}(2l+1)\sin^2\phi_l\,.$$

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 admit ψ,χ 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 through D.2.4 attempt to clarify the situation with respect to level densities, strength functions, and spin statistics.

2.5. References for Chapter 2

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3. FILE 3, REACTION CROSS SECTIONS

3.1. General Description

Reaction cross sections and auxiliary quantities are given in File 3 as functions of energy E, where E is the incident 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 (MT number); see Section 0.5 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 $a+A \rightarrow b+c+...+B$, $QM=[(m_a+m_A)-(m_b+m_c+...+m_B)](9.315016 \times 10^8)$ if the masses are in amu. (See paragraph 3.3.2).
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 paragraph 3.3.2.)
LR	Complex or "breakup" reaction flag. Indicates that additional particles not specified by the MT number will be emitted. See Sections 0.5.5 and 3.4.4.
NR,NP,E_{int}	Standard TAB1 parameters.
σ(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 cover an energy range up to a common upper limit of at least 20 MeV, and the data must extend to a lower limit of the reaction threshold or 10^{-5} eV whichever is higher. For other reactions, the cross section should start at the reaction threshold energy (with a value of 0.0 barns) and should continue up to a **common upper energy limit**.

In the case where there is a change in the representation above a given energy, *e.g.*, a change from separate reactions to MT=5 (sum of reactions not given separately in other sections), the following procedure should be used. For the cross sections in the lower energy region, there should be a duplicate point with a value of zero at the last energy for a which a non-zero cross section is given, and a point with a value of zero at the common upper energy limit. Similarly, for the cross sections in the upper energy region, there should be a duplicate point with a value of zero at the first energy for a which a non-zero cross section is given, and a zero value at the low energy limit. The evaluator should document the change in representation in the File 1 comments.

For charged-particle emission, the cross section is usually very small from the threshold (or lower limit) up to an ***effective threshold*** defined by a noticeable cross section (for example, 10^{-10} barns). The evaluator should tabulate a cross section of 0.0 in such a range in order to avoid interpolation problems.

Sometimes ENDF reactions have an apparent upper limit lower than the upper limit for the material due to changes in representation in different sections. For example, there might be a change from discrete levels to a continuum rule, or from separate reactions to MT=5. Such cross sections must be ***double valued*** at the highest energy for which the cross section is nonzero. The second cross section at the discontinuity must be zero, and it must be followed by another zero value at the upper limit. This will positively show that the cross section has been truncated. For such reactions, there will be another reaction with an artificial threshold at the discontinuity. The cross sections must be chosen in such a way that their sum is continuous.

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 at the limits of the resonance ranges or where reactions change representation), because such features cannot be realistically Doppler broadened.

3.3.2. Q Values

Accurate 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.

As an example to clarify the use of QM and QI, consider the reaction $\alpha+{}^{9}Be\rightarrow n+X$. 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 high probability by breaking up into three alpha particles (7.275 MeV is required). This pattern can be represented as follows.

Reaction	QM	QI	EX	MT
9Be(a,n_0)12C	5.702	5.702	0.000	50
9Be(a,n_1)12C	5.702	1.263	4.439	51
9Be(a,n_2)12C(3α)	-1.573	-1.952	7.654	52
9Be(a,n_3)12C(3α)	-1.573	-3.939	9.641	53
9Be(a,n_C)12C(3α)	-1.573	-1.573		91

The gamma for the second reaction is not written 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 materials 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 50,000. 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 not usually well defined in reaction evaluations since they are 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 usually not be given. 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,...), and other neutron emitting reactions such as MT=16,17,22,28,.... Specific procedures for each reaction 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 production, 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 40-100 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 components 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 in 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.

The total cross section, as well as any partial cross section, must be represented by 50,000 incident-energy points or fewer. 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, then the elastic cross section plus all nonelastic components 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. If a precise total cross section is required between the energy points provided, it is recommended that the total be calculated from the sum of the partials rather than interpolated directly from MT=1.

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 obtained by subtracting the nonelastic cross section from the total cross section. This procedure can cause problems. The result is an elastic scattering cross section that contains 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 used to prepare 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)

A 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 particular section (MT) represents (n,n'gamma). 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, 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. When inelastic photons cannot be separated from other nonelastic photons, they can be included in MF=13, MT=3.

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 0.6)30 . 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 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.

30 LR=31 is still allowed, however, to uniquely define the γ-decay when using MF=3, and MF=12 (or 15) and MF=4.

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. Energy distributions are given in File 5. 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, discrete levels, and a continuum (MT=103, 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. 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).

3.5. Procedures for Incident Charged Particles and Photons

See Table 0.1 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, σ 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, and, in this case, should be set to epsilon, *e.g.*, 10^{-38}. The first and 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's for Total Inelastic σ
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, but it should be repeated for each isotope of the element. 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.

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 must 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 2.4.22 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 will be 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.*,

$$\int_{-1}^{1} f(\mu, E)d\mu = 1$$

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,

$$f(\mu, E) = \frac{2\pi}{\sigma_s(E)}\sigma(\mu, E) = \sum_{l=0}^{NL} \frac{2l+1}{2} a_l(E) P_l(\mu)$$

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 and it is understood that $a_0 = 1.0$.

The angular distributions may be given by one of two methods, and in either the center-of-mass (CM) or laboratory (LAB) systems. Using the first method, the distributions are given by tabulating the normalized probability distribution, $f(\mu,E)$, as a function of incident energy. Using the second method, 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

$$\sigma(\mu,E)=\frac{\sigma_s(E)}{2\pi}f(\mu,E)$$

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

$$\sigma(\mu,E)=\frac{\sigma_s(E)}{2\pi}\sum_{l=0}^{NL}\frac{2l+1}{2}a_l(E)P_l(\mu)$$

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.

Elastic transformation matrices are no longer permitted in ENDF formatted files.

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. If the section contains a description of the angular distributions for elastic scattering, the transformation matrix is given first (if present) and this is followed by the representation of the angular distributions.

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 normalized 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 (NE≤2000)
NL	Highest order Legendre polynomial that is given at each energy (NL≤64)
NM	Maximum order Legendre polynomial that will be required (NM≤64) to describe the angular distributions of elastic scattering in either the center-of-mass or the laboratory system. NM should be an even number.

V_K	Matrix elements of the transformation matrices $V_K=U^{-1}_{l,m}$, if LCT=1 (data given in LAB system) $V_K=U_{l,m}$, if LCT=2 (data are given in CM system)
NP	Number of angular points (cosines) used to give the tabulated probability distributions for each energy (NP≤20l)

Other commonly used variables are given in the Glossary (Appendix A).

The structure of a section depends on the values of LTT (representation used, $a_l(E)$ or $f(\mu,E)$) but it always starts with a HEAD record of the form

```
[MAT, 4, MT/ ZA, AWR,   0, LTT,  0,  0]HEAD
```

4.2.l. Legendre Polynomial Coefficients: LTT=1 and 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/ Eint] TAB2
[MAT, 4, MT/   T,  E1,  LT,   0, NL,  0/al(E1)]LIST
[MAT, 4, MT/   T,  E2,  LT,   0, NL,  0/al(E2)]LIST
-----------------------------------------------
-----------------------------------------------
[MAT, 4, MT/   T,  ENE,  LT,   0, NL,  0/al(ENE)]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 and 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/Eint] TAB2
[MAT, 4, MT/   T,  E1 ,  LT,   0, NR, NP/μint /f(μ,E1)]TABl
[MAT, 4, MT/   T,  E2 ,  LT,   0, NR, NP/μint /f(μ,E2)]TABl
--------------------------------------
--------------------------------------
[MAT, 4, MT/   T,  ENE ,  LT,   0, NR, NP/μint /f(μ,ENE)]TABl
[MAT, 4,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

T and LT are normally zero.

4.2.3. All angular Distributions are Isotropic: LTT=0 and 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 and 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_NE,  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_1,  LT,   0,  NR,  NP/μ_int /f(μ,E_NE1)]TABl
    ------------------------------
    ------------------------------
[MAT, 4, MT/   T,  E_NE,  LT,   0,   NR, NP/μ_int /f(μ,E_NET)]TABl
           (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.

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 *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 a value of 64. If more than 64 coefficients appear to be required to obtain a non-negative distribution, a constrained Legendre polynomial fit to the data should be given. 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 interpolation scheme for $f(\mu,E)$ vs. μ should be log-linear (INT=4), and that for $f(\mu,E)$ vs. E should be linear-linear (INT=2).

Accurate angular distributions for the thermal energy range can be obtained by using File 7 or a detailed free-gas calculation. File 4 contains distributions for stationary free targets only.

The formats given above do not allow an energy-dependent transformation matrix to be given, so transformation matrices may not be given for nonelastic scattering reaction types. When a processing code wishes to transfer inelastic level angular distributions expressed as Legendre polynomial coefficients from the LAB to the CM system, or CM to LAB system, a distribution

should be generated and transformed point by point to the desired frame of reference. The point-wise angular distributions can then be converted to Legendre polynomial coefficients in the new frame of reference.

4.4. Procedures for Specific Reactions

4.4.l. Elastic Scattering (MT=2)

1. Legendre polynomial representations should be used for the elastic scattering angular distributions and discrete channel scattering, and must be given in the CM system. When this representation is given, the maximum order of the polynomial for each incident energy should be even and l_{max} must be ≤64.

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 independent of one another. Remember, processing codes operate on MT=2 data 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, this process must be done in a consistent manner. The same contributions must be subtracted from both the integrated elastic scattering and the angular distribution. Be sure that these contributions are included in the inelastic scattering cross section (both integrated data and angular distributions). 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 2000.

5. An incident energy point must be given at 10^{-5} eV. A point must be given at the highest energy point for which the angular distribution is isotropic. The highest incident energy must be the highest energy for which cross section data are given in File 3, at least 20 MeV.

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).

$$\sigma(0°) \geq \sigma_W = \left(\frac{\sigma_T}{4\pi\lambda\!\!\!^{-}}\right)^2$$

$$\sigma_W = X\ E_0 \frac{AWR^2}{(1+AWR)^2}\ \sigma_T^2 \qquad \frac{\text{barns}}{\text{steradian}}$$

where E_0 is in eV and σ_T in barns; see Appendix H for value of X.

Care should be taken to observe this inequality, especially at high energies.

4.4.2. Inelastic Scattering Cross Sections

1. Do not give angular distribution data for MT = 4.
2. Always give angular distribution data for any one of the following if they are given in File 3: MT = 51 through 91.
3. Discrete channel (two body) angular distributions (*e.g.*, MT = 2, 51 - 90, 701...) should be given as Legendre coefficients in the CM system.
4. The continuum reaction (MT = 91) should 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 Neutron 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.

4.4.4. Charged-Particle Producing Reactions

Distributions for charged particles from two-body reactions in the 600 series can be given in File 4 using the CM system, if desired. (Continuum reactions where only one charged particle is possible (*e.g.*, 649, 699, *etc*.) can also be given in File 4 using the LAB system. If angular data is needed for more complex reactions, File 6 is more appropriate.)

5. FILE 5, ENERGY DISTRIBUTION OF SECONDARY PARTICLES

5.1. General Description

File 5 is used to describe the energy distributions of secondary particles expressed as normalized probability distributions. File 5 is for incident neutron reactions and spontaneous fission only, and should not be used for any other incident particle. Data will be given in File 5 for all reaction types that produce secondary neutrons, unless the secondary neutron energy distributions can be implicitly

determined from data given in File 3 and/or File 4. 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. No data will be given for neutrons that result from excitation of discrete inelastic levels when data for these reactions are given in both File 3 and File 4 (MT=51, 52, ..., 90).

Data should be given in File 5 for MT=91 (inelastic scattering to a continuum of levels), MT=18 (fission), MT=16 (n,2n), MT=17 (n,3n), MT=455 (delayed neutrons from fission), and certain other nonelastic reactions that produce secondary neutrons. The energy distribution for spontaneous fission is given in File 5 (in sub-library 4).

File 5 may also contain energy distributions of secondary charged particle 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

$$\frac{d\sigma(E \rightarrow E')}{dE'} = m\sigma(E)\,p(E \rightarrow E') \tag{5.2}$$

where $\sigma(E)$ is the cross section as given in File 3 for the same reaction type number (MT) and m is the neutron multiplicity for this reaction (m is implicit; *e.g.*, m=2 for n,2n reactions).

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 different analytic representations;

$$p(E \rightarrow E') = \sum_{k=1}^{NK} p_k(E)\, f_k(E \rightarrow E') \tag{5.3}$$

and at a particular incident neutron energy E,

$$\sum_{k=1}^{NK} p_k(E) = 1$$

where $p_k(E)$ is the fractional probability that the distribution $f_k(E \rightarrow E')$ can be used at 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.

Secondary Energy Distribution Laws

LF = l, ***Arbitrary tabulated function***:

$$f(E \rightarrow E') = g(E \rightarrow E')$$

A set of incident energy points is given, E and $g(E \rightarrow E')$ is tabulated as a function of E'.

LF = 5, ***General evaporation spectrum***:

$$f(E \rightarrow E') = g\left(E'/\theta(E)\right)$$

$\theta(E)$ is tabulated as a function of incident neutron energy, E; $g(x)$ is tabulated as a function of x, $x = E'/\theta(E)$.

LF = 7, ***Simple fission spectrum (Maxwellian)***:

$$f(E \rightarrow E') = \frac{\sqrt{E'}}{I} e^{-E'/\theta(E)}$$

I is the normalization constant,

$$I = \theta^{3/2}\left[\frac{\sqrt{\pi}}{2} erf\left(\sqrt{(E-U)/\theta}\right) - \sqrt{(E-U)/\theta}\, e^{-(E-U)/\theta}\right]$$

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 $0 \le E' \le (E - U)$.

LF = 9, **Evaporation spectrum:**

$$f(E \rightarrow E') = \frac{E'}{I} e^{-E'/\theta(E)}$$

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 $0 \le E' \le (E–U)$

LF = 11, Energy dependent Watt spectrum:

$$f(E \to E') = \frac{e^{-E'/a}}{I} \sinh\left(\sqrt{bE'}\right)$$

I is the normalization constant,

$$I = \frac{1}{2}\sqrt{\frac{\pi a^3 b}{4}} \exp\left(\frac{ab}{4}\right)\left[erf\left(\sqrt{\frac{E-U}{a}} - \sqrt{\frac{ab}{4}}\right) + erf\left(\sqrt{\frac{E-U}{a}} + \sqrt{\frac{ab}{4}}\right)\right]$$

$$- a \exp\left[-\left(\frac{E-U}{a}\right)\right] \sinh\sqrt{b(E-U)}$$

a and *b* are energy dependent;

U is a constant introduced to define the proper upper limit for the final particle energy such that $0 \le E' \le (E\text{-}U)$

LF = 12, Energy dependent fission neutron spectrum (Madland and Nix):

$$f(E \to E') = \frac{1}{2}\left[g(E', EFL) + g(E', EFH)\right]$$

where

$$g(E', EF) = \frac{1}{3(EF \times TM)^{1/2}}\left[u_2^{3/2} E_1(u_2) - u_1^{3/2} E_1(u_1) + \gamma(3/2, u_2) - \gamma(3/2, u_1)\right]$$

$$u_1 = \left(\sqrt{E'} - \sqrt{EF}\right)^2 \Big/ TM$$

$$u_2 = \left(\sqrt{E'} - \sqrt{EF}\right)^2 \Big/ TM$$

EFL and *EFH* are constants, which represent the average kinetic energy per nucleon of the average light and heavy fragments, respectively.

TM depends upon the incident neutron energy,

$E_1(x)$ 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 Sec. 5.4.10.

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.

Note: Distribution laws are not presented for LF = 2, 3, 4, 6, 8, or 10. These laws are no longer used.

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 $0 \le E' \le E - U$ (given in the LAB 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.l.).
$\mathbf{p_k(E_N)}$	Fractional part of the particular cross section which can be described by the kth partial energy distribution at the Nth incident energy point. NOTE: $\sum_{k=1}^{NK} p_k(E_N) = 1.0$
$\mathbf{f_k(E \rightarrow E')}$	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 used in the energy-dependent fission neutron spectrum (Madland and Nix), LF = 12.
TM	Maximum temperature parameter, TM(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 (NE≤200.)
NF	Number of secondary energy points in a tabulation. (NF≤l000.)

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 following.

LF = 1, *Arbitrary tabulated function*

```
[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→E'_2),  E'_3,g(E_1→E'_3),
            ---------------------------------
            ---,E'_NF-1,g(E_1→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→E'_2),  E'_3 ,g(E_2→E'_3),----
            ----------------------------------
           ---, E'_NF-1,g(E_2→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→E'_2), E'_3,g(E_NE→E'_3)----
            --------------------------------
            --- ,E'_NF-1,g(E_NE→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.

LF = 5, *General evaporation spectrum*

```
[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 / θ(E)]TAB1
[MAT, 5, MT/ 0.0, 0.0,  0,  0, NR, NF/ x_int / g(x)]TAB1   (x=E'/θ(E))
```

LF = 7, *Simple fission spectrum (Maxwellian)*

```
[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
```

LF = 9, *Evaporation spectrum*

```
[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
```

LF = 11, *Energy-dependent Watt spectrum*

```
[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
```

LF = 12, *Energy-dependent fission neutron spectrum (Madland and Nix)*

```
[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 /TM(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.l. General Comments

Do not give File 5 data for the discrete level excitation data 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.

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.

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.

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.

Note that prompt fission spectra are given under MT=18, 19, 20, 21, and 38. The delayed fission spectra are given under MT=455. The energy distribution for prompt spontaneous fission is given in File 5 for MT=18, but in sublibrary 4. It is used with $\bar{\nu}_p$ from File 1 (MT=456) to determine the prompt spontaneous fission spectrum. The delayed spontaneous fission spectrum is determined from $\bar{\nu}_d$ from File 1 (MT=455) and the delayed energy spectrum in File 5 MT=455. Note that for the specification of spontaneous spectra no cross sections from File 3 are required.

5.4.2. LF = 1 (Tabulated Distributions)

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. LF = 7 (Maxwellian Spectrum)

A linear-linear interpolation scheme is preferred for specifying the nuclear temperature as a function of energy.

5.4.4. LF = 9 (Evaporation Spectrum)

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. LF = 11 (Watt Spectrum)

A linear-linear interpolation scheme is preferred for specifying the parameters a and b as a function of energy.

5.4.6. LF = 12 (Madland-Nix Spectrum)

A log-log interpolation scheme may be used for specifying the parameter TM 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 Eth 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.

$$U = -Q, \text{ where Q is the reaction Q-value.}$$

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

$$U = -Q \text{ , where Q is the energy required for 3-body breakup.}$$

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. θ(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:

$$E_{avail} = E + \frac{1 + AWR}{AWR} Q,$$

where E_{avail} is greater than the neutron multiplicity times the average energy of all the emitted neutron $\nu\ \overline{E}'$, where ν is the multiplicity. The mean energy should be calculated from the distribution at each value of E. This mean is analytic in the four cases given below.

LF	$\overline{E'}$
7	$\frac{3}{2}\theta - \frac{\theta^{5/2}}{I}\left(\frac{E-U}{\theta}\right)^{3/2} e^{-(E-U)/\theta}$
9	$2\theta - \frac{\theta^{3}}{I}\left(\frac{E-U}{\theta}\right)^{2} e^{-(E-U)/\theta}$
11	$\frac{1}{2I}\left\{ a\exp\left(\frac{ab}{4}\right)\sqrt{\pi\frac{a^3 b}{4}}\left(3+\frac{ab}{2}\right)\left[\frac{erf\left(\sqrt{\frac{E_r}{a}}-\sqrt{\frac{ab}{4}}\right)+erf\left(\sqrt{\frac{E_r}{4}}+\sqrt{\frac{ab}{4}}\right)}{2}\right] - 3a^2\sqrt{ab}\exp\left(-\frac{E_r}{a}\right)\left[\sqrt{\frac{E_r}{a}}\cosh\sqrt{bE_r}-\sqrt{\frac{ab}{4}}\sinh\sqrt{bE_r}\right] - 2a^2\exp\left(-\frac{E_r}{a}\right)\left[\left(\frac{E_r}{a}+\frac{ab}{4}\right)\sinh\sqrt{bE_r}-\sqrt{bE_r}\cosh\sqrt{bE_r}\right]\right\}$
	where $E_r = E-U$
12	$\frac{1}{2}(EFL + EFH) + \frac{4}{3}TM$

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 LF = 12, Energy-Dependent Fission Neutron Spectrum (Madland and Nix)

Integral over finite energy range [a,b].

Set:

$$\alpha = \sqrt{TM}\,,\ \beta = \sqrt{EF}$$

$$A = \left(\sqrt{a} + \beta\right)^2 / \alpha^2$$

$$B = \left(\sqrt{b} + \beta\right)^2 / \alpha^2$$

$$A' = \left(\sqrt{a} - \beta\right)^2 / \alpha^2$$

$$B' = \left(\sqrt{b} - \beta\right)^2 / \alpha^2$$

Then,

the integral is given by one of the following three expressions depending on the region of integration in which a and b lie.

<u>Region I</u> (a > EF, b > EF)

$$3(ET\ TM)^{1/2}\int_a^b g(E',EF)dE' =$$

$$\left[\left(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2\right)E_1(B) - \left(\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2\right)E_1(A)\right]$$

$$-\left[\left(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2\right)E_1(B') - \left(\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2\right)E_1(A')\right]$$

$$+\left[\left(\alpha^2 B - 2\alpha\beta B^{1/2}\right)\gamma(3/2,B) - \left(\alpha^2 A - 2\alpha\beta A^{1/2}\right)\gamma(3/2,A)\right]$$

$$-\left[\left(\alpha^2 B' + 2\alpha\beta B'^{1/2}\gamma(3/2,B'\right) - \left(\alpha^2 A' + 2\alpha\beta A'^{1/2}\right)\gamma(3/2,A')\right]$$

$$-\frac{3}{5}\alpha^2\left[\gamma(5/2,B) - \gamma(5/2,A) - \gamma(5/2,B') - \gamma(5/2,A')\right]$$

$$-\frac{3}{5}\alpha\beta\left[e^{-B}(1+B) - e^{-A}(1+A) + e^{-B'}(1+B') - e^{-A'}(1+A')\right]$$

<u>Region II</u> (a < EF, b < EF)

$$3(ET\ TM)^{1/2}\int_a^b g(E',EF)dE' =$$

$$\left[\left(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2\right)E_1(B) - \left(\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2\right)E_1(A)\right]$$

$$-\left[\left(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2\right)E_1(B') - \left(\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2\right)E_1(A')\right]$$

$$+\left[\left(\alpha^2 B - 2\alpha\beta B^{1/2}\right)\gamma(3/2,B) - \left(\alpha^2 A - 2\alpha\beta A^{1/2}\right)\gamma(3/2,A)\right]$$

$$-\left[\left(\alpha^2 B' - 2\alpha\beta B'^{1/2}\gamma(3/2,B'\right) - \left(\alpha^2 A' - 2\alpha\beta A'^{1/2}\right)\gamma(3/2,A')\right]$$

$$-\frac{3}{5}\alpha^2\left[\gamma(5/2,B) - \gamma(5/2,A) - \gamma(5/2,B') + \gamma(5/2,A')\right]$$

$$-\frac{3}{5}\alpha\beta\left[e^{-B}(1+B) - e^{-A}(1+A) + e^{-B'}(1+B') + e^{-A'}(1+A')\right]$$

<u>Region III</u> (a < EF, b > EF)

$$
\begin{aligned}
3(ET\ TM)^{1/2}\int_a^b g(E',EF)dE' = \\
&\left[\left(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2\right)E_1(B) - \left(\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2\right)E_1(A)\right] \\
&-\left[\left(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2\right)E_1(B') - \left(\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2\right)E_1(A')\right] \\
&+\left[\left(\alpha^2 B - 2\alpha\beta B^{1/2}\right)\gamma(3/2,B) - \left(\alpha^2 A - 2\alpha\beta A^{1/2}\right)\gamma(3/2,A)\right] \\
&-\left[\left(\alpha^2 B' + 2\alpha\beta B'^{1/2}\gamma(3/2,B'\right) - \left(\alpha^2 A' + 2\alpha\beta A'^{1/2}\right)\gamma(3/2,A')\right] \\
&-\frac{3}{5}\alpha^2\left[\gamma(5/2,B) - \gamma(5/2,A) - \gamma(5/2,B') + \gamma(5/2,A')\right] \\
&-\frac{3}{5}\alpha\beta\left[e^{-B}(1+B) - e^{-A}(1+A) + e^{-B'}(1+B') + e^{-A'}(1+A')\right]
\end{aligned}
$$

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.

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 File 4 and File 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:

$$\sigma_i(\mu, E, E') = \sigma(E) y_i(E) f_i(\mu, E, E') / 2\pi \tag{0.19}$$

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

$$\int dE' \int d\mu \quad f_i(\mu, E, E') = 1 \tag{0.20}$$

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≤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). NK≤2000.

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.

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 for 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, E_{int} Standard TAB1 parameters.

A section of 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 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. 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.

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 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/Eint]TAB2
[MAT, 6, MT/  0.0,       E1,      ND,   NA,   NW,  NEP/
              E'1, b0(E1,E'1),b1(E1,E'1),------ bNA(E1,E'1),
              E'2, b0(E1,E'2), ----------------------
             E'NEP,b0(E1,E'NEP), ------------  bNA(E1,E'NEP)]LIST
            ---------------------------------------
            <continue with LIST structures for the rest of 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).

LANG=1

If LANG=1, Legendre coefficients are used as follows:

$$f_i(\mu, E, E') = \sum_{l=0}^{NA} \frac{2l+1}{2} f_l(E, E') P_l(\mu) \tag{0.21}$$

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); instead, $f_0(E,E')$ gives the total probability of scattering from E to E′ integrated over all angles. This is just the function g(E,E′) normally given in File 5. The Legendre coefficients are stored with f_0 in b_0, f_1 in b_1, *etc*.

LANG=2

For LANG=2, the angular distribution is 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.

This formulation addresses reactions of the form

$$A + a \rightarrow C \rightarrow B + b,$$

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*

$$\varepsilon_a = E_a \times \frac{AWR_A}{AWR_A + AWR_a}$$

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*

$$\varepsilon_b = E_b \times \frac{AWR_B}{AWR_B + AWR_b}$$

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

$$f(\mu_b, E_a, E_b) = 0.5 * f_0(E_a, E_b)\left[\frac{a(E_a, E_b)}{\sinh\left(a(E_a, E_b)\right)}\left[\begin{array}{l}\cosh\left(a(E_a, E_b)\mu_b\right)\\ +r(E_a, E_b)\sinh\left(a(E_a, E_b)\mu_b\right)\end{array}\right]\right] \quad (0.22)$$

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

$$\begin{aligned} E_{b,lab} &= E_{b,cm} + \frac{AWR_a AWR_b}{(AWR_A + AWR_a)^2} E_{a,lab} + 2\frac{\sqrt{AWR_a}\sqrt{AWR_b}}{AWR_A + AWR_a}\sqrt{E_{a,lab}E_{b,cm}}\,\mu_{b,cm} \\ \mu_{b,lab} &= \sqrt{\frac{E_{b,cm}}{E_{b,lab}}}\mu_{b,cm} + \frac{\sqrt{AWR_a}\sqrt{AWR_b}}{AWR_A + AWR_a}\sqrt{\frac{E_{a,lab}}{E_{b,lab}}} \end{aligned} \quad (0.23)$$

The pre-compound fraction r, where r goes from 0.0 to 1.0, is usually computed by a model code, although it can be chosen to fit experimental data.

The formula for calculating the slope value $a(E_a,E_b)$31 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

$e_a = \varepsilon_a + S_a$	$e_b = \varepsilon_b + S_b$
$R_1 = \text{minimum}(e_a,E_{t1})$	$R_3 = \text{minimum}(e_a,E_{t3})$
$X_1 = R_1 e_b/e_a$	$X_3 = R_3 e_b/e_a$

The parameter values for light particle induced reactions as given in KA8832 are:

$C_1 = 0.04/\text{MeV}$	$C_2 = 1.8\times10^{-6}/\text{MeV}^3$
$C_3 = 6.7\times10^{-7}/\text{MeV}^4$	
$E_{t1} = 130$ 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 in MeV33 are:

31 Equation 10 of Ref. 2.

32 Table V of ref. 2.

33 Equation 4 of Ref. 2.

$$S_a = 15.68\left[A_C - A\right] - 28.06\left[\frac{(N_C - Z_C)^2}{A_A} - \frac{(N_A - Z_A)^2}{A_A}\right]$$
$$-18.56\left[A_C^{2/3} - A_A^{2/3}\right] + 33.22\left[\frac{(N_C - Z_C)^2}{A_C^{2/3}} - \frac{(N_A - Z_A)^2}{A_A^{2/3}}\right]$$
$$-0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_A^2}{A_A^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_A^2}{A_A}\right] - I_a$$

and

$$S_b = 15.68\left[A_C - A_B\right] - 28.07\left[\frac{(N_C - Z_C)^2}{A_A} - \frac{(N_B - Z_B)^2}{A_B}\right]$$
$$-18.56\left[A_C^{2/3} - A_B^{2/3}\right] + 33.22\left[\frac{(N_C - Z_C)^2}{A_C^{2/3}} - \frac{(N_B - Z_B)^2}{A_B^{2/3}}\right]$$
$$-0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_B^2}{A_B^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_B^2}{A_B}\right] - I_b$$

where

subscripts A, B, and C refer to the target nucleus, the residual nucleus, and the compound nucleus, as before,

N, Z, and A are the neutron, proton, and mass numbers of the nuclei,

I_a and 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).

The parameter $f_0(E_a,E_b)$ has the same meaning as f_0 in Eq. (6.3); that is, the total emission probability for this E_a and E_b. *The number of angular parameters (NA) is always 1 for LANG=2*, and f_0 and r are stored in the positions of b_0 and b_1, 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, S*a* and S_b will be identical.

LANG = 11-15

For LANG=11-15, a tabulated function is given for $f(\mu)$ using the interpolation scheme defined by LANG minus 10. For example, if LANG=12, use linear-linear interpolation (don't 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 $\mu_{NA/1}$ or above $\mu_{NA/2}$ is zero.

The tabulation is stored in the angular parameters as follows:

$b_0 = f_0$,
$b_1 = \mu_1$,
$b_2 = 0.5f_1(\mu_1)/f_0$,
$b_3 = \mu_2$,
...
...
$b_{NA} = 0.5f_{NA/2}(\mu_{NA/2})/f_0$.

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

$$\begin{aligned} p_i(\mu, E) &= \int dE' f_i(\mu, E, E') \\ &= 0.5 + \sum_{l+1}^{NL} \frac{2l+1}{2} a_l(E) P_l(\mu) \quad , \end{aligned} \tag{0.24}$$

where the P_l are the Legendre polynomials with the maximum order NL. Note that the angular distribution pi 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 *1n* p_i linear in μ.
NR, NE, E_{int}	standard TAB2 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
             ---------------------------
             <continue with LIST records for the
                 rest of the incident energies>
             ---------------------------
```

Note that LANG=0 is very similar to File 4, LTT=1, and LVT=0. The tabulated option is similar to File 4, LTT=2, LVT=0, 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).

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.*, nn?, pn) described using LAW=2 or 3 doesn't break up, its energy and angular distribution can be determined by 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.

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 (barns/sr) for distinguishable particles
$\sigma_{ci}(\mu,E)$	cross section for identical particles
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 and Z_2	charge numbers of the incident particle and target, respectively
s	spin (identical particles only, s = 0, 1/2, 1, 3/2, *etc*.)
A	target/projectile mass ratio
k	particle wave number (barns-1/2)
η	dimensionless Coulomb parameter

The cross sections can then be written

$$\sigma_{cd}(\mu,E)=\frac{\eta^2}{k^2(1-\mu)^2} \tag{0.25}$$

and

$$\sigma_{ci}(\mu,E)=\frac{2\eta^2}{k^2(1-\mu)^2}\left[\frac{1+\mu^2}{1-\mu^2}+\frac{(-1)^{2s}}{2s+1}\cos\eta\left(\ln\frac{1+\mu}{1-\mu}\right)\right] \tag{0.26}$$

where

$$k=\frac{A}{1+A}\left[\frac{2}{\hbar}m_1E\right]^{1/2} \tag{0.27}$$

$$\eta=Z_1Z_2\left[\left(\frac{e^4}{2\hbar^2}\right)\frac{m_1}{E}\right]^{1/2} \tag{0.28}$$

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

$$\begin{aligned}\sigma_{ed}(\mu,E)=\sigma_{cd}(\mu,E)&-\frac{2\eta}{1-\mu}\mathrm{Re}\left\{\exp\left(i\eta\ \ln\frac{1-\mu}{2}\right)\sum_{l=0}^{NL}\frac{2l+1}{2}a_l(E)P_l(\mu)\right\}\\&+\sum_{l=0}^{NL}\frac{2l+1}{2}b_l(E)P_l(\mu)\end{aligned} \tag{0.29}$$

and the cross section for identical particles is

$$\begin{aligned}\sigma_{ei}(\mu,E)&=\sigma_{ci}(\mu,E)\\&-\frac{2\eta}{1-\mu^2}\mathrm{Re}\left\{\sum_{l=0}^{NL}\left[\begin{array}{l}(1+\mu)\exp\left(i\eta\ \ln\frac{1-\mu}{2}\right)\\+(-1)^l(1-\mu)\exp\left(i\eta\ \ln\frac{1+\mu}{2}\right)\end{array}\right]\frac{2l+1}{2}a_l(E)P_l(\mu)\right\}\\&+\sum_{l=0}^{NL}\frac{4l+1}{2}b_l(E)P_{2l}(\mu)\end{aligned} \tag{0.30}$$

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

$$\sigma_{Rd}(\mu,E)=(1-\mu)\left[\sigma_{ed}(\mu,E)-\sigma_{cd}(\mu,E)\right] \tag{0.31}$$

and

$$\sigma_{Ri}(\mu,E) = (1-\mu^2)\left[\sigma_{ei}(\mu,E) - \sigma_{ci}(\mu,E)\right] \tag{0.32}$$

Then σ_R can be given as a Legendre polynomial expansion in the forms

$$\sigma_{Rd}(\mu,E) = \sum_{l=0}^{NL} \frac{2l+1}{2} c_{ld}(E) P_l(\mu) \tag{0.33}$$

and

$$\sigma_{Ri}(\mu,E) = \sum_{l=0}^{NL} \frac{4l+1}{2} c_{li}(E) P_{2l}(\mu) \tag{0.34}$$

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

$$\sigma_{NI}(\mu,E) = \int_{\mu_{\min}}^{\mu_{\max}} \left[\sigma_e(\mu,E) - \sigma_c(\mu,E)\right] d\mu \tag{0.35}$$

and

$$\begin{aligned} P_{NI}(\mu,E) &= \frac{\sigma_e(\mu,E) - \sigma_c(\mu,E)}{\sigma_{NI}(E)}, \ \mu_{\min} \le \mu \le \mu_{\max} \\ &= 0, \quad \text{otherwise,} \end{aligned} \tag{0.36}$$

where μ_{min} is -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 Eqs. (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 (Eq. 6.11, 6.12); LTP=2, residual cross section expansion as Legendre coefficients (Eq. 6.13 through 6.16); LTP=12, nuclear plus interference distribution with p_{NI} linear in μ (Eq. 6.17 and 6.18); LTP=14, tabulation with *ln* P_{NI} linear in μ (Eq. 6.17 and 6.18). LTP=15, tabulation with P_{NI} linear in μ (Eq. 6.17 and 6.18).
NR, NE, 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.

$A_i(E)$ Coefficients (a_i, b_i, or c_i as described below) in barns/sr or μ,p pairs with p dimensionless.

A subsection for LAW=5 has the following form:

```
[MAT, 6, MT/ SPI, 0.0, LIDP,  0,  NR,  NE/ Eint ]TAB2
[MAT, 6, MT/ 0.0,  E1,  LTP,  0,  NW,  NL/A1(E1)]LIST
             -------------------------------
             <continue with LIST records for the rest of the NE
                incident energies>
             -------------------------------
```

The coefficients in the text of the LIST 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}; and
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

$$P_i^{cm}(\mu, E, E') = C_n \sqrt{E'}(E_i^{\max} - E')^{(3n/2)-4} \tag{0.37}$$

where E_i^{max} is the maximum possible center-of-mass energy for particle i,
μ and E′ are in the cm system, and
C_n are normalization constants:

$$C_3 = \frac{4}{\pi(E_i^{\max})^2} \tag{0.38}$$

$$C_4 = \frac{105}{32(E_i^{\max})^{7/2}} \tag{0.39}$$

$$C_5 = \frac{256}{14\pi(E_i^{\max})^5} \tag{0.40}$$

In the laboratory system, the distributions become

$$P_i^{lab}(\mu, E, E') = C_n \sqrt{E'} \left[E_i^{\max} - \left(E^* + E' - 2\mu\sqrt{E^* E'} \right) \right]^{(3n/2)-4} \tag{0.41}$$

where μ and E' are in the laboratory system and E^* is given by

$$E^* = E \frac{A^{incident}}{(AWR + A^{exit})^2} \tag{0.42}$$

and $A^{incident}$ and A^{exit} are the mass ratios 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,

$$E_i^{\max} = \frac{M - m_i}{M} E_a \tag{0.43}$$

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 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 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

$$E_a = \frac{m_T}{m_p + m_T} E + Q \tag{0.44}$$

where m_T is the target mass,
m_p is the projectile mass,
E is the LAB energy, 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 parameters for incident energy, E.
NRM, NMU, μ_{int} normal TAB2 parameters for emission cosine, μ.
NRP, NEP, E'_{int} normal TAB1 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
             -------------------------------------
            <continue with TAB2 structures for the rest of the
                    NMU emission cosines>
            -------------------------------------
            <continue with TAB2/TAB1 structures for the rest
                  of the NE incident energies>
             -------------------------------------
```

where f(μ,E,E′) is defined as in Eq. (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/B-VI, and it will take time for detailed procedures to evolve. The following comments are in tended to clarify some features of the format.

6.3.1. Elastic Scattering

For ENDF/B-VI, neutron elastic scattering is represented by giving a cross section in File 3, MT=2 (with resonance contributions in File 2) and an angular distribution in File 4, MT=2. This representation is compatible with previous versions of the ENDF format.

Charged-particle elastic scattering uses MF=3, MT=2, and MF=6, MT=2, but the cross section in File 3 is set equal to 1.0 at all energies represented using LTP=1 and LTP=2. For LTP=12 and LTP=14, File 3 must contain $\sigma_{NI}(E)$ in barns. The elastic File 6 uses LAW=5.

Whenever possible, the nuclear amplitude expansion should be used. Note that the a and b 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 underdetermine the a's and b'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 and b 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.

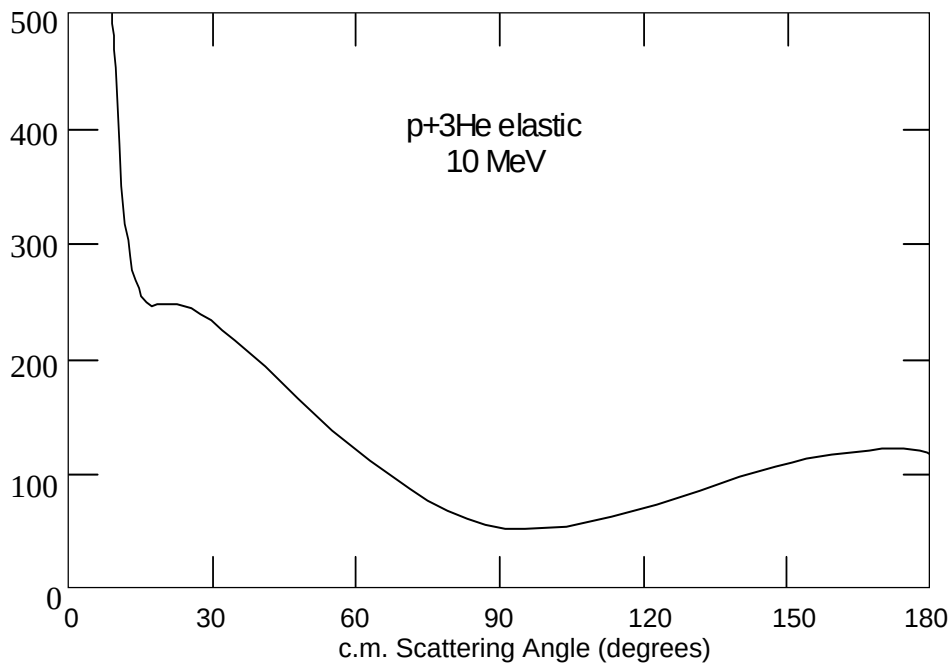

Figure 6.1 Example of Charged-Particle Elastic Scattering Cross Section

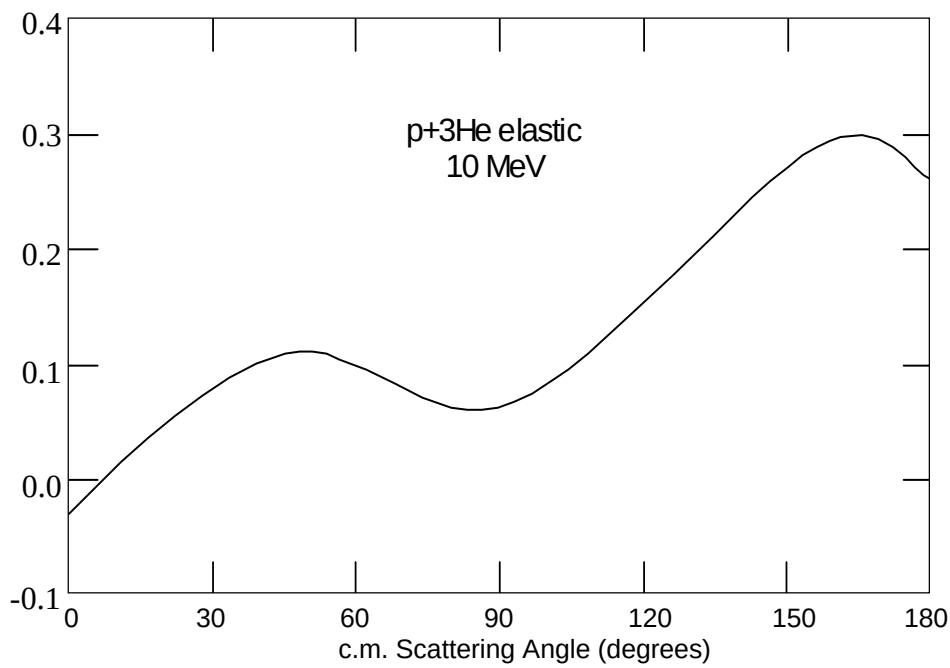

Figure 6.2 Example of Residual Cross Section for Elastic Scattering

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 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 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).

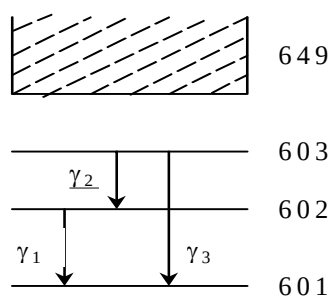

Figure 6.3
Typical Level Structure for Proton-Induced Photon Production

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.

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 LCT=3,34 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 with an element.

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34 LCT=3 is only appropriate for LAW=1 and LANG≠2.

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. This subsection is redundant, and the user should be careful to avoid double counting.

6.3.7. CM versus LAB

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 Eq. (C.5). This helps assure that the angular distribution given for each E and E′ will be fairly simple. Further more, 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.

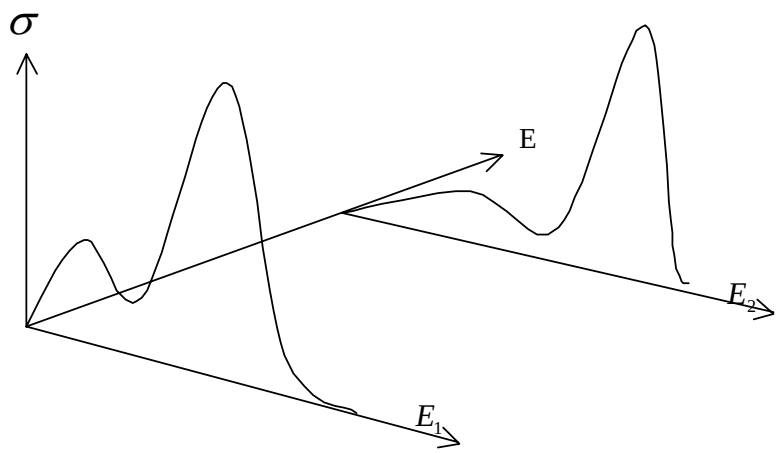


Figure 6.4
Typical Energy Spectrum Showing Levels on a Continuum

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 angle and energy, 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 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

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

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. Starting with ENDF/B-VI, 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:

$$\frac{d^2\sigma}{dEd\Omega}(E \to E',\mu,T) = \frac{1}{E}\sum_{i=1}^{E_i<E} s_i(T)\delta(\mu-\mu_i)\delta(E-E')/2\pi \tag{0.45}$$

where

$$\mu_i = 1 - \frac{2E_i}{E} \tag{0.46}$$

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.[35]

The quantity actually given in the file is

$$S(E,T) = \sum_{i=1}^{E_i<E} S_i(T) \tag{0.47}$$

which is conveniently represented as a stair-step function with breaks at the Bragg edges using histogram interpolation.

7.2.1. Formats for Coherent Elastic

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).

[35] As an example, the HEXSCAT code [Ref. 1] can be used for hexagonal lattices.

LT	Flag for temperature dependence. The data for the first temperature are given in a TAB1 record. The data for subsequent 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,E_{int}	Standard TAB1 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,Ti) ] LIST
          ---------------------------
          <repeat LIST for T2, T3, ...TLT+1>
          ---------------------------
[MAT, 7, 0 /  0.0, 0.0,    0,  0,  0,  0] SEND
```

7.2.2. Procedures for Coherent Elastic

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

$$\frac{d^2\sigma}{dE\,d\Omega}(E \to E',\mu,T) = \frac{\sigma_b}{4\pi} e^{-2EW'(T)(1-\mu)}\,\delta(E-E') \tag{0.48}$$

where

σ_b is the characteristic bound cross section (barns),

W' is the Debye-Waller integral divided by the atomic mass (eV^{-1}),

and all the other symbols have their previous meanings. The integrated cross section is easily obtained:

$$\sigma(E) = \frac{\sigma_b}{2}\left(\frac{1-e^{-4EW'}}{2EW'}\right) \tag{0.49}$$

Note that the limit of σ for small E is σ_b.

7.3.1. Format for Incoherent Elastic

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 material charge and mass parameters.
LTHR	flag indicating which type of thermal data is being represented. LTHR=2 for incoherent elastic.
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

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(α,β,T), and is defined for a moderating molecule or crystal by

$$\frac{d^2\sigma}{d\Omega\, dE'}(E \to E', \mu, T) = \sum_{n=0}^{NS} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}}\, e^{-\beta/2}\, S_n(\alpha, \beta, T) \tag{0.50}$$

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)
B	Energy transfer, β = (E′–E)/kT
α	momentum transfer, α = (E′+E–2μ sqrt(EE′)/A_0kT
A_n	Mass of the nth type atom **A_0** is the mass of the principal scattering atom in the molecule,
σ_{fn}	Free atom scattering cross section of the nth type atom

$$\sigma_{bn} = \sigma_{fn} \left(\frac{A_n + 1}{A_n} \right)^2 \tag{0.51}$$

k	Boltzmann's constant
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(α,β,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(α,β). In these cases, the short-collision-time (SCT) approximation should be used as follows:

$$S^{SCT}(\alpha,\beta,T) = \frac{e^{-\left[\frac{(\alpha-\beta)^2 T}{4\alpha T_{eff}(T)}+\frac{|\beta|}{2}\right]}}{\sqrt{4\pi\alpha\frac{T_{eff}(T)}{T}}} \tag{0.52}$$

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.

$$\left(\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{A_0}kT\right)$$

B(4) = E_{max}, the upper energy limit for the constant $\boldsymbol{\sigma}_{f0}$ (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_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) = $M_1\boldsymbol{\sigma}_{f1}$, the total free atom cross section for this atom type.

B(9) = A_1, effective mass for this atom type.

B(10) = 0.0, B(10) is not used.

B(11) = 0.0, B(11) is 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(α,β) method has sometimes been used. Using BeO as an example, the S(α,β) 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(α,β) is used for the principal atom in Eq. (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(α,β,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(α,β) is normally a symmetric function of β and only positive values are given. For ortho- and para-hydrogen 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 of 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(α,β) 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 α + β = 0. Computer precision can become a real problem in these cases. As an example, for water at room temperature, calculations using Eq. (7.6) for incident neutrons at 4 eV require working with products like $e^{80}x10^{-34}$. For liquid hydrogen at 20 Kelvin and for 1 eV transfers, the products can be $e^{300}x10^{-130}$. 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

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(α,β) is given LASYM=0, S is symmetric. LASYM=1, S is asymmetric
LLN	Flag indicating the form of S(α,β) 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≤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.
$\mathbf{T_{eff0}}$	Table of effective temperatures (K) for the short-collision-time approximation given as a function of moderator temperature T(K) for the principal atom.
$\mathbf{T_{eff1}}$,$\mathbf{T_{eff2}}$, $\mathbf{T_{eff3}}$	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(α,β), given.
$\boldsymbol{\beta_{int}}$, $\boldsymbol{\alpha_{int}}$	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(α,β) are omitted and the TAB2 and TAB1 records are not given.

7.4.2. Procedures for Incoherent Inelastic

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(α,β) function should be useful to energies as high as possible in order to minimize the discontinuities that occur when changing to the short-collision-time approximation. The β mesh for S(α,β) 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(α,β) is given should be the same for each β value of and for each temperature.

Experience has shown that temperature interpolation of S(α,β) 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

1. Y.D. Naliboff and J.V. Koppel, *HEXSCAT:Coherent Scattering of Neutrons by Hexagonal Lattices*, General Atomic report **GA-6026** (1964).

8. FILE 8, RADIOACTIVE DECAY AND FISSION PRODUCT YIELD DATA

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 8.2) and spontaneous radioactive decay data (MT=457) for the nucleus (see Section 8.3) 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.

8.1. Radioactive Nuclide Production

For any isotope, sections may be given which specify that the end product from the interaction of any incident particle or photon is radioactive. Information is given for any MT by identifying the end products in the reaction by their 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 MATP.
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	End-point 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 8.3).

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:

$n + {}^7Li \rightarrow \gamma + {}^8Li$ (ground state)

β^- (MT=102)

↘

$\underline{2.94\ 2^{\pm},0}$

${}^8Be$

↘

2α

For this example:

ZA(^{7}Li) = 3.007E+03 LIS(^{7}Li) = 0 LISO(^{7}Li) = 0

ZAP(^{8}Li) = 3.008E+03 LFS(^{8}Li) = 0

ZAN(^{8}Be) = 4.008E+03 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.

8.1.1. 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
```

8.1.2. 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/B 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).

8.2. Fission Product Yield Data (MT = 454 and 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 neutron 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 neutron energy. 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≤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 neutron 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 neutron energies.

I_i Interpolation scheme (see Appendix E) to be used between the E_{i-1} and E_i energy points.

8.2.1. 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.

8.2.2. 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 normally the independent 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 yield for each nuclide (ZAFP, FPS) can be determined by use of the branching fractions in MT=457 or directly from MT=459.

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.

8.3. 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 (=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)
$\mathbf{T_{1/2}}$	Half-life of the original nuclide (seconds).
NC	Total number of decay energies (eV) given (NC = 3 or 17).
$\mathbf{E_{"x"}}$	Average decay energy (eV) of "x" radiation, *e.g.*, for decay heat applications. The average energies must be given in an order specified in Section 8.3.2. Unknown average radiation energies are indicated by a value of –1.0.
SPI	Spin of the nuclide in its LIS state. (SPI = –77.777 = 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 (cannot be zero).

RTYP Mode of decay of the nuclide in its LIS state.

Decay modes defined:

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*, 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 (^{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 defined:

STYP	Radiation type	
0.	γ	Gamma rays
I.	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_γ,$E_{\beta-}$,$E_{e.c.}$,*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 $\int RP(E)dE = 1$.

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	[36]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	[1]Continuum spectrum normalization factor (absolute intensity/relative intensity).
FD	[1]Discrete spectrum normalization factor (absolute intensity/relative intensity).
NER	Total number of tabulated discrete energies for a given spectral type (STYP).
ER_{AV}	[37]Average decay energy of radiation produced.
NR	Number of interpolation ranges for the continuum spectrum.
NP	Number of points at which the distribution will be 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.
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.

$\{E_k,F_k\}$ is an array of 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 in an E table must be zero or blank since it is not defined.

The meaning of the F_k values in the E_k table for the allowed LB=2 is as follows:

LB=2 Fractional components fully correlated over all E_k intervals

$$\mathrm{COV}\,(X_i, X_j) = \sum_{kk'} S_i^k\, S_j^{k'}\, F_k\, F_{k'}\, X_i\, X_j$$

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.

[36] Spontaneous _v for RTYP = 6. and STYP = 5., LCON = 1 and FC =_v_p and FD = _v_d.

[37] For STYP = 2, this is the average positron energy, for STYP = 4, this includes energy of recoil nucleus.

8.3.1. 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:

```
[MAT, 8,457/    ZA,    AWR, LIS, LISO,    NST,   NSP] HEAD   (NST=0)
[MAT, 8,457/   T1/2,  ΔT1/2,    0,     0,  2*NC,     0/ (E"x",ΔE"x")[38] / 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
```

The structure of a subsection is:

```
[MAT, 8,457/   0.0, STYP,   LCON,     0,     6,    NER/
                FD,   ΔFD,   ERAV, ΔERAV,    FC,    ΔFC] LIST
[MAT, 8,457/   ER1,  ΔER1,     0,     0,    NT,     0/
             RTYP1, TYPE1,   RI1,   ΔRI1,  RIS1, ΔRIS1,
             RICC1,ΔRICC1, RICK1,ΔRICK1, RICL1,ΔRICL1] LIST
            ---------------------------------------
              ERNER, ΔERNER,    0,     0,    NT,     0/
            RTYPNER,TYPENER, RINER, RINER, ------------] LIST
```

(omit these LIST records if LCON=1)

```
[MAT, 8,457/ RTYP,   0.0,    0, LCOV,    NR,    NP/ Eint / RP(E) ] TAB1
```

(omit if LCON=0)

```
[MAT, 8,457/  0.0,   0.0,    0,   LB, 2*NPP,   NPP/ (Ek,Fk) ] 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
```

8.3.2. Procedures

1. The initial state of the parent nucleus is designated by LISO, which equals 0 for the

[38] Data must be given in order specified in Section 8.3.2.

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 non-isomeric states may be included in the count of levels.)

2. The average decay energy $\underline{E}_{"x"}$ for decay heat application is given for three general radiation types, E_{LP} (for light particles), E_{EM} (for electromagnetic radiation), and 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

$$\overline{E}_{LP} = \overline{E}_{\beta^-} + \overline{E}_{\beta^+} + \overline{E}_{e^-} + \ldots$$
$$\overline{E}_{EM} = \overline{E}_{\gamma} + \overline{E}_{x-ray} + \overline{E}_{ann.rad.} + \ldots$$
$$\overline{E}_{HP} = \overline{E}_{\alpha} + \overline{E}_{SF} + \overline{E}_{p} + \overline{E}_{n} + \ldots$$

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.
$\overline{E}_{ann.rad.}$	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 8.l).

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 will also allow 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 $\underline{\underline{E}}_{SF}$ and $\Delta \underline{\underline{E}}_{SF}$ 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 using MF = 5 in 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:

$$\sum_k F_k\, y_k = 0,$$

$$\text{where, } y_k = \int_{E_k}^{E_{k+1}} RP(E)\, dE$$

   and y_k is the energy spectrum on the uncertainty evaluation grid. $\Sigma y_k = 1$. 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' will 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

$$V_{mn} = \sigma_m \sigma_n\,,$$

$$\text{where, } \sigma_n = \int_{E_n}^{E_{n+1}} F(E)\, RP(E)\, dE$$

   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.

9. FILE 9. MULTIPLICITIES FOR PRODUCTION OF RADIOACTIVE NUCLIDES

9.1. General Description

Neutron activation cross sections can be obtained by the use of 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 (ZA P) (as defined in MF=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) 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 $a+A \rightarrow b+c+\ldots + B$. If the masses are in amu, $QM = [(m_a+m_A) - (m_b+m_c+\ldots+m_B)] \times (amu/eV)$[39].

QI Reaction Q value (eV) for the state described by the subsection. For isomeric states it is defined as QM minus the residual excitation energy of the isomer. For the ground state QI=QM.

IZAP 1000*Z+A for the product nucleus

NS Number of final states for each MT for which multiplicities are to be given.

NR Number of energy ranges. A different interpolation scheme may be given for each range. ($NR \leq 20$).

NP Total number of energy points used to specify the data ($NP \leq 5000$)[40].

[39] See Appendix H for conversion factor.
[40] 50,000 energy points are allowed for the total cross section.

E_{int}	Interpolation scheme for each energy range. (For details, see Section 0.6.2.)
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 MF=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 20 MeV. That is, multiplicities cannot be used over a portion of the incident neutron energy range with cross sections covering another portion. For negative Q reactions, 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 50,000 incident energy points are allowed for the total cross section, 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 not enter data in MF=8 and 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 MF=8 with LMF=9 as an indicator in the LIST record of the subsection for that particular MT and value of LFS must have the corresponding multiplicities in File 9.

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 (ZAP) 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) 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 a+A→b+c+...+B, if the masses are in amu,

$QM = [(m_a+m_A) - (m_b+m_c+...+m_B)]\times(amu/eV)$[41]

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.

IZAP 1000*Z+A for the product nucleus

NS Number of final states for each MT for which cross sections are to be given.

NR Number of energy ranges. A different interpolation scheme may be given for each range. (NR≤20).

[41] See Appendix H for conversion factor.

NP	Total number of energy points used to specify the data (NP≤5,000)[42].
E_{int}	Interpolation scheme for each energy range. (For details, see Section 0.4.3.)
σ(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 / σ(E)] TAB1
```

10.3. Procedures

Isomer production cross sections must be given in File 10 for those reactions described in MF=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 20 MeV. That is, cross sections cannot be used over a portion of the incident neutron energy range with multiplicities covering another portion. For negative Q reactions, 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. Although 10000 incident energy points are allowed for the total cross section, 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 would be to not enter data in MF=8 and 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 value of LFS must have the

[42] 50,000 energy points are allowed for the total cross section.

corresponding cross sections in File 10.

11. FILE 11. GENERAL COMMENTS OF PHOTON PRODUCTION

Photon production data not represented in MF=6 may be presented in four distinct files.

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→i), which need not be adjacent, including the effects of cascading from the m_0-j levels higher than j, is

$$\frac{d\sigma}{dE_\gamma}(E_\gamma, E, m_0, i, j) = \delta\left[E_\gamma - (\varepsilon_j - \varepsilon_i)\right] A_{ji}\sigma_{m_0}(E)\sum_{\alpha=1}^{m_0-j} R_{m_0 j\alpha}\ , \qquad (0.53)$$

where

σ_{m0}	=	Cross section for exciting the m_0^{th} level with incident particle energy E, taken from file 3 for MT corresponding to the m_0^{th} level,
$\delta[E_\gamma-(\varepsilon_j-\varepsilon_i)]$	=	Delta function defining the discrete gamma of energy E_γ that results from the transition level j to level i,
A_{ji}	=	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 of j→i,

$R_{m_0 j\alpha}$ = 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,

$$= \sum_{m_1=\alpha+(j-1)}^{m_0-1} \sum_{m_2=\alpha+(j-2)}^{m_1-1} \cdots \sum_{m_{\alpha-1}=j+1}^{m_{\alpha-2}-1} \sum_{m_\alpha}^{j} \prod_{l=1}^{\alpha} TP_{m_{l-1}m_l}$$

$Tp_{k,l}$ = 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→*l* level.

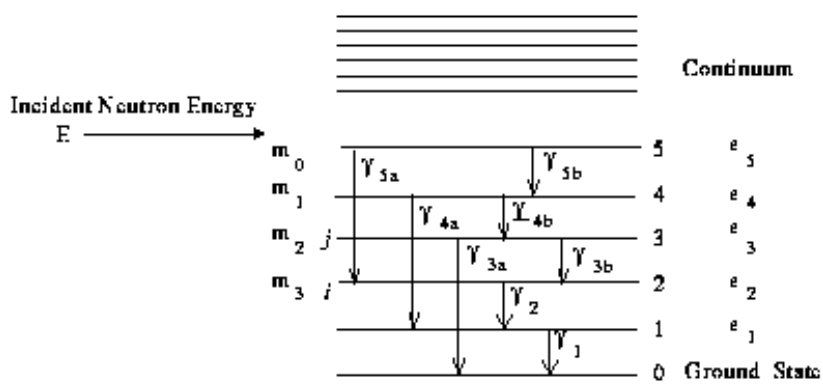
In general, $R_{m0j\alpha}$ is the sum of the products of α transition probabilities (branching ratios) leading from level m_0 through intermediate levels to level j. In the example shown for initial excitation of level m_0=5 and interest being in the resulting γ-ray due to transition

$$R_{m_0 j} = TP_{m_0 j} = TP_{52}$$
$$R_{m_0 j 2} = TP_{m_0 m_1} TP_{m_1 j} + TP_{m_0 m_2} TP_{m_2 j} = TP_{52} \cdot TP_{42} + TP_{53} TP_{32} = 0 + 0 = 0$$

between levels 2 and 1 [Eγ = $E_{\gamma 2}$ = (ε_2-ε_1)], the relevant quantities are for this example, and

$$R_{m_0 j 3} = TP_{m_0 m_1} TP_{m_1 m_2} TP_{m_2 j} = TP_{54} \cdot TP_{43} \cdot TP_{32}$$

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 Eq. (11.1) over m_0:

$$\frac{d\sigma_1}{dE_\gamma}(E_\gamma, E, i, j) = \sum_{m_0=j}^{N} \frac{d\sigma}{dE_\gamma}(E_\gamma, E, m_0, i, j) \qquad (0.54)$$

where N is the highest level that can be excited by a neutron of incident energy E [*i.e.*, $\varepsilon_N \leq$ AWR/(AWR + E)]. 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 Eq. (11.1) over i and j:

$$\frac{d\sigma_2}{dE_\gamma}\left(E_\gamma, E, m_0\right) = \sum_{j=1}^{m_0} \sum_{i=0}^{j-1} \frac{d\sigma}{dE_\gamma}\left(E_\gamma, E, m_0, i, j\right) \tag{0.55}$$

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

$$\begin{aligned}\frac{d\sigma}{dE_\gamma}\left(E_\gamma,E\right) &= \sum_{m_0=1}^{N}\frac{d\sigma_2}{dE_\gamma}\left(E_\gamma,E,m_0\right)\\ &\equiv \sum_{j=1}^{N}\sum_{i=0}^{j-l}\frac{d\sigma_1}{dE_\gamma}\left(E_\gamma,E,i,j\right).\end{aligned} \tag{0.56}$$

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,αγ) reactions, and the use of MT=103, 101, 105, 106, and 107 is recommended for these cases.

12. FILE 12. PHOTON PRODUCTION MULTIPLICITIES AND TRANSITION PROBABILITY ARRAYS

File 12 can be used to represent the neutron energy dependence of photon production cross sections by means of either multiplicities or transition probability arrays. Both methods rely upon processing codes that use neutron cross sections from File 2 and/or File 3 to generate absolute photon production cross sections.

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.

12.1. 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.

12.1.1. Option 1 (LO=1): Multiplicities

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[43]. 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

$$y_k(E) = \frac{\sigma_k^{\gamma}}{\sigma(E)} \quad \text{(photons)} \tag{0.57}$$

where E designates neutron energy and σ(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,

[43] 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.

$$y_k(E) = \frac{\sigma_k^\gamma(E)}{\sigma(E)} = \frac{\int \frac{d\sigma_k^\gamma}{dE_\gamma}\left(E_\gamma \leftarrow E\right) dE_\gamma}{\sigma(E)}$$
$$= \frac{\int \sigma(E)\, y_k\left(E_\gamma \leftarrow E\right) dE_\gamma}{\sigma(E\ )} = \int_0^{E_\gamma^{\max}} y_k\left(E_\gamma \leftarrow E\right) dE_\gamma \tag{0.58}$$

where E_γ designates photon energy (eV),

$$\frac{d\sigma_k^\gamma}{E_\gamma}(E_\gamma \leftarrow E)$$

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

$$y_k(E_\gamma \leftarrow E) = y_k(E)\, f_k(E_\gamma \leftarrow E) \quad ,$$

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 NK

$$Y(E) = \sum_{k=1}^{NK} y_k(E) \qquad \text{(photons)}$$

is also tabulated for each MT number if NK>1.

The structure of a section for LO=1 is

```
[MAT, 12, MT/  ZA, AWR, LO,  0, NK,  0] HEAD                    (LO=1)
[MAT, 12, MT/ 0.0, 0.0,  0,  0, NR, NP/ Eint / Y(E)] TAB1 [44]
          <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/ Egk,  ESk, LP, LF, NR, NP/ Eint / yk(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

[44] If the total number of discrete photons and photon continua is one (NK=1), this TAB1 record is omitted.

$$EG'_k = EG_k + \frac{AWR}{AWR+1} E_n \ .$$

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.

12.1.2. Option 2 (LO=2): Transition Probability Arrays

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.

Now define the following variables.

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 nonzero transition probabilities), NT≤NS.

ES_i Energy of the ith level, i=0,1,2... NS.
ES ≡ 0.0, ground state

TP_i $TP_{NS,i}$, probability of a direct transition from level NS to level i, i=0,1,2... (NS-1).

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 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 $E_\gamma = ES_{NS} - ES_i$, and its multiplicity is given by $y(E_\gamma \leftarrow E) = (TP_i)\ (GP_i)$. 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/ ESNS, 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.

12.2. 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 exactly span the same energy range as the combined energy range of all the $y_k(E)$. Within that range,

$$Y(E) = \sum_{k=1}^{NK} y_k(E)$$

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 in any tabulations of Y(E) or $y_k(E)$ is 1000. 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 10.
17. Tabulations of non-threshold data should normally cover at least the energy range 10^{-5} eV $\leq E \leq 2\times10^7$ eV, where practical. Threshold data should be given from threshold energy up to 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 de-excitation 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 (given in File 3 as MT=51,...) must be given from threshold energies up to the same maximum energy (no exceptions). Decay properties of all n 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 20 MeV. It is seldom that all level data can be given for neutron energies up to 15 MeV.

13. FILE 13. PHOTON PRODUCTION CROSS SECTION

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 neutron files.

13.1. 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 (b) for the photon designated by k. For the photon continuum, $\sigma_k^\gamma(E)$ is the integrated (over photon energy) cross section for the photon continuum[45] designated by k. In the continuum case,

$$\sigma_k^\gamma(E) = \int_0^{E_\gamma^{\max}} \frac{d\sigma_k^\gamma}{dE\gamma}\left(E_\gamma \leftarrow E\right) dE_\gamma \quad \text{(barns)} \tag{0.59}$$

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 b/eV. The energy distribution can be further broken down as

$$\frac{d\sigma_k^\gamma}{dE_\gamma}\left(E_\gamma \leftarrow E\right) = \sigma_k^\gamma(E)\, f_k\left(E_\gamma \leftarrow E\right), \tag{0.60}$$

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,

$$\sigma_{tot}^\gamma(E) = \sum_{k=1}^{NK} \sigma_k^\gamma(E) \quad \text{(barns)}, \tag{0.61}$$

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.

[45] 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.

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;

$$EG'_k = EG_k + \frac{AWR}{AWR+1} E_n$$

LP=2, for primary photons where the photon energy EG'_k is given by

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

```
[MAT, 13, MT/  ZA,  AWR,   0,   0,  NK,   0] HEAD
[MAT, 13, MT/ 0.0,  0.0,   0,   0,  NR,  NP/ Eint / σtotγ (E)] TAB1 [46]
           <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/  Egk,  Esk,  LP,  LF,  NR,  NP/ Eint / σkγ(E)] TAB1,
```

13.2. 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, $EG_{NK} \equiv 0.0$.
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 $ES_k \equiv 0.0$.
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, $\sigma_{tot}^{\gamma}(E)$ should exactly span the same energy range as the combined energy range of all the $\sigma_k^{\gamma}(E)$. Within that range,

$$\sigma_{tot}^{\gamma}(E) = \sum_{k=1}^{NK} \sigma_k^{\gamma}(E)$$

should hold within four significant figures. If only one energy distribution is given, either

[46] If the total number of discrete photons and photon continua is one (NK=1), this TAB1 record is omitted.

discrete or continuous (NK=1), the TAB1 record for the $\sigma_{tot}^{\gamma}(E)$ 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 1000. 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 10.

10. Tabulations of non-threshold data should normally cover at least the energy range 10^{-5} eV $\leq$ E $\leq 2\times10^{7}$ eV, where practical. Threshold data should be given from threshold energy up to $2\text{x}10^{7}$ eV, where practical.

13.3. 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 it probably will not be possible to separate the various components of the total γ production cross section. When this happens, it is preferred that the data be given as MT=3.

7. All other reactions. Data for other reactions should be given as photon production cross sections (File 13) using the appropriate MT numbers. The same general rule outlined above should be used.

14. FILE 14. PHOTON ANGULAR DISTRIBUTIONS

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,

$$\int_{-1}^{1} p_k(\mu,E)\,d\mu = 1\,,$$

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,

$$\begin{aligned} p_k(\mu,E) &= \frac{2\pi}{\sigma_k^{\gamma}(E)}\frac{d\sigma_k^{\gamma}}{d\Omega}(\Omega,E) \\ &= \sum_{l=0}^{NL}\frac{2l+1}{2}a_l^k(E)P_l(\mu) \end{aligned} \tag{0.62}$$

where

μ	=	cosine of the reaction angle in the lab 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 *l*-th Legendre coefficient associated with the discrete photon or photon continuum specified by k. (It is understood 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.

Note that File 14 assumes separability of the photon energy and angular distributions for the ***continuum*** spectrum. If this is not the case, File 16 (analogous to File 6) must be used instead of Files 14 and 15. (Since File 14 implicitly specifies an energy-angle distribution

for discrete photons, File 16 is required only for the continuum spectrum).

14.1. 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 as a tabulation.
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.

a. LI=1: Isotropic Distribution

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
```

b. LI=0: Anisotropic Distribution

If LI=0, there are two possible structures for a section, depending upon the value of LTT.

i. LTT=1: Legendre Coefficient Representation

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, which is 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/  EGk, ESk,   0,   0,   NR,  NE/ Eint ] TAB2
[MAT, 14, MT/  0.0,  E1,   0,   0,  NL1,   0/ al^k(E1)] LIST
[MAT, 14, MT/  0.0,  E2,   0,   0,  NL2,   0/ al^k(E2)] LIST
            ------------------------------------
            ------------------------------------
            ------------------------------------
[MAT, 14, MT/  0.0, ENE,   0,   0,  NLNE,  0/ al^k(ENE)] LIST
```

Note that lists of the $a_l^k(E)$ start at l=1 because $a_0^k(E) \equiv 1.0$ is always understood.

ii. LTT=2: Tabulated Angular Distributions

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 $EG_k \equiv 0.0$.

The structure of the first Ni subsections is

```
[MAT, 14, MT/ EGk,  ESk,  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 $EG_k \equiv 0.0$.

The structure of the last NK-NI subsections is

```
[MAT, 14, MT/  EGk, ESk,   0,   0,  NR,  NE/ Eint ] TAB2
[MAT, 14, MT/  0.0,  E1,   0,   0,  NR,  NP/ μint / pk(μ,E1)] TAB1
[MAT, 14, MT/  0.0,  E2,   0,   0,  NR,  NP/ μint / pk(μ,E2)] TAB1
               ---------------------------------------------------
               ---------------------------------------------------
[MAT, 14, MT/  0.0,  ENE,   0,   0,  NR,  NP/ μint / pk(μ,ENE)] TAB1
```

14.2. 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, $EG_{NK} \equiv 0.0$.
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, $\leq$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 linear-linear or log-linear (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 m 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%.

15. File 15. CONTINUOUS PHOTON ENERGY SPECTRA

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

$$\int_0^{E_\gamma^{\max}} f\left(E_\gamma \leftarrow E\right) dE_\gamma = 1 \quad ,$$

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.[47] 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:

$$f\left(E_\gamma \leftarrow E\right) = \sum_{j=1}^{NC} p_j(E)\, g_j\left(E_\gamma \leftarrow E\right) \qquad (\mathrm{eV})^{-1} \tag{0.63}$$

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
$p_j(E)$	= 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,

$$\sum_{j=1}^{NC} p_j(E) = 1.$$

The absolute energy distribution cross section, $\sigma^\gamma(E_\gamma \leftarrow E)$, can be constructed from the expression

$$\sigma^\gamma\left(E_\gamma \leftarrow E\right) = \sigma^\gamma\left(E\right) f\left(E_\gamma \leftarrow E\right) \qquad (\mathrm{b/eV}),$$

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.*,

$$g_j\left(E_\gamma \leftarrow E\right) = g\left(E_\gamma \leftarrow E\right) \quad ,$$

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.

[47] 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 NK^{th} subsection in File 12 or 13 that contains the production data for the continuum.

15.1. 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_γ int/ g(E_γ←E_1)] TAB1
[MAT, 15, MT/ 0.0,   E_2,  0,   0,  NR,  NP/ E_γ int/ g(E_γ←E_2)] TAB1
             ------------------------------
             ------------------------------
[MAT, 15, MT/ 0.0,  E_NE,  0,   0,  NR,  NP/ E_γ int/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 0.5-MeV 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).

15.2. 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. Like-wise, the interpolation scheme for $g(E_\gamma \leftarrow E)$ 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 nonzero 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 200. The limit on the number of photon energy points for $g(E_\gamma \leftarrow E)$ is 1000.

23. FILE 23. "SMOOTH" PHOTON INTERACTION CROSS SECTIONS

23.1. General Comments on Photon Interaction

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 cross-sections. 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 534-599.
EFL	Fluorescence yield (eV/photoionization). Value is zero if not a photoelectric subshell ionization cross section.
NR,NP,E_{int}	Standard TAB1 parameters (see Section 1.3.1).
σ(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 × 1000.0; also, AWR should be for the naturally occurring element.
2. Photoelectric edges will not be multi-valued. The edge will be defined by two energies 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.

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 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 losses 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 parameters.
y(E)	Yield for the particle being described (always 1 in File 26, but we keep this 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/ Eint / 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/ Eint / ET(E)] TAB1
```

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 θ vs. cos θ, 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.

a. ***Incoherent Scattering***. The cross section for incoherent scattering is given by

$$\frac{d\sigma_i(E,E',\mu)}{d\mu} = S(q;Z)\frac{d\sigma_i(E,E',\mu)}{d\mu}, \tag{0.64}$$

where $d\sigma_c/d\mu$ = the Klein-Nishina cross section[48] 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[49]).

$$q = \alpha\left[1+\left(\frac{\alpha'}{\alpha}\right)^2 - 2\mu\left(\frac{\alpha'}{\alpha}\right)\right]^{1/2} \tag{0.65}$$

where $\alpha = E_\gamma/m_0c^2$,
E_γ' = scattered photon energy,
$\mu = \cos\theta$.

The angular distribution can then easily be calculated, given a table 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.

b. ***Coherent Scattering.*** The coherent scattering cross section is given by

$$\frac{d\sigma_{coh}(E,E',\mu)}{d\mu} = \pi r_0^2\left(1+\mu^2\right)\left[\left(F(q;Z)+F'(E)\right)^2 + F''(E)^2\right], \tag{0.66}$$

where $q = \alpha[2(1-\mu)]^{1/2}$, 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 anomalous scattering factor.
$F''(E)$ = the imaginary anomalous scattering factor.

The quantity F(q;Z) is a form factor. This quantity is also easily tabulated. At high momentum transfer (q), F approaches zero. In the other limit F(0;Z)=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.

---

[48] O. Klein and Y. Nishina, Z. Phys. 52, 853 (1929).

[49] 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.

An alternative way of presenting the photon scattering data, then, 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.

28. FILE 28. ATOMIC RELAXATION DATA

28.1. General Comments on Atomic Relaxation

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 EK, the atom will emit an electron with energy E-EK, 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 EK-EL1. 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 EK-EL1-EM1, 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).

28.2. General Description

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.

28.3. 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
```

28.4 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

```
                                                                        1 0  0    0
 6.000000+3 11.9078164         -1          0          0          0 600 1451    1
 0.000000+0 0.000000+0          0          0          0          6 600 1451    2
 0.000000+0 0.000000+0          0          0          6          6 600 1451    3
 0.000000+0 0.000000+0          0          0          6          2 600 1451    4
 6-C -  0 LLNL        EVAL-DEC90 CULLEN                               600 1451    5
                      DIST-                                           600 1451    6
----ENDF/B-VI         MATERIAL  600                                   600 1451    7
-----ATOMIC RELAXATION DATA                                           600 1451    8
------ENDF-6 FORMAT                                                  600 1451    9
 converted from EADL                                                  600 1451   10
                               1        451         12          0 600 1451   11
                              28        533         17          0 600 1451   12
                                                                    600 1  0   13
                                                                    600 0  0   14
 6.000000+3 11.9078164          0          0          4          0 60028533   15
 1.000000+0 0.000000+0          0          0         54          8 60028533   16
 2.910100+2 2.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   17
 5.000000+0 0.000000+0 2.820200+2 5.614880-4 0.000000+0 0.000000+0 60028533   18
 6.000000+0 0.000000+0 2.820300+2 1.120600-3 0.000000+0 0.000000+0 60028533   19
 3.000000+0 3.000000+0 2.558900+2 4.136090-1 0.000000+0 0.000000+0 60028533   20
 3.000000+0 5.000000+0 2.644600+2 1.361900-1 0.000000+0 0.000000+0 60028533   21
 3.000000+0 6.000000+0 2.644700+2 2.710990-1 0.000000+0 0.000000+0 60028533   22
 5.000000+0 5.000000+0 2.730300+2 4.207480-3 0.000000+0 0.000000+0 60028533   23
 5.000000+0 6.000000+0 2.730400+2 1.100120-1 0.000000+0 0.000000+0 60028533   24
 6.000000+0 6.000000+0 2.730500+2 6.320080-2 0.000000+0 0.000000+0 60028533   25
 3.000000+0 0.000000+0          0          0          6          0 60028533   26
 1.756000+1 2.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   27
 5.000000+0 0.000000+0          0          0          6          0 60028533   28
 8.990000+0 6.700000-1 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   29
 6.000000+0 0.000000+0          0          0          6          0 60028533   30
 8.980000+0 1.330000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   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                          1 0  0    0
 6.000000+3 11.9078164         -1          0          0          0 600 1451    1
 0.000000+0 0.000000+0          0          0          0          6 600 1451    2
 5.438673-4 1.00000+11          0          0        113          6 600 1451    3
 0.000000+0 0.000000+0          0          0          6         14 600 1451    4
 6-C -  0 LLNL        EVAL-DEC89 CULLEN                               600 1451    5
                      DIST-                                           600 1451    6
----ENDF/B-VI         MATERIAL  600                                   600 1451    7
-----ELECTRO-ATOMIC DATA                                              600 1451    8
------ENDF-6 FORMAT                                                  600 1451    9
 converted from EEDL                                                  600 1451   10
                                1        451         24          0 600 1451   11
                               23        526         37          0 600 1451   12
                               23        527         31          0 600 1451   13
                               23        528         64          0 600 1451   14
                               23        534         12          0 600 1451   15
                               23        536         14          0 600 1451   16
                               23        538         15          0 600 1451   17
                               23        539         15          0 600 1451   18
                               26        526        353          0 600 1451   19
                               26        527        197          0 600 1451   20
                               26        534        120          0 600 1451   21
                               26        536        151          0 600 1451   22
                               26        538        155          0 600 1451   23
                               26        539        155          0 600 1451   24
                                                                   600 1  0   25
                                                                   600 0  0   26
 6.000000+3 11.9078164          0          0          0          0 60023526   27
 0.000000+0 0.000000+0          0          0          1        101 60023526   28
        101          2                                               60023526   29
 1.000000+1 3.063510+9 1.258930+1 2.498030+9 1.584890+1 2.036940+9 60023526   30
 1.995260+1 1.660950+9 2.511890+1 1.354370+9 3.162280+1 1.104370+9 60023526   31
 3.981070+1 9.008210+8 5.011870+1 7.347880+8 6.309570+1 5.993570+8 60023526   32
 7.943280+1 4.889770+8 1.000000+2 3.991460+8 1.258930+2 3.258180+8 60023526   33
 1.584890+2 2.659610+8 1.995260+2 2.171000+8 2.511890+2 1.772160+8 60023526   34
 3.162280+2 1.447630+8 3.981070+2 1.183030+8 5.011870+2 9.667950+7 60023526   35
 6.309570+2 7.900840+7 7.943280+2 6.458900+7 1.000000+3 5.282720+7
  …
 6.000000+3 11.9078164          0          0          1          0 60026526  223
 1.100000+1 5.438673-4          0          2          1          2 60026526  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         16 60026526  227
         16          2                                               60026526  228
 0.000000+0 1.000000+1         12          0          4          2 60026526  229
-1.000000+0 5.000000-1 9.999990-1 5.000000-1                         60026526  230
 0.000000+0 1.000000+3         12          0         54         27 60026526  231
-1.000000+0 7.349540-3-6.350000-1 1.014680-2-3.300000-1 1.408430-2 60026526  232
-7.500000-2 1.996880-2 1.350000-1 2.832790-2 3.000000-1 3.982680-2 60026526  233
 4.300000-1 5.580130-2 5.350000-1 7.828660-2 6.225000-1 1.108190-1 60026526  234
 6.925000-1 1.559570-1 7.500000-1 2.204030-1 7.950000-1 3.078220-1 60026526  235
 8.325000-1 4.339260-1 8.625000-1 6.085020-1 8.875000-1 8.591520-1 60026526  236
 9.080000-1 1.212620+0 9.250000-1 1.713720+0 9.390000-1 2.413930+0 60026526  237
 9.510000-1 3.432260+0 9.610000-1 4.874960+0 9.690000-1 6.802370+0 60026526  238
 9.760000-1 9.598280+0 9.820000-1 1.360430+1 9.870000-1 1.914880+1 60026526  239
 9.915001-1 2.744700+1 9.956001-1 4.014720+1 9.999990-1 6.259920+1 60026526  240
 0.000000+0 2.000000+3         12          0         64         32 60026526  241
-1.000000+0 3.008670-3-9.000000-1 3.301630-3-5.350000-1 4.906250-3
```

```
…
6.000000+3 11.9078164          0          0          1          0 60026534  775
1.100000+1 5.438673-4          0          1          1          2 60026534  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          7 60026534  779
         7          2                                               60026534  780
0.000000+0 2.910100+2          0          0          4          2 60026534  781
1.000000-2 1.111110+1 1.000000-1 1.111110+1                        60026534  782
0.000000+0 2.973140+2          0          0          4          2 60026534  783
3.152220-2 3.265060-1 3.152220+0 3.143760-1                        60026534  784
0.000000+0 1.995260+3          0          0         28         14 60026534  785
1.000000-1 7.771360-3 6.309570+0 7.133700-3 1.412540+1 6.229690-3 60026534  786
3.162280+1 5.440240-3 6.309570+1 4.054250-3 8.912520+1 3.138130-3 60026534  787
1.258930+2 2.429030-3 1.778280+2 1.605960-3 2.511890+2 1.061790-3 60026534  788
3.162280+2 7.491710-4 3.758380+2 5.767510-4 4.869680+2 3.895820-4 60026534  789
6.309570+2 2.631530-4 8.521260+2 2.098710-4                        60026534  790
0.000000+0 3.981070+4          0          0         70         35 60026534  791
1.000000-1 7.237010-3 6.309570+0 6.655140-3 1.412540+1 5.837310-3 60026534  792
3.162280+1 5.119990-3 6.309570+1 3.846900-3 8.912520+1 2.990940-3 60026534  793
1.258930+2 2.325440-3 1.496240+2 1.886340-3 1.938660+2 1.378130-3
…
2.06836+10 4.46563-21 2.51189+10 3.13693-21 3.16228+10 2.30613-21 60026539 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
```

30. INTRODUCTION TO DATA COVARIANCE FILES

30.1. 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 for 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/V-IV, 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 large cost. The data uncertainties may also be reduced, often at large cost, 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), the neutron cross sections (Files 3 and 10), energy distributions (File 4) and angular 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 in the other cases there are restrictions. In some cases such as inelastic scattering one may employ the subterfuge of pseudo-discrete levels to treat a continuum using the formats and procedures of File 3 and 33.

Since covariance files will 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 the 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 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 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 new LB=8 format allows 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 evaluator-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 new file-30 format provides an alternate way to avoid the effects of artificial energy boundaries.

It is appropriate to define uncertainty quantities[50]. 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) ΔX is the probability that the true numerical value of X lies in the range ΔX at X. The marginal density function f(X) is the average over all other independent variable Y, Z, ... 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", <g(X)>, 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:

$$< X >= \int X \; f(X)\, dX$$

In practice, one often uses the same symbol for a physical quantity, its expected value, and its value in a particular data set. In this Chapter, the last is written X = <X> + δX, where <δX>=0. In this language the cross section, *etc.*, quantities in ENDF-6 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 and ENDF-6 formatted cross section and some more-recently realized "better" evaluation, or any cross-section imprecision induced by ENDF-6 procedures, or the widths of any physical distributions such as the fission neutron multiplicity distribution P(v).

The following quantities are defined that relate to the second moments of the density function. Here <X> and <Y> 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 δX = X - <X>.

---

[50] 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.

$$\mathrm{Cov}(X,Y) = <\delta X\,\delta Y>$$

$$= \iint (X - <X>)(Y - <Y>)\,F(X,Y)\,dX\,dY,$$ the covariance between X and Y,

$$\mathrm{Var}(X) = \mathrm{Cov}(X,X) = <\delta X^2>,$$ the standard error or uncertainty in <X>,

$$s(X) = \left[\mathrm{Var}(X)\right]^{1/2},$$ the variance of X,

$$\rho(X<Y) = \mathrm{Cov}(X<Y)/\{s(X)\,s(Y)\},$$ the correlation coefficient between X and Y.

The relative standard error, $s(X)/\langle X\rangle$, the relative variance $\mathrm{Var}(X)/<X>^2$, and the relative covariance, $\mathrm{Cov}(X,Y)/(<X><Y>)$, are 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.

30.1. FILE 30. DATA COVARIANCES OBTAINED FROM PARAMETER COVARIANCES AND SENSITIVITIES

30.1.1. General Description

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 multi-group 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 30.1.4.) 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 prejudge 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 30.1.3 below, this generality also facilitates various mathematical operations, such as diagonalizing the parameter covariance matrix.

30.1.1.1. 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,

$$\sigma_i' \equiv \frac{\partial \sigma}{\partial \left(\ln \alpha_i\right)} = \alpha_i \frac{\partial \sigma}{\partial \alpha_i} \tag{0.67}$$

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 Eq. (30.7).

As discussed in detail in Section 30.1.2.3, a ***sub-section*** 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 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 stand-alone (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≠30) ENDF definitions.

30.1.1.2. 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 File 3. One can treat $\bar{\nu}$ data in File 1 in the same way as cross sections.

Some interesting points arise with respect to distributions, for example tabulated data in File 4 for elastic scattering. If the derivatives of the normalized angular distribution *p(θ)* with respect to a given parameter are large, they should be described in a subsection with (MFSEN,MTSEN) = (4,2).

Note that since *p(θ)* 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 γ(θ) (barns/steradian) at angle θ is formed as a product,

$$\gamma(\theta) \equiv d\sigma/d\Omega = \sigma p(\theta)\,, \tag{0.68}$$

So that

$$\frac{\partial\gamma(\theta)}{\partial\alpha_i} = \sigma\frac{\partial p(\theta)}{\partial\alpha_i} + p(\theta)\frac{\partial\sigma}{\partial\alpha_i}\,. \tag{0.69}$$

Multiplying both sides of Eq. (30.3) by α_1, and recalling the notation of Eq. (30.1), one gets,

$$\gamma_i'(\theta) = \sigma p_i'(\theta) + \sigma_i' p(\theta)\,. \tag{0.70}$$

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 Eq. (30.4) will be omitted.

Just as one is permitted to employ a Legendre representation of *p(θ)* 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(θ)* itself is given in tabular form. As mentioned above $p_i'(\theta)$ must integrate to zero, so the magnitude of the implied zero-th 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 Eq. (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.

30.1.1.3. Multi-grouped Sensitivities

Multi-group 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

$$g = \int dE\, dE'\, d\Omega\, \gamma_i\left(E,E',\theta\right)\omega\left(E,E',\theta\right), \tag{0.71}$$

where ω is some weighting function. As discussed below, one frequently is interested in the uncertainty in such multi-group quantities, and to obtain this uncertainty, one will first need to calculate the derivative of g with respect to the parameter α_i.

$$g'_i = \frac{\partial g}{\partial(\ln\alpha_i)} = \alpha_i \int dE\, dE'\, d\Omega \frac{\partial\gamma\left(E,E',\theta\right)}{\partial\alpha_i}\omega\left(E,E',\theta\right),$$

or

$$g'_i = \int dE\, dE'\, d\Omega\, \gamma'_i\left(E,E',\theta\right)\omega\left(E,E',\theta\right), \tag{0.72}$$

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, Equation (30.5), can be used, with few modifications, to calculate the parameter sensitivity of multigroup constants, 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.

30.1.2. 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.

30.1.2.1. 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 data-block "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 non-zero, 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 different evaluation 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.

30.1.2.2. 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(2,1+K, K=2,NCS2}] LIST
   [MAT,30, 2/ PARM3, 0.0,  0,  0, NCS3,  3/ {RCOV(3,2+K, 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 filing of the MP^{th} 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 MP^{th} parameter (or optionally just a zero) is entered in the first floating-point field of the LIST.

30.1.2.3. 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. These 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 30.1.2.1.) 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 30.1.1.2. 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).

30.1.3. Additional Procedures

30.1.3.1. 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.

30.1.3.2. Parameter Values

Because many models are nonlinear, 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 30.1.2.2. 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.

30.1.3.3. Eigenvalue Representation

By use of eigenvalue methods[51], 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.

[51] For example, the SSIEV routine described in B.T. Smith, et. al., *Matrix Eigenvalue Routines - EISPACK Guide*, 1976.

30.1.3.4. 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.

30.1.3.5. 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 $\sigma(EG_i)$. (Alternative approaches exist.)

3.1.4. Multigroup Applications of Parameter Covariances

Given the relative covariances, $RCOV(\alpha_i,\alpha_j) \equiv Cov(\alpha_i,\alpha_j)/\alpha_i\alpha_j$, from (MF30, MT2), and the multigrouped sensitivities g'_{mi} from Eq. (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 30.1.2.1.) 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,

$$\begin{aligned}
\mathrm{Cov}\left(g_m, g_n\right) &= \sum_{ij} \frac{\partial g_m}{\partial \alpha_i} \frac{\partial g_n}{\partial \alpha_j} \mathrm{Cov}(\alpha_i, \alpha_j) \\
&= \sum_{ij} \alpha_i \alpha_j \frac{\partial g_m}{\partial \alpha_i} \frac{\partial g_n}{\partial \alpha_j} \mathrm{Cov}(\alpha_i, \alpha_j) / \alpha_i \alpha_j \qquad (0.73) \\
&= \sum_{ij} g'_{mi}\, g'_{nj}\, \mathrm{RCOV}(\alpha_i, \alpha_j)\,.
\end{aligned}$$

Equation (30.7) gives the desired multigroup covariance matrix in terms of the multigrouped (logarithmic) sensitivities from Eq. (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 $Cov(g_m,g_n)$ becomes prohibitively large (10^8 items), while the sensitivity matrix g'_{mi} (containing 500000 items) and parameter covariance matrix $RCOV(\alpha_i,\alpha_j)$ (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, y. A typical number of such quantities might also be around 50. The covariance matrix D(y) for the integral quantities is related (again in the first-order approximation) to the cross section covariance matrix D(g), with elements given by Equation (30.7), by the familiar propagation of errors relation,

$$D(y) = S\ D(g)\ S^T \tag{0.74}$$

where S is the 50 × 10000 sensitivity matrix relating the integral quantities y to the multigroup cross sections g. S can be obtained from standard neutronics analyses. If we introduce a 10000 × 50 matrix R, having elements g'_{mi}, Equation (30.7) can be re-written in matrix form,

$$D(g) = R\,D(\alpha)R^T$$

Equation (30.8) can then becomes

$$D(y) = S\left[R\,D(\alpha)\,R^T\right]S^T = T\,D(\alpha)\,T^T \tag{0.75}$$

The product matrix $T = S\,R$, which contains the direct sensitivity of the integral data to the nuclear-model parameters, is very compact, having about the same size as the covariance matrix $D(\alpha)$. Note that in evaluating the matrix products in Equation (30.9) one actually never need calculate the full 10000 × 10000 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 $D_{33}(y)$ based on conventional sensitivity and uncertainty analysis (*i.e.*, based on Files 3 and 33 only) with analogous data $D_{30}(y)$ 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.

31. FILE 31. COVARIANCES OF THE AVERAGE NUMBER OF NEUTRONS PER FISSION

31.1. General Description

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 $\bar{\nu}$, 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, $\bar{\nu}_d$, and the average number of prompt neutrons per fission, $\bar{\nu}_p$, respectively.

The average number of neutrons per fission is given as a function of incident energy for induced fission. This energy dependence may be given by tabulating the values as a function of incident neutron 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

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 $\bar{\nu}$ or its covariance components. There, NC- and NI-type sub-subsections for spontaneous fission neutron multiplicity have no energy variables present.

"NC-type" sub-subsections for spontaneous fission $\bar{\nu}$, MT=452, 255, 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" sub-subsections 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 33.3 concerning the ordering and completeness of sections of File 33 apply to sections of File 31: $\bar{\nu}$ (MAT,31,452), $\bar{\nu}_d$ (MAT,31,455) and $\bar{\nu}_p$ (MAT,31,456).

Note that in File 1 $\bar{\nu}$ (MT=452), $\bar{\nu}_d$ (MT=455) and $\bar{\nu}_p$ (MT=456) satisfy the relation:

$$\bar{\nu}(E) = \bar{\nu}_d(E) + \bar{\nu}_p$$

Therefore, if one of these quantities is "derived" in terms of the other two, it is permissible to use "NC-type" sub-sections with LTY=0 to indicate that it is a "derived redundant cross section". See section 33.2.1.a. 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 $\bar{\nu}_d$ is much smaller than $\bar{\nu}_p$, it should never be evaluated by subtracting $\bar{\nu}_p$ from $\bar{\nu}$.
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 $\bar{\nu}$ for spontaneous fission of ^{252}Cf and the $\bar{\nu}$(E) for the major fissile materials by use of NC-type sub-subsections 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.

32. FILE 32, COVARIANCES OF RESONANCE PARAMETERS

32.1. General Description

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-5 to the Breit-Wigner representations (LRF=1 or 2), in ENDF-6 formats covariances may also be given for the Reich-Moore (LRF=3) and Adler-Adler (LRF=4) 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 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 energy. 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.

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 or 4 for LRU=1 (resolved parameters) and to LRF=1 for LRU=2 (unresolved parameters).

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,   0, LFW,  NER] 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,   0, LFW,  NER] 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 sub-subsections as defined in Chapter 33.2 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-5, as described in Section 32.2.1 below. If LCOMP≠0, then NLS=0 and subsection formats are as shown in Sections 32.2.2 and 32.2.3.

32.2.1 Compatible resolved resonance subsection format.

This format differs from that used for ENDF-5 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). 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 sub-subsections 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,    0.0,
                                (DJDN1,DJDG1,DJDF1=0.0)
```

<three physical records for each resonance through resonance NRS>] LIST

<a similar list record for each additional 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.

32.2.2 General resolved resonance subsection formats.

Following the record that starts with the target spin, SPI, if it states LCOMP≠0, the next card of a subsection defines for that isotope and energy range how many (NSRS) sub-sections will occur for covariances among parameters of specified resonances and how many (NLRS) sub-sections are to contain data on long-range parameter covariances. The complete structure of an LCOMP=1 subsection is as follows:

<f NRO≠0, a control record and NI sub-subsections for energy-dependent covariances of the scattering radius>

```
[MAT,32,151/ SPI,  AP,   0, LCOMP,  NLS,    0] CONT  (LCOMP=1,NLS=0)
[MAT,32,151/AWRI, 0.0,   0,     0, NSRS, NLRS] CONT
```

<NSRS sub-subsections each giving covariances among specified parameters of enumerated sets of resonances>

<NLRS sub-subsections each giving long-range covariances contributions for stated energy regions for a particular type of resonance parameter>

Covariance formats for NSRS-type sub-subsections

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 to 4 are allowed, there is no segregation by L-value, 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 following paragraphs cover the formats for the NSRS sub-subsections for the various (LRF) resonance formulations for resolved parameters (LRU=1). LRF=1 through 4 are allowed.

<u>LRF=1,2, LRU=1.</u> 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 sub-sections 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 is covariance data.

ER_1, AJ_1, GT_1, GN_1, GG_1, GF_1,
…
…
ER_{NRB}, AJ_{NRB}, GT_{NRB}, GN_{NRB}, GN_{NRB}, GG_{NRB}, GF_{NRB},

Resonance parameter variances and

V_{11}, V_{12}, ... $V_{1,MPAR*NRB}$, V_{22},
..., $V_{2,NPAR*NRB}$, V_{33},

covariances for all resonances listed.	...,	$V_{MPAR*NRB,MPAR*NB}$, 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.

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 sub-section.
ER	Lab system energy of the kth resonance (in this block).
$\mathbf{AJ_k}$	Floating-point value of the spin for the kth resonance.
$\mathbf{GT_k}$	Total width (eV) for the kth resonance. GT=GN+GG+GF+GX.
$\mathbf{GN_k}$	Neutron width of the kth resonance.
$\mathbf{GG_k}$	Gamma-ray width for the kth resonance.
$\mathbf{GF_k}$	Fission width of the kth resonance.
$\mathbf{V_{mn}}$	Variance (eV^2) or covariance matrix element, row m and column, n≥m. If j≤MPAR is the parameter index (j=4 for fission width) for the kth resonance in the block, m=j+(k-1)×MPAR. The indexing is the order defined above under MPAR.

LRF=3, LRU=1. 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.

LRF=4, LRU=1. 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 sub-subsection 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,
GRF1,  GIF1,  DEC1, DWC1,     GRC1,  GIC1,
------------------------------------
DETNRB, DWTNRB, GRTNRB, GITNRB, DEFNRB, DWFNRB,
GRFNRB, GIFNRB, DECNRB, DWCNRB, GRCNRB, GICNRB,
 V11,  V12, -------------, V1,MPAR*NRB,    V22,
-----------------------, V2,NPAR*NRB,    V33,
----------, VMPAR*NRB,MPAR*NB,      0.0,   0.0] LIST
```

Parameters for each reference in the block.

Resonance parameter variances for all resonances listed.

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, DWT = DWF = DWD = v,
GRT, GIT, GRF, GIF, GRC, GIC

<u>Format for Long-Range Covariance Sub-subsections (LRU=1)</u>. Here are described the forms that the sub-subsections 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.

Here each sub-subsection 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 following table 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 COV[Γ_α(i),Γ_α(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.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \delta_{ij} \sum_{k=1}^{NE-1} S_i^k \, F_{\alpha k}^{(-1)} \, \Gamma_\alpha^2(i)$$

LB=0 Absolute covariance components correlated only within each E interval.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k=1}^{NE-1} P_{j,k}^{i,k} \, F_{\alpha k}^{(0)}$$

LB=1 Relative covariance components correlated only within each E interval

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k=1}^{NE-1} P_{j,k}^{i,k} \, F_{\alpha k}^{(1)} \, \Gamma_\alpha(i)\,\Gamma_\alpha(j)$$

LB=2 Fractional covariance components fully correlated over all E intervals with variable magnitude.

$$Cov\left[\Gamma_{\alpha}(i)\Gamma_{\alpha}(j)\right] = \sum_{k,k'=1}^{NE1} P_{j,k'}^{i,k} F_{\alpha k}^{(2)} F_{\alpha k'}^{(2)} \Gamma_{\alpha}(i)\Gamma_{\alpha}(j)$$

LB=5 Relative covariance components in an upper triangular representation of a symmetric matrix.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k,k'=1} P^{i,k}_{j,k'} F^{(5)}_{\alpha kk'} \Gamma_\alpha(i)\Gamma_\alpha(j)$$

Note that the $F^{(-1)}$, $F^{(1)}$, and $F^{(5)}$ parameters have the dimensions of relative covariances, the $F^{(0)}$ are absolute covariances, and the $F^{(2)}$ are relative standard deviations.
The S and P are dimensionless operations defined in Section 33.2

The sub-subsection format for LB=–1, 0, 1, or 2 is:

```
[MAT,32,151/  0.0,  0.0,  IDP,  LB, 2*NE,  NE/{Ek,F(LB)}] LIST
```

For LB=5 the requisite format is

```
[MAT,32,151/  0.0,  0.0,  IDP,  LB,   NT,  NE/{Ek},{Fkk(5)}] LIST(LB=5)
```

In the above:

LB Indicator of covariance pattern as defined above.
NE Number of energies in the parameter table for a given sub-section.
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=μ
2	Γ_n	Γ_n	Γ_n	v
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_{11}, F_{12}, ..., $F_{1,NE-1}$; F_{22}, $F_{2,NE-1}$; $F_{NE-1,NE-1}$

32.2.3 Unresolved resonance subsection 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.

<u>Correspondence Between Files 2 and 32. Completeness of File 32.</u>

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≠0, LRU=1 subsections, any selection of the resonances shown in File 2 for consistent resonance formulations may be listed in NSRS-type sub-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 NLRS-type sub-subsection must cover the entire energy range (EL,EH) of the subsection. However, any desired covariance components may be null.
5. NLRS-type sub-subsections may be included in any order in LCOMP≠0, LRU=1 subsections.

<u>Obtaining Cross Section Covariances From File 32 and File 33.</u>

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 non-zero 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 the average parameters. See B.L. Broadhead and H.L. Dodds [Ref. 2].

Example For Mat 3333.

The nucleus of concern in this example has resonances represented by LRF=2 for the energy range (1,50). 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. Table 32.1 shows the File 2 for the example, and Table 32.2 shows the corresponding file 32.

In File 32, there are included three NSRS-type sub-subsections and four NLRS-type sub-subsections. 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

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 sub-subsection refers only to the 5-eV resonance, and conveys the following covariance contribution:

E_r	0.5×10^{-6}	0	0	0
Γ_n		1×10^{6}	1×10^{6}	0.2×10^{6}
Γ_γ		1×10^{6}	0.0	2.0×10^{6}
Γ_f		0.2×10^{6}	2.0×10^{6}	4×10^{6}

The third block covers Γ_n covariances for the 30 and 40 eV resonances.

The first NLRS sub-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 sub-subsection fills the "hole" in the table just above (with the value 16×10^{-6}). The second sub-subsection expresses the expected resonance-to-resonance uncorrelated fluctuation in Γ_γ. The third and fourth sub-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 of 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. +0   5.00 +1    LRU=1    LRF=2    NRO=0   NAPS=0333332151 CONT
  1.0 +0   0.6  +0        0        0    NLS=1        0333332151 CONT
  2.7 +2   0.0  +0      L=0    LRX=0 6*NRS=30    NRS=5333332151
 .1.0 +0   1.5  +0  4.04 +0  3.0  +0  0.04 +0  1.0  +0333332151
  5.0 +0   1.5  +0  0.07 +0  0.01 +0  0.04 +0  0.02 +0333332151
  1.5 +1   0.5  +0  0.08 +0  0.01 +0  0.04 +0  0.03 +0333332151
  3.0 +1   1.5  +0  7.04 +0  1.0  +0  0.04 +0  6.0  +0333332151
  4.0 +1   1.5  +0  6.04 +0  5.0  +0  0.04 +0  1.0  +0333332151 LIST
  0.0 +0   0.0  +0        0        0        0        0333332  0 SEND
  0.0 +0   0.0  +0        0        0        0        03333 0  0 FEND
```

Example 32.2. 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. + 0  5.00 + 1    LRU=1    LRF=2    NRO=0   NAPS=0333332151 CONT
  1.0 + 0  0.6 + 0         0  LCOMP=1    NLS=0        0333332151 CONT
  2.7 + 2  0.0 + 0         0        0   NSRS=3   NLRS=4333332151 CONT
  0.0 + 0  0.0 + 0    MPAR=4                1652   NRB=1333332151
 -1.0 + 0  1.5 + 0  4.04 + 0  3.0 + 0 0.04 + 0  1.0 + 0333332151
  1.0 + 0 -1.5 + 0   0.0 + 0 -0.2 + 0  4.0 + 0  0.0 + 0333332151
 -1.0 + 0  0.0 + 0   0.0 + 0  0.8 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0    MPAR=4                16*   NRB=1333332151
  5.0 + 0  1.5 + 0  0.07 + 0 0.01 + 0 0.04 + 0 0.02 + 0333332151
  0.5 - 6  0.0 + 0   0.0 + 0  0.0 + 0  1.0 - 6  -1.0 -6333332151
 -0.2 - 6  0.0 + 0  -2.0 - 6  4.0 - 6  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0    MPAR=2                22*    NRB=2333332151
  3.0 + 1  1.5 + 0  7.04 + 0  1.0 + 0  0.04 + 0 6.0 + 0333332151
  4.0 + 1  1.5 + 0  6.04 + 0  5.0 + 0  0.04 + 0 1.0 + 0333332151
  2.0 - 3  0.0 + 0   0.0 + 0  0.0 + 0  1.0 - 3  0.0 + 0333332151
 -0.5 - 4  2.0 - 3   0.0 + 0  2.0 - 3  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0     IDP=3     LB=1   2*NE=4     NE=2333332151
 -2.0 + 0  1.0 - 2   5.0 + 1  0.0 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0     IDP=3    LB=-1   2*NE=8     NE=4333332151
 -2.0 + 0  1.0 - 2   1.0 + 0  0.0 + 0  1.0 + 1  1.0 - 2333332151 LIST
  5.0 + 1  0.0 + 0   0.0 + 0  0.0 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0     IDP=2     LB=5     NT=6     NE=3333332151
  1.0 - 5  2.0 + 1   5.0 + 1  1.0 - 4  1.0 - 4  2.0 - 4333332151 LIST
  0.0 + 0  0.0 + 0     IDP=4     LB=1   2*NE=4     NE=2333332151
  1.0 - 5  4.0 - 4   5.0 + 1  0.0 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0         0        0        0        0333332  0 SEND
  0.0 + 0  0.0 + 0         0        0        0        03333 0  0 FEND
```

52 *NVS+6*NRB

REFERENCES

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)

33. FILE 33, COVARIANCES OF NEUTRON CROSS SECTIONS

33.1. General Description

File 33 contains the covariances of neutron cross section information appearing in File 3. It is intended to provide a measure of the "accuracies and their correlations" of the data in File 3, and does not indicate the precision with which the data are entered in the File 3. Since ENDF/B represents our knowledge of the microscopic data, the File 33 is used to give the covariances of these microscopic data. 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.

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.

Table 33.1
Analogies Between File 33 Covariances Within One Section and Uncertainties in a Hypothetical Experiment [53]

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

Example: If there is 2% uncertainty due to statistics (short-range), 2% due to multiple scattering (medium-range) and, 1% due to geometry (long-range), cite a 3% uncertainty for a discrete measurement (one group covering a small energy range); ≈2.5% over an energy range encompassing several measurements (several groups

[53] 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.

which together cover a 1- to 2-MeV range); and closer to 1% average over the entire energy range.

3.2. Formats

File 33 is divided into sections identified by the value of MT. Within a section, (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	Nonzero 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 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
```

3.2.1. Subsections

Each subsection of the section (MAT,33,MT) is used to describe a single covariance matrix. It is the covariance matrix of the energy-dependent cross sections given in section (MAT,3,MT) and energy-dependent cross sections given in section (MAT1,MF1,MT1) of the ENDF tape. [If MF1=0, then in the subsection (MAT1,10,MT1.LFS1)]. The values of MAT1, XMF1 = Float(MF1), MT1, and XLFS1 =Float(LFS1) if MF1=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" sub-sections. 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 MF for 2nd energy-dependent cross section of pair for which correlation matrix is given. If MF1=MF, XMF1 = 0.0 or blank.
XLFS1	Floating point equivalent for final excited state of 2nd energy-dependent cross section, For MF1=10, XLFS1 = 10; if MF1≠10, XLFS1 = 0.0 or blank.
MAT1	MAT for 2nd energy-dependent cross section
MT1	MT for 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 the ENDF/B tape (MAT,3,MT) and (MAT1,MF1,MT1,[LFS1]) is:

```
[MAT,33,MT/ MF1, 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>
```

3.2.2. Sub-subsections

The "NC-type" and "NI-type" sub-subsections have different structures.

The "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/B tape. The major purpose of the "NC-type" sub-subsections is to eliminate from the ENDF/B tape a large fraction of the mostly redundant information which would otherwise be needed if only "NI-type" sub-subsections were used.

The "NI-type" sub-subsections are used to describe explicitly various components of the covariance matrix defined by the subsection.

I. <u>"NC-type" sub-subsections</u>

The "NC-type subsections may be used to describe the covariance matrices in energy ranges where the cross sections in (MAT,3,MT) can be "derive" 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

a.) <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" the covariances of these cross sections are given in File 33 wholly in terms of "NI-type" sub-subsections. [In general the linear relationship given in an LTY=0 sub-subsection applies not only to the range of energy specified, but also over the whole range of the file.]

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}[54].

{CI, XMTI} **Array of pairs consisting of coefficient CI and a value of XMTI, (MTI given as a floating point number). The pair of numbers indicate 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:**

$$\sigma_{MT}^{MAT}(E) = \sum_{i=1}^{NC1} C_i \times \sigma_{MT}^{MAT}(E) \quad .$$

[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] CONT                (LTY=0)
[MAT,33,MT/  EL,  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 33.3.2-a-3). In such cases the subsection may be thought of as describing in part several covariance matrices.

b.) <u>LTY=1, 2 and 3, "Covariances of Cross Sections Derived via Ratio Measurements to Standard Cross Sections"</u>.

Many important cross sections of ENDF/B are based on measurements of cross sections ratios. When an evaluated cross section is obtained from such measurements, covariances so generated between the cross sections for the two reactions may become important. This is a primary origin of ENDF-6 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 to those standards. 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.

[54] The Notation {AI,BI} stands for A_1, B_1; A_2, B_2; ...; A_i, B_i in a list record.

In order efficiently to represent in File 33 the covariances that depend on "absolute" ratio measurements to standards, evaluators may use "NC"-type sub-subsections with LTY=1, 2 and 3 in appropriate File 33 subsections. [In other cases of covariance components induced by ratio measurements, it is necessary for the evaluator to represent the covariance components that arise may be found in the literature.[55]]

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,

$$\sigma_a(E) = \alpha(E)\ \sigma_S(E)\ , \quad \text{for } (E1 \le E < E2)$$

The evaluated ratio itself is assumed to be independent of the standard cross section evaluation because the relevant measurements are similarly independent. If so, then

$$\mathrm{Rvar}[\sigma_a(E)] = \mathrm{Rvar}[\alpha(E)] + \mathrm{Rvar}[\sigma_S(E)], \quad \text{for } (E1 \le E < E2)$$

$$\mathrm{Rvar}[\sigma_a(E),\sigma_a(E')] = \mathrm{Rvar}[\alpha(E),\alpha(E')] + \mathrm{Rvar}[\sigma_S(E),\sigma_S(E')],$$

$$\text{for } (E1 \le E < E2) \text{ and } (E1 \le E' < E2)$$

$$\mathrm{Rvar}[\sigma_a(E),\sigma_S(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_S(E')], \quad \text{for } (E1 \le E < E2) \text{ and } (E1 \le E' < E2)$$

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 o the energy E′.

A cross section $\sigma_a(E)$ may be obtained from measurements relative to (MATS,MTS) energy region ($E1 \le E < E2$) and cross section $\sigma_b(E')$ from (MATS′,MT′) in energy region ($E1' \le E' < E2'$). 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:

$\mathrm{Rvar}[\sigma_a(E),\sigma_b(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_{S'}(E')]$, for $(E1 \le E < E2)$ and $(E1' \le E < E2')$, zero otherwise;

$\mathrm{Rvar}[\sigma_a(E),\sigma_{S'}(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_{S'}(E')]$, for $(E1 \le E < E2)$ and all E′ ,zero otherwise;

$\mathrm{Rvar}[\sigma_S(E),\sigma_b(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_{S'}(E')]$, for $(E1' \le E' < E2')$ and all E, zero otherwise;

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,

---

[55] 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)

R. W. Peele, "Uncertainties and Correlations in Evaluated Data Sets Induced by the Use of Standard Cross Sections", **NBS Special Publication 425**, *Conf. on Nuclear Cross Sections and Technology*, p.173, R. A. Schrack and C. D. Bowman, eds. (1975)

Rcov[σ_a(E), σ_x(E')] = Rcov[σ_S(E), σ_x(E;)], for (E1 $\leq$ E < E2) and all σ_S(E′), zero otherwise.

The right side may nonzero for many (MATX, MTX), and discretion may be required to avoid generation in cross section processing of negligible but nonzero multigroup covariances 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,MT;MAT,3,MT,0) 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. (LFS=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,MT;MAT,3,MT,0).

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 in over its complete energy range. Therefore, in the File 33 of the material MAT, in subsection contsining 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,MT; MAT,3,MT,0)] 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,MTS,[LFSS]; MAT,MT) of the File (MFS+30) of the "standard" material MATS and LTY=3 sub-subsection in the File 33 subsection (MAT,MFT; MAT,3,MT,0)] 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 (NEI-1) 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 WE_i in the interval $E_i \leq E < E_{i+1}$. 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 sub-section 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,0) 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,0); 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,0) 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 ENDF/B and are not restricted to the special set of "standard cross sections" maintained in the ENDF/B library. The "standard cross sections of ENDF/B" 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.

II. "NI-type" Sub-subsections

The "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 a flag, the 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 $\{E_k, F_k\}\{E_l, F_l\}$.

a. Flag LB=0-4

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, $\{E_l,F_l\}$.LT=0, when the table contains is a single array $\{E_k,F_k\}$. LT≠0, when 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 a 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/ {Ek, Fk}{El, Fl}] LIST
```

The E_n 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. 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 section in (MAT,3,MT) at energy E_i and Y_j refer to the cross section in (MAT1,3,MT1) at energy E_j. The contribution of the sub-subsection to the covariance matrix 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

$$Cov\left(X_i,Y_i\right)=\sum_k P_{j;k}^{i;k}F_{xy;k}$$

LB=1 Fractional components correlated only within each E_k interval

$$Cov\left(X_i,Y_i\right)=\sum_k P_{j;k}^{i;k}F_{xy;k}X_iY_j$$

LB=2 Fractional components correlated over all E_k intervals

$$Cov\left(X_i,Y_i\right)=\sum_{k,k'} P_{j;k}^{i;k}F_{xy;k}F_{xy;k'}X_iY_j$$

LB=3 Fractional components correlated over E_k and E_l intervals

$$Cov\left(X_i,Y_i\right)=\sum_{k,l} P_{j;l}^{i;k}F_{x;k}F_{y;l}X_iY_j$$

LB=4 Fractional components correlated over all E_l intervals within each E_k interval

$$Cov\left(X_i,Y_i\right)=\sum_{k,l,l'} P_{j;k,l'}^{i;k,l}F_kF_{xy,l}F_{xy,l'}X_iY_j$$

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≠0, *i.e.*, two E tables, the E_k and the E_l tables.

The dimensionless operators P in the above definitions are defined in terms of the operator S as follows:

$$P_{j;m,n,...}^{i;k,l,...} \equiv S_i^k\, S_i^l \ldots S_j^m\, S_j^n \ldots ,$$

where $S_i^k \equiv 1$, when $E_k \le E_i \le E_{k+1}$ and
$S_i^k \equiv 0$, when the energy E_i is outside the range of E_k to E_{k+1} of an E_k table.

b.) <u>Flag LB=5</u>. 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:

$$Cov\left(X_i,Y_i\right)=\sum_{k,k} P_{j;k}^{i;k}F_{xy;k,k}X_iY_j$$

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/ {Ek}{Fk,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

$$NT = NE + (NE-1)^2 = NE(NE-1) + 1$$

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

$$NT = NE + [NE\ (NE-1)]/2 = [NE\ (NE+1)]/2$$

c.) <u>Flag LB=6</u>. 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:

$$Cov\left(X_i, Y_i\right) = \sum_{k,l} P_{j;l}^{i;k} F_{xy;k,l} X_i Y_j$$

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 P is as defined for other LB's. A single "stacked" list of energies $\{E_{kl}\}$ 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 $\{E_{kl}\}\{F_{k,l}\}$. 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, NT, NER/ {`E_{kl}`}{`$F_{k,l}$`}] LIST` (LB=6)

The matrix elements $F_{k,l}$ are ordered by rows in the array $\{F_{k,l}\}$:

$$\{F_{k,l}\} = F_{1,1}, F_{1,2}, \ldots, F_{1,NEC-1}; F_{2,1}, \ldots, F_{2,NEC-1}; \ldots; F_{NER-1,1}, F_{NER-1,2}, \ldots, F_{NER-1,NER-1}$$

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:

$$NT = NER + NEC + (NER-1)(NEC-1) = 1 + NER*NEC.$$

d.) <u>Flag LB=8, Short Range Variance Representation</u>. 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 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 arrays $\{E_k, F_k\}\{E_l,F_l\}$.
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 sub-section 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)

Only one E_k table is required. The F_k values for LB=8 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} for the LB=8 component are just F_k and the off diagonal elements are zero.

In general, each F_k characterizes an uncorrelated contribution to the absolute variance of the indicated cross section averaged over any energy interval (sub-group) ΔE_j that includes a portion of the energy interval ΔE_k. The variance contribution VAR_{jj} from an LB=8 sub-subsection to the processed group variance for the energy group (E_j,E_{j+1}) is inversely 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

$$VAR_{jj} = F_k\, \Delta E_k/\Delta Ej\ , \text{ where } E_k \le E_j \le E_{j+1} \le E_{k+1}$$

Note that the VAR_{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 sub-subsections.

3.2.3. 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] HEAD` (NL=0)

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 File 3, 4 or 5, 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≠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" sub-section 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.) <u>Sections</u>. 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 identified by the set of numbers: (MAT,MT;MAT1,MF1,MT1,[LFS1]); the first pair of numbers indicated the section and the second set of numbers appears in the appropriate fields, XMF1, XLFS1, MAT1 and MT1, of the CONT record which begins every subsection. [When MT≠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. When MAT1=0, when according to procedure 33.3.1-b-2 means that MAT1=MAT, and XMF1=0.0 meaning MF1=MF-30, only subsections for which MT1>MT shall 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.

c.) Sub-subsections. 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.

1. "NC-type" sub-sections. 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-subsection. However, in ENDF-6 formats it is permitted to have overlapping (E1,E2) ranges for LTY≥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.

2. "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:

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[MAT,MT; MAT1,MF1,MT1,(LFS1)]
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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 procedure 33.3.1-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,0) 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 paragraph 33.3.2.b below concerning the desirability of explicitly representing some zero covariances.) This procedure and procedure 33.3.1-b-4 guarantee that every section of File 33, (MAT,33,MT), starts with the subsection (MAT,MT; 0,3,MT,0).

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-subsection.

3. "NC-type" sub-subsections with LTY=0 must be given only in subsections of the type (MAT,MT; 0,3,MT,0), *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,0) 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 33.3.3.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,0), 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, similar to procedure 33.3.2-a-1, there must also be a subsection (MAT,MT; 0,3,MT,0) 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,0) in the File (MF1+30) for material MAT1.

33.3.3. Other Procedures

a.) "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.

b.) 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.

c.) 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.

d.) "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.

e.) 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 of 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 intergroup 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.

f.) 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.

1. 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.
2. 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.

g.) 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.

h.) 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.

i.) 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.

j.) 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′ continuum), may also be treated in this way.

k.) 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.

l.) The components of a lumped reaction need not have adjacent MT-numbers.

m.) 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.

n.) 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.

o.) An LB=8 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[56]. The Doppler effect in reactor applications smooths cross sections on an energy scale too narrow to be of concern for LB=8 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 nonphysical full correlation between neighboring fine-group cross sections, the problem that the LB=8 format was designed to solve. The LB=8 format 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 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/B-VI covariance files).

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 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 Sub-sections. 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 specifies absolute covariances, it should not be employed near reaction thresholds. In particular, for threshold reactions having an effective threshold above 0.1 MeV, LB=8 should not be employed for incident energies less than 1 MeV above the effective threshold.

[56] 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 sub-section. Covariance data in such cases may best be represented in File 30.

33.4. Examples

We illustrate here the use of File 33 by means of two concrete examples.

a. Use of LTY=1 and LTY=2 "NC-type" subsections

Let us consider the 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 section of ^{239}Pu at the energy E_i.

   a. From 10^{-5} eV to an energy ES, X_i was 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 ES 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 $X_i = R_iY_i$, 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 section of ^{239}Pu at the energy E_i. In this evaluation, Z_i was 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 $Z_i = a_iX_i$.

In this evaluation then, only 3 quantities were evaluated: A_i from 10^{-5} eV to ES, R_i from Es 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: COV(A_i,A_j), COV(R_i,R_j) and 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 COV(A_i,a_j) can be neglected.

Let us denote relative covariance matrices such as COV(A_iA_j)/(A_iA_j) as $\langle dA_i,dA_j\rangle$, and similarly for the other quantities.

From 10^{-5} to ES, since $X_i = A_i$ and $Z_i = a_iX_i$, we have:

$$\langle dX_i\cdot dX_j\rangle = \langle dA_i\cdot dA_j\rangle$$
$$\langle dX_i\cdot dZ_j\rangle = \langle dA_j\cdot dA_j\rangle$$
$$\langle dZ_i\cdot dZ_j\rangle = \langle da_i\cdot da_j\rangle + \langle dA_i\cdot dA_j\rangle$$

From ES to 20 MeV, since $X_i = R_iY_i$ and $Z_i = a_iX_i$, we have

$$\langle dX_i\cdot dX_j\rangle = \langle dR_i\cdot dR_j\rangle + \langle dY_i\cdot dY_j\rangle$$
$$\langle dX_i\cdot dZ_j\rangle = \langle dR_i\cdot dR_j\rangle + \langle dY_i\cdot dY_j\rangle$$
$$\langle dX_i\cdot dY_j\rangle = \langle dY_i\cdot dY_j\rangle$$
$$\langle dZ_i\cdot dZ_j\rangle = \langle da_i\cdot da_j\rangle + \langle dR_i\cdot dR_j\rangle + \langle dY_i\cdot dY_j\rangle$$
$$\langle dZ_i\cdot dY_j\rangle = \langle dY_i\cdot dY_j\rangle$$

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 $<dA_i \cdot dA_j>$, $<dR_i \cdot dR_j>$ and $<da_i \cdot da_j>$ 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:

$<dA_j \cdot dA_j> \rightarrow \{E_k^A, F_k^A\}$
$<dR_j \cdot dR_j> \rightarrow \{ER_k^R, FR_k^R\}$
$<da_j \cdot da_j> \rightarrow \{E_K^a, F_k^a\}$

Whether one or more "NI-type" sub-subsection is used, each one of the E tables used in the sub-subsections can be written as:

$\{E_k^A, F_k^A\} = \{1.0E\text{-}5, F_1^A ; ...; E_k^A, F_k^A ; ...; ES, 0.0; 2.0E+7, 0.0\}$,
$\{E_k^R, F_k^R\} = \{1.0E\text{-}5, 0.0; ES, F_k^R ; ...; E_k^R, F_k^R ;...; 2.0E+7, 0.0\}$,
$\{E_k^a, F_k^a\} = \{1.0E\text{-}5, F_1^a ; F_k^a ; ...; E_k^a, F_k^a ;...; 2.0E+7, 0.0\}$,

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 $<dA_i \cdot dA_j>$, $<dR_i \cdot dR_j>$ and $<da_i \cdot da_j>$. 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

```
9.42390+4 2.36999+2         0         0         0       NL=3126433 18 HEAD
0.00000+0 0.00000+0    MAT1=0     T1=18       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=0LB=1     NY=14      NE=7           126433 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;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 0.00000+0126433 19 <dYi×dYj>
0.00000+0 0.00000+0         0         0         0          0126433  0 SEND
      (1264,102;0,102)
```

Example 33.2. (continued) **File 33 with "NC-type" LTY=1 sub-subsections.**

```
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=61254331-2 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
```

b. 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:

$$<d\sigma_i^T \cdot d\sigma_j^T> \rightarrow \{E_k^T, F_k^T\} ,$$

with $\{E_k^T, F_k^T\} = \{1.0E\text{-}5, F_1^T ; ...; E_k^T, F_k^T ;...; 2.0E+7, 0.0\}$,

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:

$$<d\sigma_i^E \cdot d\sigma_j^E> \rightarrow \{E_k^E, F_k^E\} ,$$

with $\{E_k^E, F_k^E\} = \{1.0E\text{-}5, 0.0; 8.5E+6, F_k^E ; ...; E_k^E, F_k^E ;...; 2.0E+7, 0.0\}$.

3. Inelastic cross sections (MT=4), σ_i^I, were evaluated from threshold, 4.8 MeV, to 8.5 MeV and:

$$<d\sigma_i^i \cdot d\sigma_j^I> \rightarrow \{E_k^I, F_k^I\} ,$$

with $\{E_k^I, F_k^I\} = \{1.0E\text{-}5, 0.0; 4.8E+6, F_k^I ; ...; E_k^I, F_k^I ;...; 8.5E+6, 0.0; 2.0E+7, 0.0\}$,

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:

$$<d\sigma_i^C \cdot d\sigma_j^C> \rightarrow \{E_k^C, F_k^C\} ,$$

with $\{E_k^C, F_k^C\} = \{1.0E\text{-}5, F_1^C ; ...; E_k^C, F_k^C ;...; 2.0E+7, 0.0\}$,

5. The (n,α) cross sections (MT=107), σ_i^α, were evaluated from threshold, 6.18 MeV to 20 MeV and:

$$<d\sigma_i^\alpha \cdot d\sigma_j^\alpha> \rightarrow \{E_k^\alpha, F_k^\alpha\} ,$$

with $\{E_k^\alpha, F_k^\alpha\} = \{1.0E\text{-}5, 0.0; 6.18E+6, F_k^\alpha ; ...; E_k^\alpha, F_k^\alpha ;...; 2.0E+7, 0.0\}$,

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.

a. MT=51

The inelastic scattering to the first excited state, σ_1^{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: σ_i^{51} =

σ_1^I. This is permissible because MT=4 has only "NI-type" sub-subsection in this energy range.

From 8.5 MeV to 20 MeV, MT=51 was evaluated and:

$$<d\sigma_i^{51} \cdot d\sigma_j^{51}> \rightarrow \{E_k^{51}, F_k^{51}\} ,$$

with $\{E_k^{51}, F_k^{51}\}$ = {1.0E-5, 0.0; 8.5E+6, F_k^{51} ; ...; E_k^{51}, F_k^{51} ;...; 2.0E+7, 0.0},

b. MT=91

From 8.5 to 20 MeV, the continuum inelastic, σ_1^{91}, was "derived" as: $\sigma_i^{91} = \sigma_i^{I} - \sigma_i^{51}$. However, we cannot use this relationship for purposes of File 33 because in this energy range σ_i^{I} is indicated in the file as being already "derived."

Therefore, for 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-subsection.

```
     (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+0-1.00000+0 1.02000+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 0.00000-0 8.50000+6 8.00000-6 1.50000+6 2.50000-5112733  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
LIST
 1.00000+0 1.00000+0-1.00000+0 2.00000+0-1.00000+0 1.02000+2112733  4
-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 0.00000-0112733  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 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
```

34. FILE 34. COVARIANCES FOR ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES

34.1. Introduction

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 need 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(μ).

In ENDF-6 formats there is no provision for covariance components linking the angular distribution parameters for different materials, though a MAT1(=0) field is provided.

34.2. Formats

The general structure of File 34 follows the normal pattern, with sections for 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=3, 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, LVT, LTT,  0, NMT1] HEAD          (LVT=0)
              <subsection for MT1 = MT>
            ----------------------------
            ----------------------------
              <NMT1th 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 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.

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 item ,
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.s in the LIST.

{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,     0,   NI1] CONT [57]
[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
```

[57] In this first sub-section, 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/B file corresponding to a particular material. (The information contained in File 34 for L *or* L1 nonzero 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).

35. FILE 35. COVARIANCES FOR ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES

35.1. Introduction

File 35 contains covariance matrices for the energy distribution of secondary neutrons given in File 5. The data in File 5 are given in the Laboratory system, and are expressed as normalized probability distributions.

Since there is usually very fragmentary 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 neutron energy. It is therefore proposed that only a few (at most 4 or 5) 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. In this first attempt at dealing with covariance matrices of secondary energy distributions, no covariances between the different incident energy ranges will be 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 v_(E) in File 1 are allowed in File 35.

35.2. Formats

Each subsection covers a covariance matrix for an incident neutron energy range, and the complete incident energy range is covered by the NK subsections.

A new type of LB subsection is defined (LB=7), since in File 35 it is natural to specify the covariance matrices as absolute covariances rather than 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 neutron energies, and defining NE-1 energy intervals for outgoing neutrons. The value of E'_1 in the array must be the lowest outgoing neutron energy possible at E_1; E'_{NE} in the array must be the highest outgoing neutron 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

$$\{F_{k,k'}\} \equiv F_{1,1}, F_{1,2}; F_{2,2}, F_{2,3}, \ldots, \ldots; F_{NE-1,NE-1} .$$

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 points on the unity-normalized probability distribution

$$Cov\left(p\left(E \to E'_i\right), p\left(E \to E'_j\right)\right) = \sum_{k,k'} P^{i,k}_{j,k'} F_{k,k'}$$

is:

where $E_1 \leq E \leq E_2$, and the P values are defined so that only the term in the sum for $E'_k \leq E'_l \leq E'_{k+1}$ and $E'_k \leq E'_l \leq E'_{K'+1}$ is non-zero.

35.3. Procedures

Because probability distributions must remain normalized to unity, covariance matrices in File 35 must satisfy a constraint in addition to being symmetric. This constraint is that the sums of the elements in any row of the matrix, therefore also of any column, must be zero. Therefore, if one were to divide the outgoing energy of a distribution into n energy ranges, it would only be necessary to give the covariance matrix of the probabilities in n-1 energy ranges. The remainder of the full covariance matrix could be obtained from the above constraint.

There is a procedural objection to the above suggestion. It is that, for the covariance file, if no information is provided in the file, this does not imply anything as far as the uncertainties in the data are concerned. Therefore, it is necessary to provide redundant information in File 35 for each covariance matrix of a secondary energy distribution and to require that each covariance matrix in File 35 meets the above constraint. The sum of each row or column should be $<10^{-5}$ on the evaluator's energy grid. [Note that this condition must also be met with processed data on the user's energy grid].

If $F_{k,k'}$ are the covariance elements defined above for the normalized spectral yields Y_k on the evaluator's grid {E'_k}, but the above constraint has not been applied, corrected values $\hat{F}_{k,k'}$ may be obtained from the following relation.

$$\hat{F}_{k,k'} = F_{k,k'} - S_k Y'_k - S'_k Y_k + Y_k Y'_k \sum_j S_j$$

where $$S_k = \sum_i F_{i,k}$$

The secondary energy distribution uncertainty analysis using the "hot-cold" technique of Gerstl, et al., (see References) 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

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 Seminar-Workshop, August 22-24, 1978*, C. R. Weisbin, et al., Eds, Radiation Shielding Information Center report, Oak Ridge National Laboratory **ORNL/RSIC-42** (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).

40. FILE 40. COVARIANCES FOR PRODUCTION OF RADIOACTIVE NUCLEI

40.1. General Description

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.

Section

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
```

Subsection

Each subsection has the following structure:

```
[MAT,40, MT/  QM,  QI,   0, LFS,  0, NL] CONT
                <sub-subsection for L=1>
            --------------------------
            --------------------------
                <sub-subsection 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) with given final state (LFS) and the energy-dependent cross sections given in section (MAT1,MF1,MT1) (and for a given final state (LFS1), if MF1=10). The values of MAT1, MF1, MT1, and LSF1 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 given in (MAT, 10, MT) LFS and (MAT1,MF1, MT1) LFS1 is:

```
[MAT,40,MT/ XMF1, XLFS1, MAT1, MT1, NC, NI] CONT
                <sub-sub-subsection for nc = 1>
            -------------------------------
            -------------------------------
                <sub-sub-subsection for nc = NC>
                <sub-sub-subsection for ni = 1>
            -------------------------------
            -------------------------------
                <sub-sub-subsection for ni = 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.

40.3.1. Ordering of Sections, Subsections, Sub-subsections, and Sub-sub-subsections

a. Sections: The sections in File 40 are ordered by increasing value of MT.

b. Subsections: Within a section, (MAT,40,MT), the subsections are ordered by increasing value of LFS.

c. 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.

1. **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.**
2. 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.

3. 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.
4. 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).

40.3.2. 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, MT, MF=10, LFS), in File 40 of MAT;
b. (MAT1, MT1, LFS1; MAT1, MT1, MF1, LFS1), in File (MF1+30) of MAT1;
c. (MAT1, MT1, LFS1; MAT, MT, MF=10, LFS), also in File (MF1+30) of MAT1.

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_o is mass of the principal scattering atom in molecule.	7
ABN	Abundance (weight fraction) of an isotope in this material.	2,32
AC	Channel radius	2
AC_1, AC_2, AC_3, AC_4, BC_1, BC_2	Background constants for the Adler-Adler radiative capture cross section.	2
AF_1, AF_2, AF_3, AF_4, BF_1, BF_2	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
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
AT_1, AT_2, AT_3, AT_4, BT_1, BT_2	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.	2
AWI	Projectile mass in neutron units.	1
AWP	Product mass in neutron units.	6

Parameter	Definition	Chapter
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.	5
$b_i(E,E')$	Representation of angular part of $f_i(\mu,E,E')$.	6
$B_i(N)$	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
	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
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
DJDF	Covariance of AJ and GF.	32
DJDG	Covariance of AJ and GG.	32
DJDN	Covariance of AJ an GN.	32
DN^2	Variance of GN.	32
DNDF	Covariance of GN and GF.	32
DNDG	Covariance of GN and GG.	32

* The subscript r denotes the rth resonance.

Parameter	Definition	Chapter
DWC_r^*	Value of Γ/2, (v), used for the radiative capture cross section.	2
DWF_r^*	Value of Γ/2, (v), used for the fission cross section.	2
DWT_r^*	Value of Γ/2, (v), 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 (Appendix E).	all
E_{th}	Threshold energy.	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-department fission spectrum	5
EFL	Constant in energy-department 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
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

Parameter	Definition	Chapter
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
ER_{AV}	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
$g_j(E_\gamma \leftarrow E)$	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	3
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

Parameter	Definition	Chapter
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
$GP_{j,i} \equiv Gp_i$	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 ate 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
I_i	Interpolation scheme (see Appendix E) to be used between the E_{i-1} and E_i energy points.	8
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
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	

Parameter	Definition	Chapter
LASYM	Flag indicating whether asymmetric S(α,β) is given.	
LAT	Flag indicating which temperature has been used to compute α and β.	7
LAW	Distinguishes between different representations of f_i, the normalized product energy-single distribution	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.	3,8,9,10,4 0
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
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(α,β).	7
LMF	File number for this MT containing multiplicity or cross section.	8

Parameter	Definition	Chapter
LNU	Indicates representation of $\bar{\nu}$(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 Appendix F).	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
LVT	Specifies whether a transformation matrix given for elastic scattering.	4
L1	Integer to be used as a flag or a test. Number of Legendre coefficients.	1 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
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

Parameter	Definition	Chapter
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…MTRE4	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
	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

Parameter	Definition	Chapter
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
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 θ(E) (file 5) 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
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

Parameter	Definition	Chapter
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
	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

Parameter	Definition	Chapter
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
$P_k(E_N)$	Fractional part of cross section that can be described by the kth partial distribution of the nth incident-energy point.	5

Parameter	Definition	Chapter
p(μ,E)	$\frac{2\pi}{\sigma_s(E)}\frac{d\sigma}{d\Omega}(\Omega,E)$	4
PAR	Parity π of target nuclide.	8
PCP(E)	Charged-particle penetrability.	2
PMT	Floating point value for PMT.	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 a 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 $\int RP(E)dE=1$.	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(α,β,T)	Defined (for a moderating molecule) by the relation. $$\frac{d^2\sigma}{d\Omega dE'}(E \to E',\mu,T) = \sum_{n=0}^{NS} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}} e^{\beta/2} S_n(\alpha,\beta,T)$$	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 8.3).	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 ≤E′≤E-U (given in the Lab system).	5
V_k	Matrix elements of the transformation matrices.	4
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′/θ(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

Parameter	Definition	Chapter
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
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	Designation of the original nuclide.**	all
ZAI	(Z,A) designation for an isotope.**	2,32
ZAFP	(Z,A) identifier for a particular fission product.**	8
ZAN	(Z,A) designation of the next nuclide in the chain.**	8
ZAP	(Z,A) designation of the product nuclide.**	8
ZSYMA	Test representation of material: Z-chemical symbol-A	8
ZSYMAM	Text representation of material Z-chemical symbol-A-state.	1
α	Momentum transfer, $\alpha = \left(E' + E - 2\mu\sqrt{EE'}\right)\Big/A_0 kT$.	7
β	Energy transfer, β = (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
$\bar{\nu}$(E)	Total average number of neutrons formed per fission event.	1
σ(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, $\sigma_{bn} = \sigma_{fn}\left(\frac{A_n + 1}{A_n}\right)^2$	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

** (ZA=(1000.0*Z) + A).

Parameter	Definition	Chapter
$\sigma_{m_0}(E)$	Neutron cross section for exciting m_o^{th} 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)	$\frac{C}{\sqrt{E}}(AT_1 + AT_2/E + A_3/E^2 + AT_4/E^3 + BT_1 * E + BT_2 * E^2)$	2
σ_W	Wick's limit cross section in units of barns/steradian.	4
$\frac{d\sigma(\Omega,E)}{d\Omega}$	Differential scattering cross section in units of barns/steradian.	4
$\frac{d\sigma_k^\gamma}{d\Omega}$	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 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 beware of the few differences. In the following table, those MT numbers restricted to neutrons incident 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 0.0 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 0.5.3 and 0.5.4.

MT		Description	Comments
1	(n,total)	Neutron total cross sections. Sum of MT=2, 4, 5, 11, 16-18, 22-26, 28-37, 41-42, , 44-45, 102-117.	Redundant. Undefined for incident charged particles.
2	(z,z_0)	Elastic scattering cross section for incident particles.	
3	(z,nonelastic)	Nonelastic neutron cross section. Sum of MT=4, 5, 11, 16-18, 22-26, 28-37, 41-42, , 44-45, 102-117.	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 version 5.
10	(z,continuum)	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.	
12-15		Unassigned.	
16	(z,2n)	Production of two neutrons and a residual[58]. Sum of MT=875-891, if they are present.	
17	(z,3n)		
18	(z,fission)		
19	(n,f)		
20	(n,nf)	Second-chance fission[59].	
21	(n,2nf)	Third-chance 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.	

[58] The "residual" is the remainder after the reaction specified by MT has taken place (for example, A-1 after an n,2n reaction on target A). This "residual" may break up further if LR>0.

[59] Note that the partial fission cross section are not defined for incident charged particles.

MT		Description	Comments
24	(z,2nα)	Production of two neutrons and an alpha particle, plus a residual.	
25	(z,3nα)	Production of three neutrons and an alpha particle, plus a residual.	
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[2].	
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.	

MT		Description	Comments
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.
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.	For incident ^{3}He particles, this is inelastic scattering (MT=750 is undefined).
107	(z,α)	Production of an alpha particle, plus a residual. Sum of MT=800-849, if they are present.	For incident alpha particles, this is inelastic scattering (MT=800 is undefined).
108	(z,2α)	Production of 2 alpha particles, plus a residual.	

MT		Description	Comments
109	(z,3α)	Production of 3 alpha particles, plus a residual.	
110		(Unassigned)	
111	(z,2p)	Production of 2 protons, plus a residual.	
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.

MT		Description	Comments
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.
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,...)	$\overline{\mu}_L$, 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, $\overline{E}, \overline{\sigma}$, 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.

MT		Description	Comments
451	(z,...)	Heading or title information; given in File 1 only.	
452	(z,...)	$\bar{\nu}_T$, average total (prompt plus delayed) number of neutrons released per fission event.	
453		(Unassigned)	
454	(z,...)	Independent fission product yield data.	
455	(z,...)	$\bar{\nu}_d$, average number of delayed neutrons released per fission event.	
456	(z,...)	$\bar{\nu}_p$, average number of prompt neutrons released per fission event.	
457	(z,...)	Radioactive decay data.	
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)	

MT		Description	Comments
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	($1s^{1}/_{2}$) subshell photoelectric or electro-atomic cross section.	
535	L1	($2s^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
536	L2	($2p^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
537	L3	($2p^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
538	M1	($3s^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
539	M2	($3p^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
540	M3	($3p^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
541	M4	($3d^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
542	M5	($3d^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
543	N1	($4s^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
544	N2	($4p^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
545	N3	($4p^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
546	N4	($4dp^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
547	N5	($4d^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
548	N6	($4f^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
549	N7	($4f^{7}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
550	O1	($5s^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	

MT		Description	Comments
551	O2	($5p^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
552	O3	($5p^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
553	O4	($5d^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
554	O5	($5d^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
555	O6	($5f^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
556	O7	($5f^{7}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
557	O8	($5g^{7}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
558	O9	($5g^{9}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
559	P1	($6s^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
560	P2	($6p^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
561	P3	($6p^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
562	P4	($6d^{3}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
563	P5	($6d^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
564	P6	($6f^{5}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
565	P7	($6f^{7}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
566	P8	($6g^{7}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
567	P9	($6g^{9}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
568	P10	($6h^{9}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
569	P11	($6h^{11}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
570	Q1	($7s^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	

MT		Description	Comments
571	Q2	($7p^{1}/_{2}$) subshell photoelectric or elctro-atomic cross section.	
572	Q3	($7p^{3}/_{2}$) 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.	
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.	
	…		
	…		

MT		Description	Comments
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.	
	…		
891	$(z,2n_c)$	Production of 2 neutrons in the continuum not included in the above discrete representation.	
892-999		(Unassigned)	

LR Flags

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)

SUMMARY

Version 6 formats and procedures are recommended for all new evaluations. Version 6 format is the only format allowed for incident charged particles. It must be taken into account, however, that many version 5 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 version 6. A few MT numbers allowed for 5 have now been removed and must be replaced. Other MT numbers are allowed only in version 5 and these are ***not*** defined here--the reader is referred to the version 5 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 version 6 and, hopefully to associate them with the proper files. For explicit information on usage, see Sections 0.0, 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
l-Methane	33
s-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

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): LRU=1, LRF=1

D.1.1.1. Elastic Scattering Cross Sections[60]

$$\sigma_{n,n}(E) = \sum_{l=0}^{NSL-1} \sigma_{n,n}^{l}(E) \ ,$$

where

$$\sigma_{n,n}^{l}(E) = (2l+1)\frac{4\pi}{k^2}\sin^2\phi_l + \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}^2 - 2\Gamma_{nr}\Gamma\sin^2\phi_l + 2(E-E'_r)\Gamma_{nr}\sin 2\phi_l}{(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2}$$

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, $\varphi_l(E)$, 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/B 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

[1] Processing codes should sum the cross section, as shown, 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 2.4.23 and 2.4.24.)

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{NLS-1} \sigma_{n,\gamma}^{l}(E)$$

where

$$\sigma_{n,\gamma}^{l}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\,\Gamma_{\gamma r}}{\left(E - E_r'\right) + \frac{1}{4}\Gamma_r^2}$$

and $\boldsymbol{\Gamma_{\gamma r}}$, the radiative capture width, is constant in energy

D.1.1.3. Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{l=0}^{NLS-1} \sigma_{n,f}^{l}(E) \quad ,$$

where

$$\sigma_{n,f}^{l}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{fr}}{\left(E - E'_r\right)^2 + \frac{1}{4}\Gamma_r^2}$$

and $\boldsymbol{\Gamma_{fr}}$, 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/B 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 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.

$$NRS = \sum_{J=JMIN}^{J=JMAX} NR_J \ ,$$

where

$$JMAX = l + I + \frac{1}{2}$$

and

$$\begin{aligned} JMIN &= \left| l - I - \frac{1}{2} \right| \quad \text{if } l \geq I \\ &= \left| I - l - \frac{1}{2} \right| \quad \text{if } I \geq l \\ &= \left| \left| I - l \right| - \frac{1}{2} \right| \end{aligned}$$

$\Gamma_{nr}(|E_r|) \equiv GN_r$ 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.

$$\Gamma_{nr} = \frac{P_l(E)\,\Gamma_{nr}\left(|E_r|\right)}{P_l\left(|E_r|\right)}$$

$\Gamma_r = \Gamma_{nr}(E)+\Gamma_{\gamma r}+\Gamma_{fr}+\Gamma_{xr}$ 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:

$$\Gamma_{xr} = \Gamma_r - \Gamma_{nr} - \Gamma_{\gamma r} - \Gamma_{fr} \quad \text{at} \quad E = E_r$$

The following quantities are given in File 2 for each resonance:

E_r	= ER, the resonance energy
J	= AJ, the angular momentum ("spin") of the resonance state
I	= SPI, the angular momentum ("spin") of the target nucleus
g_J	= statistical factor (2J+1)/2(2I+1)
$\Gamma_{nr}(\|E_r\|)$	= GN, the neutron width
$\Gamma_{\gamma r}$	= GG, the radiation width
Γ_{fr}	= GF, the fission width and
$\Gamma_r(\|E_r\|)$	= GT, the total width evaluated at the resonance energy.

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:

$$E'_r = E_r + \frac{S_l\left(|E_r|\right) - S_l\left(E\right)}{2P_l\left(|E_r|\right)}\,\Gamma_{nr}\left(|E_r|\right).$$

The fact that the 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.

$$k = \frac{\sqrt{2m_n}}{\hbar}\,\frac{AWRI}{AWRI + 1.0}\sqrt{|E|},$$

The neutron wave number in the center-of-mass system is given as:

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.)

S_l is the shift factor,

$$S_0 = 0, \qquad S_2 = -\frac{18+3\rho^2}{9+3\rho^2+\rho^4},$$

$$S_1 = -\frac{1}{1+\rho^2}, \quad S_3 = -\frac{675+90\rho^2+6\rho^4}{225+45\rho^2+6\rho^4+\rho^6}.$$

(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 2.11a-c). In ENDF, the positive-energy formulas are used, but the absolute value of E is used in SLBW and MLBW. For the Hybrid R-Function, Section 2.2.1.4, all shifts are set to zero, and this is also an option for the General R-matrix, Section D.1.5.2.

P_l is the penetration factor,

$$P_0 = \rho, \qquad P_2 = \frac{\rho^5}{9+3\rho^2+\rho^4},$$

$$P_1 = \frac{\rho^3}{1+\rho^2}, \quad P_3 = \frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6}.$$

For higher *l*-values, the 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, $\Gamma(E)= \Gamma(|E_r|)P_l(E)/P_l(|E_r|)$, 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.

φ_l is the (negative of a) hard-sphere phase shift,

$$\phi_0 = \hat{\rho},$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho},$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\left\{\frac{3\hat{\rho}}{3-\hat{\rho}^2}\right\},$$

$$\phi 3 = \hat{\rho} - \tan^{-1}\left\{\frac{\hat{\rho}\left(15-\hat{\rho}\right)^2}{15-6\hat{\rho}^2}\right\}.$$

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.

ρ and $\hat{\rho}$ are defined as k × RADIUS, where RADIUS is defined as follows:

Let *a* = channel radius in units of 10^{-12} cm
= 0.123 $AWRI^{1/3}$ + 0.08 [61] (D.0)

[2] The channel radius, strictly speaking, involves $A^{1/3}$ (the target mass in amu), and not $(AWRI)^{1/3}$, but as long

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.

---

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).

If NRO = 0 (AP energy-independent)

NAPS = 0 $\rho = ka$; $\hat{\rho} = k\,AP$

NAPS = 1 $\rho = \hat{\rho} = k\,AP$

If NRO = 1 (AP energy-dependent)

NAPS = 0 $\rho = ka$; $\hat{\rho} = k\,AP(E)$

NAPS = 1 $\rho = \hat{\rho} = k\,AP(E)$

NAPS= 2 $\rho = k\,AP$; $\hat{\rho} = k\,AP(E)$

D.1.2. Multilevel Breit-Wigner (MLBW): LRU=1, LRF=2

The equations are the same as **SLBW**,[62] except that a resonance-resonance interference term is included in the equation for elastic scattering of *l*-wave neutrons, $\sigma_{n,n}^{l}(E)$:

$$\frac{\pi}{k^2}\sum_J^{\cdot} g_J \sum_{r=2}^{NR_j}\sum_{s=1}^{r-1}\frac{2\Gamma_{nr}\Gamma_{ns}\left(\left(E-E_r'\right)\left(E-E_s'\right)+\frac{1}{4}\Gamma_r\Gamma_s\right)}{\left(\left(E-E_r'\right)^2+\left(\Gamma_r/2\right)^2\right)\left(\left(E-E_s'\right)^2+\left(\Gamma_s/2\right)^2\right)}. \qquad (.76)$$

This form, which has 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 2.4.14)

$$\frac{\pi}{k^2}\sum_J^{\cdot} g_J \sum_{r=1}^{NR_J}\frac{G_r\Gamma_r+2H_r\left(E-E_r'\right)}{\left(E-E_r'\right)^2+\left(\Gamma_r/2\right)^2} \qquad (.77)$$

where

$$G_r=\frac{1}{2}\sum_{\substack{s=1\\(s\neq r)}}^{NR_J}\frac{\Gamma_{nr}\Gamma_{ns}\left(\Gamma_r+\Gamma_s\right)}{\left(E_r'-E_s'\right)^2+\frac{1}{4}\left(\Gamma_r+\Gamma_s\right)^2}, \qquad (.78)$$

$$H_r=\sum_{\substack{s=1\\(s\neq r)}}^{NR_J}\frac{\Gamma_{nr}\Gamma_{ns}\left(E_r'-E_s'\right)}{\left(E_r'-E_s'\right)^2+\frac{1}{4}\left(\Gamma_r+\Gamma_s\right)^2} \qquad (.79)$$

For the user who does not require ψ- and χ-broadening, the following equations, which are mathematically identical to the MLBW equations, require less computing time: (See Section 2.4.19)

$$\sigma_{n,n}(E)=\sum_{l=0}^{NLS-1}\sigma_{n,n}^{l}(E) \qquad (.80)$$

$$\sigma_{n,n}^{l}(E)=\frac{\pi}{k^2}\sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}}\sum_{J=|l-s|}^{l+s}g_J\left|1-U_{nn}^{lsJ}(E)\right|^2 \qquad (.81)$$

[3] Including footnote on page D.1.

$$U_{nn}^{lsJ}\left(E\right) = e^{-2i\phi_l}\left(1 + \sum_{r=1}^{NR_{sJ}} \frac{i\,\Gamma_{nr}^{lsJ}}{E_r' - E - i\,\Gamma_r/2}\right) \qquad (.82)$$

D.1.3 Reich-Moore (R-M): LRU = 1, LRF = 3

This description of the ENDF Reich-Moore formalism differs from previous versions by using notation in closer agreement with References 1 and 5. 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*:

$$\sigma_{nb} = \frac{\pi}{k^2} g_n \left|\delta_{nb} - U_{nb}\right|^2 \qquad (.83)$$

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, 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

$$\sigma_T(E) = \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \,\mathrm{Re}\left(1 - U_{lsJ\,lsJ}\right) \qquad (.84)$$

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 imposes additional "conservation rules" *l′* = *l* and *s′* = *s* which are actually just simplifying assumptions, with some basis in theory and experiment. The six-fold summation then reduces to the familiar form

$$\sigma_{nn}(E) = \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-1/2\right|}^{I+1/2} \sum_{J=|l-s|}^{l+s} g_J \left|1 - U_{lsJ\,lsJ}\right|^2 . \qquad (.85)$$

The absorption (non-elastic) cross section is obtained by subtraction:

$$\sigma_{abs}(E) = \sigma_T(E) - \sigma_{nn}(E) . \qquad (.86)$$

Fission is obtained from the collision matrix by summing Eq. (D.8) over all incident *lsJ* values and over the two exit fission channels, *b* = f1 and *b* = f2,

$$\sigma_f(E) = \frac{2\pi}{k^2}\sum_{l=0}^{NLS}\sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}}\sum_{J=|l-s|}^{l+s} g_J\left[\left|U_{nf1}^{lsJ}\right|^2 + \left|U_{nf2}^{lsJ}\right|^2\right]. \qquad (.87)$$

The Reich-Moore formalism is described in Reference 2. Here we repeat the level-matrix form of the collision matrix as given in the earlier versions of this manual:

$$U_{nb}^{J} = e^{-i(\phi_n+\phi_b)}\left[2\left((I-K)^{-1}\right)_{nb} - \delta_{nb}\right] \quad , \qquad (.88)$$

where

$$(I-K)_{nb} = \delta_{nb} - \frac{i}{2}\sum_r \frac{\Gamma_{nr}^{1/2}\,\Gamma_{br}^{1/2}}{E_r - E - i\,\Gamma_{\gamma r}/2}. \qquad (.89)$$

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*.

If we define a matrix ρ by the equation

$$\rho_{nb} = \delta_{nb} - \left((1-K)^{-1}\right)_{nb} \qquad (.90)$$

then the various cross sections take the following forms:

Total:

$$\sigma_T(E) = \frac{2\pi}{k^2}\sum_{l\,s\,J} g_J\left[(1-\cos 2\phi_l) + 2\mathrm{Re}(\rho_{nn}e^{-2i\phi_l})\right]. \qquad (.91)$$

Elastic:

$$\sigma_{nn} = \frac{\pi}{k^2}\sum_{l\,s\,J} g_J\left[2 - 2\cos 2\phi_l + 4\mathrm{Re}(\rho_{nn}e^{-2i\phi_l}) - 4\mathrm{Re}(\rho_{nn}) + 4|\rho_{nn}|^2\right]. \qquad (.92)$$

Absorption (fission plus capture):

$$\sigma_{n,abs}(E) = \frac{4\pi}{k^2}\sum_{lsJ} g_J\left[\mathrm{Re}(\rho_{nn}) - \left|\rho_{nn}\right|^2\right] \qquad (.93)$$

Fission:

$$\sigma_{nf}(E) = \frac{4\pi}{k^2}\sum_{lsJ} g_J\left[\left|\rho_{nf_1}\right| + \left|\rho_{nf_2}\right|^2\right] \qquad (.94)$$

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.

Footnote 1 applies to the Reich-Moore formalism also. Until this revision, the format did not permit the specification of channel spin; therefore, if an evaluation includes $l > 0$ resonances for $l > 0$ 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 $s = l - 1/2$ channels, and to use the same potential-scattering radius in the missing $l + 1/2$ channels. See Sections 2.4.23 and 2.4.24.) Having the ability to specify which channel spin is intended 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 $s = l - 1/2$ and positive AJ implies $s = l + 1/2$. When AJ = 0, one and only one of $l - 1/2$ or $l + 1/2$ 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): LRU=1, LRF=4

The formulae, taken from References 3 and 4, are given for the total, radiative capture, and fission cross sections. They have been slightly re-cast 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 2.4.15. Since only s-waves are considered, higher ***l***-wave contributions to the potential scattering must be put into File 3 by the evaluator.

1. Total Cross Section:

$$\sigma_T(E) = \frac{4\pi}{k^2}\sin^2\phi_0 + \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{NRS}\frac{\nu_r\left(G_r^T\cos 2\phi_0 + H_r^T\sin 2\phi_0\right) + \left(\mu_r - E\right)\left(H_r^T\cos 2\phi_0 - G_r^T\sin 2\phi_0\right)}{\left(\mu_r - E\right)^2 + \nu_r^2} + AT_1 + AT_2/E + AT_3/E^2 + AT_4/E^3 + BT_1E + BT_2E^2\right]. \quad (.95)$$

2. Radiative Capture Cross Section:

$$\sigma_{n,\gamma}(E) = \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{NRS}\frac{\nu_r G_r^\gamma + \left(\mu_r - E\right)H_r^\gamma}{\left(\mu_r - E\right)^2 + \nu_r^2} + AC_1 + AC_2/E + AC_3/E^2 + AC_4/E^3 + BC_1E + BC_2E^2\right] \quad (.96)$$

3. Fission Cross Section:

$$\sigma_{n,f}(E) = \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{NRS}\frac{\nu_r G_r^f + (\mu_r - E)H_r^f}{(\mu_r - E)^2 + \nu_r^2} + AF_1 + AF_2/E + AF_3/E^2 + AF_4/E^3 + BF_1E + BF_2E^2\right] \quad (.97)$$

Although the format uses different names for μ and v for each reaction, they are equal:

$DET_r = DEF_r = DEC_r = \mu_r$

$DWT_r = DWF_r = DWG_r = v_r$

D.1.5. General R-Matrix (GRM): LRU = 1, LRF=5

D.1.5.1. Calculation of the R-matrix elements

The basic element in an R-matrix calculation is the contribution of a single

$$R_{c,d,\lambda} = \frac{\gamma_{\lambda,c}\,\gamma_{\lambda,d}}{E_\lambda - E_{c.m.} - (i/2)\Gamma_{\gamma,\lambda}}$$

resonance to the R-matrix,

or in terms of the laboratory quantities defined in Section 2.2.1.4.2,

$$R_{c,d,\lambda} = \frac{AG_{\lambda,c}\,AG_{\lambda,d}}{ER_\lambda - E_{lab} - (i/2)\,GG_\lambda}$$

The matrix itself is obtained by summing over the appropriate λ-values and adding in the background R-matrix:

$$R_{c,d} = \Sigma_\lambda R_{c,d,\lambda} + RBK_{c,d}\,.$$

If there are altogether N channels, then the calculation will involve N(N + 1)/2 distinct R-matrix elements, $R_{c,d}$, since the matrix is symmetric. Those elements with different J and π in the two channels are zero, and the remaining ones can be rearranged in diagonal blocks labeled by J and π. The information needed to compute the elements of each block is contained in the spin-group list, together with the background R-matrix list, which specifies how the evaluation deals with distant-level effects.

Since the format gives the channel indices for each spin-group, i.e., each Jπ sub-matrix, explicitly in the spin-group list, the using code is relieved of the necessity of doing any angular momentum bookkeeping. The evaluator needs to be concerned with the details of the multiple sums over ***l***, ***l′***, s, s′, and J, but the user needs only to invert the sub-matrices specified by each spin-group, and then sum the partial cross sections according to the MT-list. Unlike the SLBW, MLBW, and Reich-Moore formalisms, here the burden of specifying ***all*** the necessary channels is on the evaluator, not the processing codes.

Following the usual procedure, the background R-matrix is assumed to be diagonal and non-zero only in the incident neutron channels, i.e., those for which PMT=SMT=2 in the spin-group list.

$$RBK_{c,d} = RBK_n \delta_{c,n} \delta_{c,d}\,,$$

where n stands for an incident neutron channel.

Three different representations are allowed for the background R-matrix:

a. a tabulated complex function of the energy,

b. the logarithmic parameterization used in SAMMY,

$$RBK_n = R0_n + R1_n\,E + R2_n\,E^2 - S1_n\,[EU_n - ED_n] - [S0_n + S1_n\,E]\;\mathbf{ln}[\{EU_n - E\}/\{E - ED_n\}]$$

c. a statistical parameterization using R_∞ (RIN), a strength function (SF), the energy interval (INT) over which the explicit resonances are given, the interval midpoint (EBAR) and an average gamma width (AVGG) over that interval (references 6 and 10):

$$RBK_n = RIN_n + 2SF_n\,[\mathrm{arctanh}[2\,(E - EBAR)/INT]$$

$$+ i\,[AVGG\ INT/\{(INT)^2 - 4(E - EBAR)^2\}]\Big]$$

D.1.5.2. Calculation of the U-matrix elements

The collision, or U-matrix, is obtained by the usual inversion formula from the R-matrix:

$$U = \Omega\, P^{1/2}\, [1 - R\,(L - B)]^{-1}\, [1 - R(L^* - B)]\, P^{-1/2}\, \Omega$$

$\Omega = \exp(-i\theta)$, $L = S + iP$

It has the same diagonal block structure as the R-matrix, but its elements are complicated functions of all the R-matrix elements involved in the inversion. In addition to the R-matrix elements, this step in the calculation requires phase shifts, penetrabilities, shift factors, nuclear radii, and boundary-condition parameters. These are specified in the following lists, or are calculated by the using code, depending on the options specified by the evaluator.

As an option, the shift factor may be set to zero. In R-matrix theory, the shift factor occurs because the underlying complete set of nuclear states on which the theory is built do not coincide with the actual nuclear states, due to the artificial boundary condition imposed on the former. In practice, only the ***form*** of the theory is used, and not its basic theoretical content, so that for neutron cross section evaluation in ENDF, the shift is an irrelevant artifact and can be ignored. It is true that a shifted and a resonance that is not shifted fitted to the same experimental data will have slight shape differences, but these will have no technological significance. Eliminating the shift also removes one barrier to the use of R-matrix parameters in multigroup slowing-down and self-shielding codes, which naively assume that a resonance energy ER will be associated with a Lorentzian bump at that energy. Anti-resonances, and strange channel-interference patterns will still cause problems in such applications, but will at least occur in the expected locations.

For the same reason, it is recommended that the boundary-condition parameter be set to zero. With S = B = 0, the above formula reduces to

$$U = \Omega\, P^{1/2}\, [1 - iRP]^{-1}\, [1 + iRP]\, P^{-1/2}\, \Omega$$

which can often reproduce experimental data as well as the more general form above.

It is assumed that the phase shifts in

$$\Omega = \exp(-i\theta)$$

are either hard-sphere values, or the ones defined in the phase-shift list. That is, hard-sphere values are assumed to be ***included*** in the tabulated values, and are not to be added by the user.

D.1.5.3. Calculation of the channel cross section

Each element of a U-sub-matrix, $U_{c,d}$, defines a channel-to-channel cross sections,

$$\sigma_{c,d} = \frac{\pi g_c}{k^2} \left| \delta_{c,d} - U_{c,d} \right|^2$$

These cross sections are not observable, but are the ingredients for ones that are. The statistical factor depends on *c* through *J*.

D.1.5.4. Calculation of the PMT-cross sections (Particular MT-values)

An observable PMT-cross section is obtained by summing the channel-to-channel cross section over all the incident channels, and over those exit channels belonging to a particular MT-value, PMT. Both of these summations are defined by the MT-list, which tells which channels are incident, SMT=PMT=2, and which channels belong to each PMT. The code used needs only to keep track of the indices, and is not required to book keep the angular momentum quantum numbers.

$$\sigma_{PMT} = \sum_{c \text{ in } n,\ d \text{ in } PMT} \sigma_{c,d}$$

D.1.5.5. Calculation of the SMT-cross sections (Summed MT-values)

The complete reaction cross sections, corresponding to the summed-MT's, are then obtained by summing over the appropriate PMT's. The MT-list specifies which PMT's belong to each SMT.

$$\sigma_{SMT} = \Sigma_{PMT\ in\ SMT}\ \sigma_{PMT}$$

The elastic cross section, SMT=2, is the same as its only component, σ(PMT=2). The same is true of the fission cross section, SMT=PMT=18.

D.1.5.6. Calculation of the total cross section

The total cross section is obtained from the diagonal elements corresponding to the incident channels. It cannot be obtained by summing partial cross sections because radiative capture is not calculated according to the above scheme, but is treated as an eliminated channel. Hence its cross section is not available for summing.

$$\sigma_{TOT} = \sum_{c\,\mathrm{in}\,n} \frac{2\pi g_c}{k^2}\left[\,1 - \mathrm{Re}\,U_{c,c}\,\right]$$

The summation here is over all channels belonging to SMT=PMT=2.

D.1.5.7. Calculation of the capture cross section

This is obtained as the total cross section minus the sum of all the SMT-cross sections:

$$\sigma_{CAP} = \sigma_{TOT} - \Sigma_{SMT}\,\sigma_{SMT}$$

If the eliminated width were read in as the sum of the capture width and some other reaction width(s), the above difference cross section would correspond to the sum of those reactions. This fact is exploited in the Hybrid R-function formalism to simplify the treatment of competitive reactions, which often do not require the complication of a full R-matrix treatment.

D.1.5.8. Calculation of the absorption cross section

$$\sigma_{ABS} = \sigma_{TOT} - \sigma_{SMT=2}$$

If the inelastic cross section, $\sigma_{SMT=4}$, is not zero, it is necessary also to subtract it.

D.1.5.9. Calculation of the angular distributions

These may be found from the Blatt and Biedenharn formalism. However, the summations required do not lend themselves to expression in terms of channel indices, the way the integrated cross sections do. If the angular distributions are calculated directly from the scattering amplitudes, one has to deal with magnetic quantum numbers in addition to α, *l*, s, and J. If one eliminates the magnetic quantum numbers ala Blatt and Biedenharn, the sums over *l*, s, and J are each treated differently and do not stay together in neat channel packages. To utilize these formulas, it is necessary to pick apart the c's and d's and extract the quantum numbers. The format has not been optimized for that, although the information is contained in the MT- and spin-group-lists. To use the angular distribution formula, the code needs to perform the indicated 9-fold summation, and to locate a given U-matrix element from its seven arguments α_1, α_2, l_1, l_2, s_1, s_2, and J. To facilitate the summation, the limits are given explicitly in the following paragraph.

Using a normalization in which B_0 is also the angle-integrated cross section, the Blatt and Biedenharn formula is[63]

$$\frac{d\sigma_{\alpha,\alpha'}}{d\Omega} = \sum_L \frac{2L+1}{4\pi} B_L P_L(\mu)$$

$$B_L = \frac{\pi}{(2i+1)(2I+1)(2L+1)\,k^2} \sum \left\{ ss' l_1 l'_1 l_2 l'_2 J_1 J_2 \right\}$$
$$\times (-1)^{s-s'} \overline{Z}_{l_1 J_1 l_2 J_2; sL} \overline{Z}_{l'_1 J_1 l'_2 J_2; s'L}$$
$$\times \left[\delta_{\alpha l_1 s, \alpha' l'_1 s'} - U_{\alpha l_1 s J_1, \alpha' l'_1 s' J_1} \right]$$
$$\times \left[\delta_{\alpha l_2 s, \alpha' l'_2 s'} - U_{\alpha l_2 s J_2, \alpha' l'_2 s' J_2} \right]$$

where $P_L(\mu)$ is a Legendre polynomial in $\cos \theta_{\alpha\alpha'}$, and

$$Z_{l_1 J_1 l_2 J_2; sL} = \sqrt{(l_1+1)(2l_2+1)(2J_1+1)(J_2+1)} \times (l_1 l_2 00; L0)\, W(l_1 J_1 l_2 J_2; sL)$$

($l_1 l_2 00;L0$) and *W* are the Clebsch-Gordan and Racah coefficients.

From outside to inside, the sum limits are

1) $0 \le L \le 2*(\text{NLSC-1})$, where NLSC-1 is a cutoff value chosen by the evaluator to converge the angular distributions. (See Sections 2.4.23 and 2.4.24).
2) $|I - i| \le s \le I + i$ (incident spins)
3) $|I' - i'| \le s' \le I' + i'$ (exit spins)
4) $0 \le l_1 \le \text{NLSC-1}$
5) $0 \le l'_1 \le \text{NLSC-1}$
6) $|L - l_1| \le l_2 \le \min\{\text{NLSC-1}, L+l_1\}$
7) $|L - l'_1| \le l'_2 \le \min\{\text{NLSC-1}, L+l'_1\}$
8) $\max\{|l_1 - s|, |l'_1 - s'|\} \le J_1 \le \min\{l_1 + s, l'_1 + s'\}$
9) $\max\{|l_2 - s|, |l'_2 - s'|, |L - J_1|\} \le J_2 \le \min\{l_2 + s, l'_2 + s', L + J_1\}$

D.1.6 Hybrid R-function (HRF): LRU=1, LRF=6

The formulae are from standard R-matrix theory, References 1, 5, and 6, augmented by the single-level Breit-Wigner formalism for the calculation of competitive reactions. The mixing of the two methods is indicated by the term "hybrid." As in the previous section, D.1.5, R, S, and U are center-of-mass quantities, written in terms of laboratory widths and energies.

[63] Sum variables in curly brackets. This formula is not applicable to either capture or fission. Both $d\sigma/d\Omega$ and B_L are center-of-mass quantities, in terms of laboratory widths and energies.

D.1.6.1. Elastic Scattering Cross Section

$$\sigma_{n,n}(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_{n,n}^{lsJ}(E)$$

$$\sigma_{n,n}^{lsJ}(E) = \frac{\pi}{k^2} g_J \left|S_{lsJ}(E)\right|^2$$

where $S_{lsJ}(E) \equiv 1 - U_{lsJ}(E)$

$$U_{lsJ}(E) = \exp(-2i\delta_{lsJ}) \frac{1 + iP_{lsJ}(E) R_{lsJ}(E)}{1 - iP_{lsJ}(E) R_{lsJ}(E)}, and$$

$$S_{lsJ}(E) = \frac{(1 - \exp(-2i\delta_{lsJ})) - iP_{lsJ}(E) R_{lsJ}(E)(1 + \exp(-2i\delta_{lsJ}))}{1 - iP_{lsJ}(E) R_{lsJ}(E)}$$

$$R_{lsJ}(E) = \sum_{r=1}^{NLSJ} \frac{\Gamma_{nr}(|E_r|)}{2P_{lsJ}(|E_r|)\left[E_r - E - i\Gamma_{er}(|E_r|)/2\right]} + R_{lsJ}^0(E)$$

The eliminated width, Γ_{er}, in the denominator of the R-function is a constant, evaluated at the resonance energy. It is the sum of the partial widths for capture and competitive reactions (see Section 2.2.1-4). Its omitted energy-dependence has a negligible effect on the shape of the elastic resonances. If the flag LPS is 0, the phase shift δ_{lsJ} will be calculated from the hard-sphere formulas. If LPS=1, tabulated phase shifts will be supplied in every channel. This permits parameterization of optical-model evaluations. Hard-sphere values depend on the channel- dependent radius AC. The formulas of section D.1.1 are used with $\rho = \hat{\rho} = k \times AC$ being dependent on *l*, s and J. Note that the above equations are all scalar. No matrix inversion is required. The background R-function $R_{lsJ}^0(E)$, if supplied, must be tabulated, although the analytic formulae of Section 2.2.1.4.3 may be used as a guide.

As in the footnote on page D.1, the processing codes must sum over all channels, whether they contain resonances or not. The evaluator must specify suitable values of NLS and NLSC to converge the cross-section and angular-distribution calculations.

D.1.6.2. Partial Reaction Cross Sections

The following formulas are the same as SLBW, except that an explicit sum on channel spin has been introduced, so that the same J-value can occur in two different channels, ls_1J and ls_2J:

$$\sigma_{n,x}(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_{n,x}^{lsJ}(E)$$

$$\sigma_{n,x}^{lsJ}(E) = \frac{\pi}{k^2} g_J \sum_{r=1}^{NLSJ} \frac{\Gamma_{nr}(E)\Gamma_{xr}(E)}{(E - E'_r)^2 + \frac{1}{4}\Gamma_r^2} \quad ,$$

x can represent any of four reaction types:

a) Radiative capture

$\Gamma_{xr}(E) = \Gamma_{\gamma r}$, a constant in energy

b) Fission

$\Gamma_{xr}(E) = \Gamma_{fr}$, a constant in energy. This convention is the same as that used in the SLBW and MLBW formalisms.

c) Inelastic scattering

$$\Gamma_{xr}(E) = \Gamma_{n'r} \frac{P_{l'}\left(E - E_p^*\right)}{P_{l'}\left(\left|E_r - E_p^*\right|\right)}.$$

E_p^* is the laboratory threshold energy for exciting the pth level in the target nucleus. It is determined from the Q-value in File 2 (QRE_n) by

$$E_p^* = -\frac{AWRI + 1}{AWRI} Q.$$

$P_{l'}$ is to be calculated using the AC values for the first channel in the file. The prime on the subscript *l* denotes the fact that an inelastically-scattered neutron may have a different *l*-value from the incident neutron. *l′* is the library quantity $ALRE_n$. AWRI is the same as for the incident neutron, because the reduced mass in an inelastic channel is (essentially) the same as in the incident channel. $P_{l'}$ is zero if its argument is a negative incident energy. If its argument is a negative resonance energy, $P_{l'}$ is evaluated at the absolute value of its argument.

d) Charged-particle scattering

The charged-particle penetrability will be supplied by the evaluator as a tabulated function of the incident neutron's laboratory energy. The conversion from the charged-particle

channel energy to the neutron's energy is discussed in Section D.3.1(c). This choice of energy eliminates the need for the user to do any conversion, and the energy-dependent charged-particle exit width is simply

$$\Gamma_{xr}(E) = \Gamma_{cpr} \frac{P_{cpl's'J'}(E)}{P_{cpl's'J'}(|E_r|)}$$

The choice also eliminates the need to specify an exit mass ratio, AWRIC, an exit Q-value, or an exit channel radius, as these are incorporated by the evaluator into the tabulated penetrability.

D.1.6.3. Total Reaction Cross Section

This is calculated as the sum of the above partial reaction cross sections,

$$\sigma_R(E) = \sum_x \sigma_{n,x}(E).$$

In the important case that radiative capture is the only reaction specified (NFRE = NIRE = NCRE = 0), the total reaction cross section is also the radiative capture cross section, and is to be calculated from the R-function formula

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_{n,\gamma}^{lsJ}(E) \quad ,$$

where

$$\sigma_{n,\gamma}^{lsJ}(E) = \frac{\pi}{k^2} g_J \left(1 - \left| U_{lsJ}(E) \right|^2\right) = \frac{\pi}{k^2} g_J \left[2 \operatorname{Re} S_{lsJ}(E) - \left| S_{lsJ}(E) \right|^2 \right].$$

This formula is applicable also in the "trivial" case of pure elastic scattering (NGRE = NFRE = NIRE = NCRE = 0). This formula, when applicable, eliminates all reference to the SLBW formalism, and reduces the hybrid R-function to a "pure" R-function.

D.1.6.4. Total Cross section

The total cross section is calculated as the sum of the elastic scattering and total reaction cross section defined above,

$$\sigma_T(E) = \sigma_{n,n}(E) + \sigma_R(E)$$

In the two special cases noted in D.1.6.3, the total cross section may also be calculated from the mathematically-equivalent form:

$$\sigma_T(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_T^{lsJ}(E), \text{ and}$$

$$\sigma_T^{lsJ}(E) = \frac{2\pi}{k^2} g_J \left(1 - \operatorname{Re} U_{lsJ}(E)\right) = \frac{\pi}{k^2} g_J \operatorname{Re} S_{lsJ}(E).$$

These special cases are standard R-function theory, as no use is made of the single-level Breit-Wigner formalism (see Section D.3.3.).

D.1.6.5. The Angular Distribution of Elastically-Scattered Particles

Scattering-matrix theory predicts an angular distribution which varies across a resonance. For some applications this variation might be worth calculating. The general formula of Blatt and Biedenharn, Reference 7, reduced to the present case of an R-function that is diagonal in *l*, s, and J is (center of mass):

$$\frac{d\sigma}{d\Omega} = \sum_{L}^{NLS-1} \frac{2L+1}{4\pi} B_L(E) P_L(\cos\theta) \quad \text{barns/steradian},$$

where

$$B_L(E) = \frac{\pi}{(2i+1)(2I+1)(2L+1)k^2} \sum_{s l_1 l_2 J_1 J_2} \overline{Z}^2(l_1 J_1 l_2 J_2; sL)\, S_{l_1 s J_1}(E)\, S^*_{l_2 s J_2}(E),$$

$$\overline{Z}(l_1 J_1 l_2 J_2; sL) = \sqrt{(2l_1+1)(2l_2+1)(2J_1+1)(2J_2+1)}\, (l_1 l_2 00; L0)\, W(l_1 J_1 l_2 J_2; sL),$$

and *i* is the neutron spin (1/2). Here ($l_1 l_2$00; L0) and W(l_1J$_1$$l_2J_2$l;sL) are Clebsch-Gordan and Racah coefficients, respectively.

The limits on the summation variables are as follows, from outside to inside:

1) $0 \le L \le 2$ (NLSC-1), where NLSC-1 is the highest partial wave required to specify the angular distribution. It may be necessary to calculate U_{lsJ} for non-resonant channels which contribute just hard-sphere or optical-model scattering, $U_{lsJ} = \exp(-2i\delta_{lsJ})$.
2) $|I - ½| \le s \le I + ½$
3) $0 \le l_1 \le$ NLSC-1
4) $|L - l_1| \le l_2 \le \min\{\text{NLSC-1}, L + l_1\}$
5) $|l_1 - s| \le J_1 \le l_1 + s$
6) $\max\{|l_2 - s|, |J_1 - L|\} \le J_2 \le \min\{l_2 + s, J_1 + L\}$

D.2. THE UNRESOLVED RESONANCE REGION: LRU=2, LRF=1 or 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. <u>Elastic Scattering Cross Section</u>

$$\sigma_{n,n}(E) = \sum_{l=0}^{NLS-1} \sigma^l_{n,n}(E),$$

$$\sigma^l_{n,n}(E) = \frac{4\pi}{k^2}(2l+1)\sin^2\phi_l + \frac{2\pi^2}{k^2}\sum_J^{NJS}\left[\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_n}{\Gamma}\right\rangle_{l,J} - 2\overline{\Gamma}_{nl,J}\sin^2\phi_l\right]$$

The asymmetric term in $E - E'_r$ is assumed to average to zero under the energy-averaging denoted by < >.

b. <u>Radiative Capture Cross Section</u>

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{NLS-1} \sigma^l_{n,\gamma}(E),$$

$$\sigma^l_{n,\gamma}(E) = \frac{2\pi^2}{k^2}\sum_J^{NJS}\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_\gamma}{\Gamma}\right\rangle_{l,J}$$

c. <u>Fission Cross Section</u>

$$\sigma_{n,f}(E) = \sum_{l=0}^{NLS-1} \sigma^l_{n,f}(E),$$

$$\sigma^l_{n,f}(E) = \frac{2\pi^2}{k^2}\sum_J^{NJS}\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_f}{\Gamma}\right\rangle_{l,J}.$$

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 re-written as

$$\left\langle \frac{\Gamma_n \Gamma_n}{\Gamma} \right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{nl,J}}{\overline{\Gamma}_{l,J}} \right) R_{n,l,J}$$

$$\left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{\gamma l,J}}{\overline{\Gamma}_{l,J}} \right) R_{\gamma l,J} \text{ , and}$$

$$\left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{fl,J}}{\overline{\Gamma}_{l,J}} \right) R_{fl,J}$$

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 (31c), where $\overline{\Gamma}_{nlJ} = \langle \Gamma_n(l,J) \rangle$. Degrees of freedom are discussed in Section 2.4.20.

The average total width, at energy E, is

$$\overline{\Gamma}_{l,J} = \overline{\Gamma}_{nl,J} + \overline{\Gamma}_{\gamma l,J} + \overline{\Gamma}_{fl,J} + \overline{\Gamma}_{xl,J} \text{ ,}$$

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 describe 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 8, their parenthesized indices will be used. Section D.2.3 contains a table of equivalences to the notation used in D.2.1 and Section D.2.4 compares the present discussion with those previously given.

D.2.2.1. Sums and Averages

In an energy interval Δε, let the resonances be identified by a subscript λ = 1, 2, … 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

$$\rho(x) = N(x)/\Delta\varepsilon \,, \qquad (.98)$$

and their level spacing is

$$D(x) = 1/\rho(x) \,. \qquad (.99)$$

If y_λ is some quantity associated with each resonance, λ, the sum of the y-values over the
subset x is

$$\sum\nolimits_\lambda^x y_\lambda \,. \qquad (.100)$$

In this section, the summation index λ is written as a subscript, and the range of the summation is indicated by the superscript x. Equation (D.25) says "sum the quantity y over every resonance in the interval Δε 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

$$\langle y \rangle^x = \left[1/N(x)\right] \sum\nolimits_\lambda^x y_\lambda \qquad (.101)$$

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:

$$\Gamma_{n\lambda}(l,J,s) = \Gamma^l_{n\lambda}(J,s)\sqrt{E}\;\nu_l(E) \qquad (.102)$$

where $v_l = P_l/\rho$
$v_0 = 1$,
$v_1 = \rho^2/(1+\rho^2)$
$v_2 = \rho^4/(9+3\rho^2+\rho^4)$
and $\rho = ka$, *a* being the channel radius.

Assuming additivity of partial widths,

$$\Gamma^l_{n\lambda}(J) = \Sigma_s \Gamma^l_{n\lambda}(J,s) \qquad (.103)$$

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,[64]

$$\left\langle \Gamma_n^l(J) \right\rangle = \sum_s \left\langle \Gamma_n^l(J, \not{s}) \right\rangle = \mu_{l,J} \left\langle \Gamma_n^l(J, \not{s}) \right\rangle \qquad (.104)$$

[64] This is not true for the individual resonances

Equation (D.29) 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 ±1/2 subject to the additional vector sum

$$\vec{s} = \vec{l} + \vec{J} \qquad (.105)$$

which may again restrict $\mu_{l,J}$ to the value one.[65]

The other new notation is the line through the quantum number s, meaning that the quantity $\left\langle \Gamma_n^l(j,\not{s}\right\rangle$ 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 v_l only depends on *l*,

$$\begin{aligned} \left\langle \Gamma_n(l,J)\right\rangle &= \left\langle \Gamma_n^l(J)\sqrt{E}v_l\right\rangle && \text{a.)} \\ &= \mu_{l,J}\left\langle \Gamma_n^l(J,\not{s})\sqrt{E}v_l\right\rangle && \text{b.)} \\ &= \mu_{l,J}\left\langle \Gamma_n^l(J,\not{s})\right\rangle\overline{\sqrt{E}v_l} && \text{c.)} \end{aligned} \qquad (.106)$$

where the bar over $\sqrt{E}v_l$ 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.

$$S(l,J,s) = \left\langle \Gamma_n^l(J,s)\right\rangle^{l,J,s} \Big/ D(l,J,s)\,. \qquad (.107)$$

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

$$S(l,J,s) = \left\langle \Gamma_n^l(J,s)\right\rangle^{l,J} \Big/ D(l,J)\,. \qquad (.108)$$

If the parity π were used as an explicit quantum number, *l* could be dropped,

$$S(l,J,s) = \left\langle \Gamma_n^l(J,s)\right\rangle^{J,\pi} \Big/ D(J,\pi)\,, \qquad (.109)$$

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

$$S\left(l,J,\not{s}\right) = \sum_{\lambda}^{l,J} \Gamma_{n\lambda}^l(J,s)\big/\Delta\varepsilon \qquad (.110)$$

where we use the assumed independence of $\left\langle \Gamma_n^l(J,\not{s})\right\rangle$ on s to get the same result on the left-hand-side.

[65] For example, if I = 1/2, $\mu_{1,2}$ = 1.

The strength function S(*l*,J) is defined as

$$S(l,J) = \sum_s S(l,J,s) \qquad \text{(a)}$$
$$= \mu_{l,J}\, S(l,J,s) \qquad \text{(b)} \qquad (.111)$$

The corresponding sum and average forms are

$$S(l,J) = \sum_\lambda^{l,J} \Gamma_{n\lambda}^l(J) \big/ \Delta\varepsilon \qquad \text{(a)}$$
$$= \left\langle \Gamma_n^l(J)^{l,J} \right\rangle \Big/ D(l,J) \qquad \text{(b)} \qquad (.112)$$

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):

$$S(l) = \frac{\sum_{Js} gS(l,J,s)}{\sum_{Js} g} \qquad (.113)$$

This equation occurs in Lynn, Reference 1, as 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

$$S(0) = \sum_\lambda^{l=0} (g\Gamma_n^0)_\lambda \big/ D\ (l=0) \qquad (.114)$$

and later generalized by Saplakoglu et al. Reference 9, to the p-wave form

$$S(1) = (1/\Delta\varepsilon)(2l+1)^{-1} \sum_\lambda^{l=1} (g\Gamma_n^1)_\lambda\,. \qquad (.115)$$

For expository purposes, it is clearer to start from (31). The sum on J and s is for fixed *l*:

$$\sum_{Js} \equiv \sum_{s=I-\frac{1}{2}}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} . \qquad (.116)$$

It is important to note that the outer sum on channel spin is correct as written. It goes over the values I±½ if I≥½ , and over the single value ½, if I=0. It is ***not*** further constrained by Equation (D.30) 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 (D.41) can be rewritten:

$$\Sigma_{Js}\, y(\not{s}) = \tilde{\Sigma}_{l,J}\, \mu_{lJ}\, y(\not{s}) \qquad (.117)$$

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 8, reminds us that J goes over its full range, "once-only":[66]

[7] Reference 8 has this written incorrectly.

$$\sum_{J}^{\sim} = \sum_{J=\left|l-I-\frac{1}{2}\right|}^{l+I+1/2} \quad \text{if } l \geq I \qquad \text{(a)}$$

$$= \sum_{J=\left|I-l-\frac{1}{2}\right|}^{l+I+1/2} \quad \text{if } I \geq l \qquad \text{(b)} \qquad (.118)$$

The denominator in Equation (D.38) can be shown to be

$$\Sigma_{Js} g = 2l + 1 , \qquad (.119)$$

or, since g is independent of s,

$$\Sigma_J \mu_{l,J}\, g = 2l + 1 . \qquad (.120)$$

G-P assume, and later approximately justify by comparison to experiment, that S(*l*,J,*s*) is also independent of J. With this, Equation (D.38) becomes

$$\begin{aligned} S(l) &= (2l+1)^{-1} \sum_{Js} gS(l,\cancel{J},\cancel{s}) = S(l,\cancel{J},\cancel{s}) \quad \text{(a)} \\ &= S\left(l,J\right)\big/\mu_{l,J} , \quad \text{(b)} \end{aligned} \qquad (.121)$$

using Equation (D.36.b).

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,

$$\begin{aligned} S(l) &= (2l+1)^{-1} \sum_{Js} gS(l,\cancel{J},\cancel{s}) \quad \text{(a)} \\ &= (2l+1)^{-1} \sum_{Js} \sum_{\lambda}^{l,J} g\Gamma_{n\lambda}^{l}(J,s)/\Delta\varepsilon \quad \text{(b)} \\ &= (2l+1)^{-1} \sum_{J} \sum_{\lambda}^{l,J} g\Gamma_{n\lambda}^{l}(J)/\Delta\varepsilon \quad , \quad \text{(c)} \end{aligned} \qquad (.122)$$

The right hand side of Equation (D.47c) says to sum $\Gamma^{l}_{n\lambda}(J)$ over all possible values of J, which is what is meant by Equations (D.39) and (D.40). We can suppress the explicit J's and write, as in Equation (D.40),

$$S(l) = (1/\Delta\varepsilon)(2l+1)^{-1} \sum_{\lambda}^{l} (g\Gamma_{n\lambda}^{l})_{\lambda} \qquad (.123)$$

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,

$$S(l) = (2l+1)^{-1} \left\langle g\Gamma_{n}^{l} \right\rangle^{l} \Big/ D(l) \quad . \qquad (.124)$$

Otherwise, all the notation is correct: D(*l*) is the spacing of *l*-wave resonances without regard to their J-values, and the average $< >^{l}$ 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 $\left\langle \Gamma_{n}^{l}(J) \right\rangle$. As Equation (37b) 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

G-P emphasize that

$$\rho(l) = \Sigma_J \rho(l,J) \qquad (.125)$$

which, together with the assumption

$$\rho(l,J) = K(l)(2J+1) \ , \qquad (.126)$$

leads to

$$\rho(l) = \rho(l,J) \frac{(2l+1)}{g} \omega_{I,l} , \qquad (.127)$$

where

$$\omega_{I,l} = (l+1)/(2l+1) \quad \text{for } l \le I$$
$$= (I+1)/(2I+1) \quad \text{for } l \ge I \qquad (.128)$$

and is unity if l=0 or I=0.

The reader is referred to Reference 8 for a fuller discussion but here we can point out that, for a given parity, ρ(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

$$\rho(0,J) = \rho(2,j) = \rho(4,j) = \ldots, \text{ and}$$
$$\rho(1,J) = \rho(3,j) = \rho(5,j) = \ldots \qquad (.129)$$

The further assumption of parity-independence makes ρ(l,J) totally independent of l. As a result, G-P's K(l) from Equation (D.51) is independent of l, and

$$\rho(l) = C(2l+1)\,\omega_{I,l} \ , \qquad (.130)$$

where C depends on the nuclear species by not on any quantum numbers.

D.2.2.5. Gamma Widths

In the limited energy range of a few keV 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 μ=1, the sum is found to have a μ≥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 in Chapter 2, Section 2.4.20, the following values should be used:

1. Neutron width, 1. ≤ AMUN ≤ 2., and specifically, AMUN= $\mu_{l,J}$.
2. Radiation width, AMUG=0.
3. Fission width, 1. ≤ AMUF ≤ 4., to be determined by comparison with experiment. Only integral values are permitted, although non-integers occur in some analyses.
4. Competitive width, 1. ≤ 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 $\tilde{I}$ 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 D.1	in D.2.1	in D.2.2	Definition
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		ρv_l	Penetration factor.
	$D_{l,J}$	$D(l,J)$	Average level spacing for a subset of resonances with given *l* and J.
	$\overline{\Gamma}^0_{nl,J}$	$\left\langle \Gamma^l_n(J) \right\rangle^{l,J}$	The *l*-wave reduced width, averaged over all resonances with given *l* and J.
	$\overline{\Gamma}_{nl,J}$	$\left\langle \Gamma_n(l,J) \right\rangle^{l,J}$	The average neutron width. In practice, the energy-dependence of this quantity is not averaged, but extracted before averaging.

D.2.4. Comparison with previous editions of ENDF-102

D.2.4.1. ENDF-102, October 1970 edition

1. Equation (1). $D_{observed}$ is $D(l)$.

2. Line 9. *l* is not the angular momentum of "the incident neutron." The incident neutrons carry all angular momenta. *l* is the orbital angular momentum of the resonance, or more precisely, of the channel or channels which are involved. The resonant l^{th} phase shift will interfere with the non-resonant ones in angular distributions, but not in angle-integrated cross sections.

3. Equation (2)

   ρ_J is $\rho(l,J)$; ρ_{obs} is $\rho(l)$; Σ is $\tilde{\Sigma}_J$.

4. Equation (3). D_J is $D(l,J)$ and the right-hand-side should have a factor $\omega_{l,l}$.

5. Page D-11, line 1. "Level-spacing" means $D(l,J)$. Line 8. The statement "If we assume the s-wave strength function is independent of J..."presumably means assuming S(0,J) is independent of J, since the s-wave strength function itself, S(0), is a sum over J-states and is therefore "independent" of J by definition.

Equation 4 means

$$S(0) = S(0,J,s) = S(0,J)/\mu_{0,J}$$

which because $\mu_{0,J}= 1$ implies

$$S(0) = S(0,J) = \langle \Gamma^0_n(J) \rangle^{0,J}/D(0,J) \ .$$

Equation 5 is trickier because $\mu_{l,J}$ is not identically equal to 1, and the discussion appears to give the user the option of getting $D(l,J)$ from Equation (3) and "the corresponding reduced neutron width" from Equation (5), or of using the ENDF/B

convention, Equation (6).

The problem lies in the failure to distinguish $\Gamma^l_n(J)$ from $\Gamma^l_n(J,s)$. Equation (6) states the "ENDF/B convention":

$$\left\langle \Gamma^l_{nJ} \right\rangle = \left\langle \Gamma^0_{nJ} \right\rangle \sqrt{E}\ \nu_l \mu_{lJ} \quad .$$

(Here and in the following, $\sqrt{E}$ and $\boldsymbol{\nu_l}$ are average values appropriate to the energy interval.)

We know that the correct relationship is

$$\left\langle \Gamma_n(l,J) \right\rangle = \left\langle \Gamma^l_n(J,\not{s}) \right\rangle \sqrt{E}\ \nu_l \mu_{lJ}$$

$$= \left\langle \Gamma^l_n(J) \right\rangle \sqrt{E}\ \nu_l$$

If we assume that $\left\langle \Gamma^l_{nJ} \right\rangle$ in Equation (6) is to agree with experiment, $\left\langle \Gamma^{0l}_{nJ} \right\rangle$ then must be

$$\left\langle \Gamma^l_n(J,s) \right\rangle = \left\langle \Gamma^l_n(J) \right\rangle \Big/ \mu_{I,J} \ .$$

If we use a subscript E to denote an ENDF-convention quantity,

$$\left\langle \Gamma^{0l}_{nJ} \right\rangle \rightarrow \left\langle \Gamma^{0l}_{nJE} \right\rangle = \left\langle \Gamma^{0l}_{nJ}\ \text{actual} \right\rangle \Big/ \mu_{I,J}$$

and now

$$\frac{\left\langle \Gamma^0_{nJ} \right\rangle^l}{D_{l,J}} \text{ in (5) means } \frac{\left\langle \Gamma^{0l}_{nJE} \right\rangle}{D_{l,J}} = \frac{\left\langle \Gamma^0_n \text{ actual} \right\rangle^l_J}{D_{l,J}\ \mu_{l,J}}$$

which is correct. Thus an ENDF reduced width $\left\langle \Gamma^{0l}_{nJE} \right\rangle$ will sometimes be half what an experimentalist would measure.

In the notation of D.2.2., Equation (24) is

$$\left\langle \Gamma_n(l,J) \right\rangle^{l,J} = \left\langle \Gamma^l_n(J,s) \right\rangle^{l,J} \sqrt{E}\ \nu_l\ \mu_{l,J}$$

and $\Gamma^l_n(J)$ is the reduced width determined by experiment.

For p-waves,

$$S(1) = S(1,J)/\mu_{1,J} = \left\langle \Gamma^1_n(J) \right\rangle^{1,J} / D(1,J)\mu_{1,J} \ ,$$

and Equation (5) would read:

$$S_1 = \frac{\left\langle \Gamma^1_n(J_1) \right\rangle^{1,J_1}}{D(1,J_1)\mu_{1,J_1}} = \frac{\left\langle \Gamma^1_n(J_2) \right\rangle^{1,J_2}}{D(1,J_2)\mu_{1,J_2}} = \ldots$$

6. The October 1970 edition uses three different symbols for the reduced width. In a unified notation:

page D-9 $\quad \overline{\Gamma}^0_{nl,J} = \left\langle \Gamma^l_n(J) \right\rangle_{l,J}$

page D-11 $\quad \left\langle \Gamma^0_n \right\rangle^{l=1}_J = \left\langle \Gamma^l_n(J) \right\rangle_{l,J}$

page D-12 $\quad \left\langle \Gamma^{0l}_{nJ} \right\rangle = \left\langle \Gamma^l_n(J,\not{s} \right\rangle_{l,J}$

D.2.4.2. Comments on ENDF-102, October 1975 edition, Section D.2.1

1. Equation (1). $D_{l,\text{observed}}$ is D(*l*).
2. Same as comment 2 on the 1970 edition; above.
3. Equation (2). D_{obs} is D(*l*); $\rho_{l,\text{obs}}$ is ρ(*l*); Σ_J is $\tilde{\Sigma}_J$.
4. "All allowed *l*-values label the same set of resonances" means ρ(*l*,J) does not depend on *l* (for given parity).
5. Equation (3). $(2J + 1)^{-1}$ is missing from the right hand side.
6. Page D-12, second equation:

The quantity $\langle g\Gamma^l_n\rangle$ is $\left\langle g\Gamma^l_n(J)\right\rangle^l$. The bracket $\langle\rangle^l$ means summed over all J-values. The other two brackets are for particular J-values, *i.e.*,

$$\left\langle g\Gamma^l_n\right\rangle = \left\langle g\,\Gamma^l_n(J)\right\rangle^l$$
$$= \frac{g\left\langle\Gamma^l_n(J)\right\rangle^{l,J}}{\omega_{I,l}\,\mu_{l,J}} = \frac{g\left\langle\Gamma^l_n(J,\not{s})\right\rangle}{\omega_{I,l}}$$

7. "The strength functions for a given *l*-value but different J-values" means S(*l*,J). These are not all equal--it is the ratio $S(l,J)\mu_{l,J}$ which is independent of J.
8. Equation (D.6) should read:

$$\left\langle\Gamma_n(l,J)\right\rangle = \left\langle\Gamma^l_n(J,\not{s})\right\rangle\sqrt{E}\;\nu_l\,\mu_{l,J}$$
$$= \left[\left\langle\Gamma^l_n(J)\right\rangle\right]\sqrt{E}\;\nu_l$$

where $\Gamma^l_n(J)$ is the reduced width determined by experiment. That is, the relation involving $\mu_{l,J}$ is only valid for an ***average*** width, and hence $\sqrt{E}\;\nu_l$ must also be some appropriate average value. The quantum number s should be exhibited when μ is used.

D.3 The Competitive Width

D.3.1 Penetrability Factor for the Competitive Width in the Resolved Resonance Region

A. <u>SLBW and MLBW</u>

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

$$\Gamma_{xr}(E) = \Gamma_{n'r}(E) = \frac{P_l\left(E - E_1^*\right)\Gamma_{xr}\left(\left|E_r\right|\right)}{P_l\left(\left|E_r - E_1^*\right|\right)}, \text{ if } E \geq E_1^*$$

excited state, corrected for recoil, so that

and

$$\Gamma_{xr} = 0 \quad \text{if } E < E_1^*$$

where E_1^* is (AWRI+1)/AWRI times the excitation energy of the first excited state, E_1^{ex} ($E_1^{ex} = -QX$ 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 $\Gamma^l_{n'}$ 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 General R-matrix and Hybrid R-function formalisms allow for this possibility (see Sections D.1.5 and D.1.6).

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. *E.g.*, when two inelastic levels can be reached,

$$\Gamma_{xr}(E) = \frac{P_{l_1}(E - E_1^*)\Gamma_{n_1'r}\left(\left|E_r\right|\right)}{P_{l_1}\left(\left|E_r - E_1^*\right|\right)} + \frac{P_{l_2}(E - E_2^*)\Gamma_{n_2'r}\left(\left|E_r\right|\right)}{P_{l_2}\left(\left|E_r - E_2^*\right|\right)},$$

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

$$\begin{aligned} \Gamma_{xr}(E) &= 0 && \text{if } E < E_1^* \\ &= \Gamma_{xr}\left(\left|E_r\right|\right) && \text{if } E \geq E_1^* \end{aligned}$$

and then make some provision to handle the resultant discontinuity in the cross section.

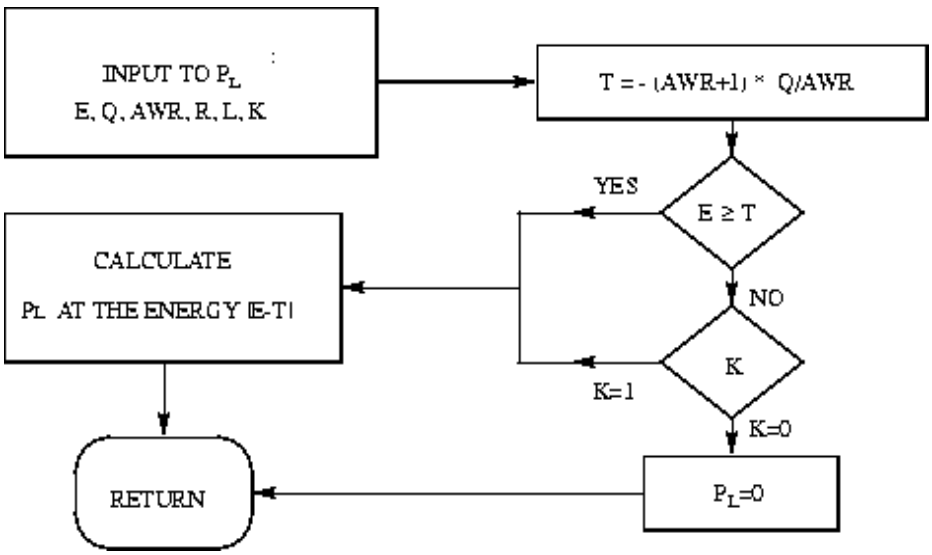
Users who are unable to handle this degree of complexity, and would like to use GT_R from File 2 as the total width without regard for whether the competitive process is energetically possible or not should at least be aware of the problem.

B. When the <u>Adler-Adler and Reich-Moore</u> 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 is used above the thermal region, the same comments apply as for the SLBW/MLBW formalism.

C. General R-matrix and Hybrid R-function formalisms allow multiple reaction channels, in addition to the elastic channel. The above discussion of penetrabilities pertains here also. For purposes of coding the penetrability factor as a subroutine, one possibility is to supply six arguments, an energy E, a Q-value Q, a mass ratio AWR, a radius R, an *l*-value L, and a sentinel K. Inside the subroutine, one calculates the threshold T= -(AWR +1.0) Q/AWR and then branches on K. If K=0, signaling an "incident" energy, the penetrability will be set to 0 if E is below threshold, but if K=1, signaling a "resonance" energy, the penetrability will be calculated at the absolute value of E-T. Thus an inelastic width would be calculated as

$$GINE\left(E\right) = GIN\left(\left|E_r\right|\right)\frac{P\left(E,Q=E^*,AWR,R,L,K=0\right)}{P\left(ER,Q=E^*,AWR,R,L,K=1\right)}$$

where P is a subroutine or function statement.



For both the R-formalisms, the evaluator must supply any Coulomb penetrabilities as tabulated functions of the incident neutron's laboratory energy. This choice keeps the energy consistent with that used in all other ENDF quantities and simplifies the problem of interpolating in the tables.

The evaluator will most likely calculate the Coulomb penetrabilities as functions of the center-of-mass energy in the exit channel, $E_{cm,exit}$. This is related to the center-of-mass energy in the incident channel by

$$E_{cm,inc} = E_{cm,exit} - Q$$

and the incident laboratory energy is

$$E_{lab,inc} = \frac{AWRI+1}{AWRI}E_{cm,inc} = \frac{AWRI+1}{AWRI}\left[E_{cm,exit} - Q\right] \quad .$$

In case the evaluator obtains his Coulomb penetrabilities as functions of the charged-particle laboratory energy, $E_{lab,exit}$, one more transformation is required:

$$E_{cm,exit} = \frac{\text{AWRIC}}{\text{AWRIC}+1}\ E_{\text{lab,exit}}\ ,$$

where AWRIC is the mass ratio in the exit channel.[67] In this case,

$$E_{lab,inc} = \left(\frac{\text{AWRI}+1}{\text{AWRI}}\right)\left[\frac{AWRIC}{AWRIC+1}E_{lab,exit} - Q\right]$$

These formulas enable the evaluator to supply the charged-particle penetrabilities as functions of the incident neutron's laboratory energy. This leaves to the user only the task of incorporating the dependence on the individual resonance energies, Section D.3.1.

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 $<\Gamma_n\Gamma_\gamma/\Gamma>$ 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 $<\Gamma_x>=0$ 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 2.4.20.)

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 $\Gamma_n + \Gamma_\gamma + \Gamma_f$, 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.

[8] For an n,p reaction AWRIC = $M_{daughter}/m_p \approx$ AWRI; but for an n,α reaction, AWRIC = $M_{daughter}/m_\alpha \approx$ (AWRI-3)/4.

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,

$$\sigma_{n,t}(E) = \frac{\pi}{k^2}\sum_J g_J \frac{\Gamma_{nr}\Gamma_r}{\left(E - E_{r'}\right)^2 + \frac{1}{4}\left(\Gamma_r/2\right)^2},$$

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 General R-matrix and Hybrid R-function do 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. Depending on what non-elastic channels are specified, the total cross section may be calculated either as the sum of the partial cross sections, or from {1-ReU(*l*sJ)}, as described in Sections D.1.5.6 and D.1.6.4. 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:

$$A = \frac{m_2}{m_1} , \qquad (.131)$$

$$A' = \frac{m_3}{m_1} , \qquad (.132)$$

$$\beta = \left(\frac{A(A+1-A')}{A'} \left[1 + \frac{1+A}{A} \frac{Q}{E_1} \right] \right)^{1/2} \qquad (.133)$$

$$\gamma = \frac{A'}{A+1-A'} \beta , \qquad (.134)$$

$$\frac{\varepsilon_3}{\varepsilon_1} = \frac{A'}{A^2} \beta^2 , \qquad (.135)$$

$$\varepsilon_1 = \left(\frac{A}{A+1} \right)^2 E_1 , \qquad (.136)$$

$$\mu_3 = \mu , \qquad (.137)$$

$$\frac{\varepsilon_4}{\varepsilon_1} = \frac{A'}{A+1-A'} \frac{\varepsilon_3}{\varepsilon_1} , \qquad (.138)$$

$$\mu_4 = -\mu , \qquad (.139)$$

$$\frac{E_3}{E_1} = \frac{A'}{(1+A)^2} \left(\beta^2 + 1 + 2\beta\mu \right) , \qquad (.140)$$

$$\omega_3 = \frac{1+\beta\mu}{\sqrt{\beta^2 + 1 + 2\beta\mu}} , \qquad (.141)$$

$$\frac{E_4}{E_1} = \frac{A+1-A'}{(1+A)^2} \left(\gamma^2 + 1 - 2\gamma\mu \right) , \qquad (.142)$$

$$\omega_4 = \frac{1-\gamma\mu}{\sqrt{\gamma^2+1-2\gamma\mu}} \,. \qquad (\ .143)$$

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.

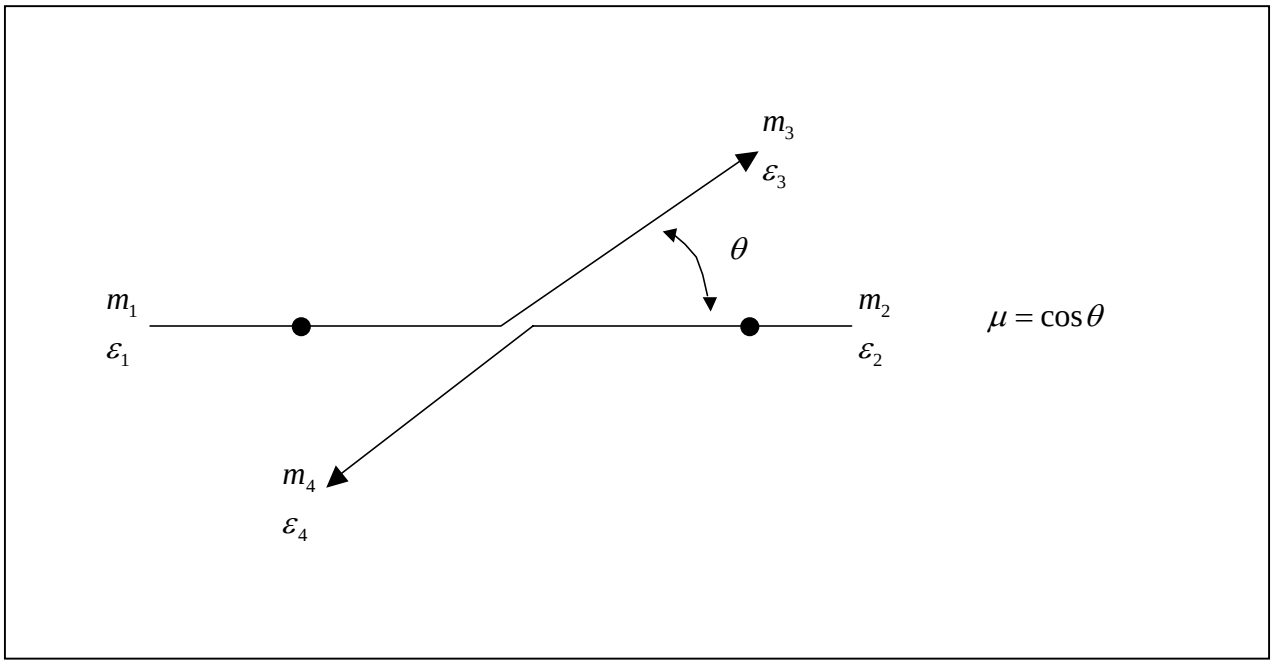

Figure E.1
Kinematics Variables for Two-Particle Reactions
Center-of-Mass System

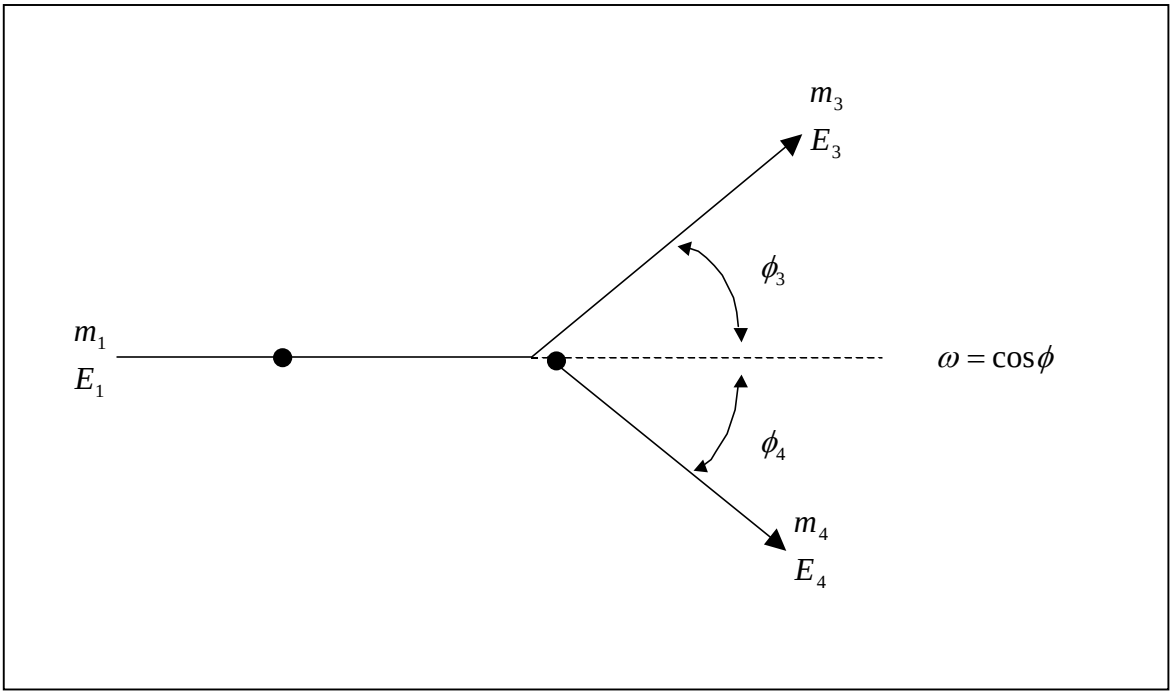

Figure E.2
Kinematics Variables for Two-Particle Reactions
Laboratory System

APPENDIX F

Summary of Important ENDF Rules

General

1. Cross sections for all significant reactions should be included.
2. The data in ENDF 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.**

File 2 - Resonance Parameters

1. Only one energy region containing resolved resonance parameters can be used, if needed.
2. The cross section from resonance parameters is 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 cross section space and not in unresolved resonance parameter space. Any INT 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.**

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.

(Exceptions MT=26, 46-49, 719, 739, 759, 779, and 799 are not included in the MT=1.)

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 at zero cross sections at the threshold energy.**

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-value 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 File 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.

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 + File 3 summation scattering cross section σ_s divided by 2π.
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. When the elastic scattering is represented by Legendre coefficients, an energy-independent transformation matrix must be given to perform a CM to laboratory conversion.
4. **Angular distributions for continuum and other reactions must be given as tabulated distributions in the Lab system.**
5. **The angular distribution, whether specified as a Legendre expansion or a tabulated distribution, must be everywhere positive.**
6. **Angular distribution data should be given at the minimum number of incident energy points that will accurately describe the energy variation of the distributions.**

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 + File 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	Section	Variable	Max	Definition of Number
1	451	NXC	350	Card images in directory
	452	NC	4	Polynomial terms in expansion of $\bar{\nu}$
	455	NCD	4	Polynomial terms in expansion of $\bar{\nu}_d$
	456	NCP	4	Polynomial terms in expansion of $\bar{\nu}_p$
All	All	NR	20	Interpolation ranges
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
		NLS	4	*l*-values
		NLCS	20	*l*-values which must be given to converge reaction
3	All≠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 ≠1	NP	50,000 5,000	Energy points
14	All	NL	64	Highest order Legendre polynomial
All other	All	NP	10,000	Mesh size

APPENDIX H

Recommended values of Physical Constants to be Used in ENDF

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 site68.

These are supplemented by the mathematical constants from **MathSoft69** (Source 2).

Atomic masses not given in the CODATA recommended values should be taken from the **Atomic Mass Tables** of G. Audi and A. Wapstra70 (Source 3).

68 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/.

69 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.

70 G. Audi and A. H. Wapstra, Nucl. Phys. A. 595, 409 (1995). The Web site, maintained by the Atomic Mass Data Center, is located at http://csnwww.in2p3.fr/groupes/massatom/masseval.html.

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.

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.

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.

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
$\alpha^{-1} = \hbar c / e^2$	inverse fine-structure constant	137.035 999 76	1
u	atomic mass constant (amu)	$931.494\ 013 \times 10^{6}$ eV	1
h	Plank's constant	$4.135\ 667\ 27 \times 10^{-15}$ eV s	1
$\hbar$	Planck's constant/2π	$6.582\ 118\ 89 \times 10^{-16}$ 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

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	3.016 049 268 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 4.
Conversion Factors

Convert	Conversion Factor	Source
amu $\rightarrow$ eV	$9.314\,940\,13 \times 10^{8}$	1

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 5.
Derived quantities whose values were formerly given in the body of the Manual

Location	Value previously given in Manual	Units for value	Expression
page 0.18	0.998 62		m_p/m_n
	1.996 26		m_d/m_n
	2.989 60		m_t/m_n
	2.989 03		m_{3He}/m_n
	3.967 13		m_a/m_n
Page 4.7	3.0560×10^{-8}	1 / (eV barn steradian)	$2\ m_n / (\hbar^2 (4\pi)^2)$
Eq. (6.9)	$4.784\,53 \times 10^{-6}$	$(10^{-12}\ \text{cm})^2$ eV / amu	$2 / \hbar^2$
Eq. (6.10)	$2.480\,58 \times 10^{4}$	eV / amu	$e^4 / 2\hbar^2 = 1 / (2\ \alpha^2)$
page D.3	$2.196\,771 \times 10^{-3}$	10^{-12} cm $(\text{eV})^{-1/2}$	$\sqrt{2m_n}/\hbar$