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 June 2005

Section	Page	Update
0.7.3		New record type: INTG (N. Larson)
2.		Replacement of LRF=5 and 6 with LRF=7 format for R-Matrix parameters. Miscellaneous corrections. (N. Larson)
32.		Addition of LCOMP=2 format for resonance-parameter covariance matrices (N. Larson)
Appendix D		Addition of D.1.7, Equations for LRF=7 format. Deletion of Sections D.1.5 and D.1.6. Other miscellaneous corrections. (N. Larson)

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 codes[4] 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 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.

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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.

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, and 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 and Debye-Waller integral. Finally, scattering law data for inelastic incoherent scattering are given, using the $S(\alpha,\beta)$ formalism and the short-collision-time approximation.

[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).

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 electrons[11] 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,

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

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

[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)

The distribution function *f(μ,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→n+α must be classified as the reaction $^3H(d,n)^4He$ (MT=50) rather than the reaction $^3H(d,n\alpha)$ (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:

$$\text{MT207} = \text{MT107} + 3\times\text{MT91}.$$

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 n^{th} value of *x*,
y(n) is the n^{th} value of *y*,
NP is the number of pairs (*x* and *y*) given,
INT(m) is the interpolation scheme identification number used in the m^{th} range,
NBT(m) is the value of *n* separating the m^{th} 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

$$\sigma = \frac{A}{E}\exp\left[-\frac{B}{\sqrt{E-T}}\right] \tag{0.1}$$

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

$$B = \frac{\ln \dfrac{\sigma_2 E_2}{\sigma_1 E_1}}{\dfrac{1}{\sqrt{E_1 - T}} - \dfrac{1}{\sqrt{E_2 - T}}} \tag{0.2}$$

and

$$A = \exp\left[\frac{B}{\sqrt{E_1 - T}}\right]\sigma_1 E_1 \tag{0.3}$$

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

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

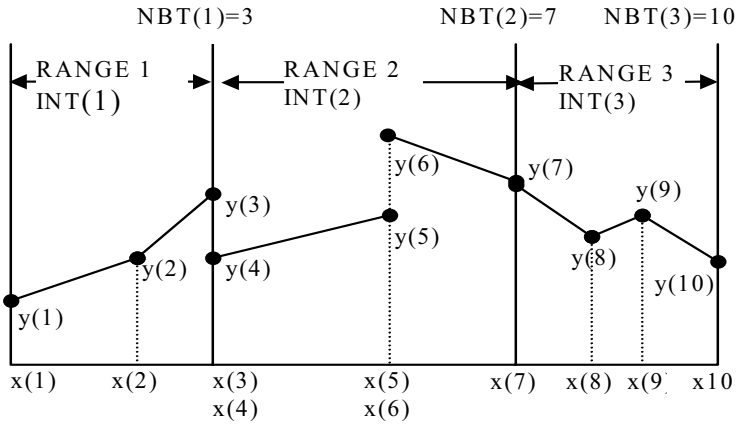
Next consider an energy distribution represented as a two-dimensional function of E and E' $f(E,E')$. Using a simple Cartesian interpolation, the function is represented by a series of tabulated functions $f(E,E')$. The simple "graph paper" rules are used for interpolating for $f(E')$ at each El. An 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 k^{th} 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.

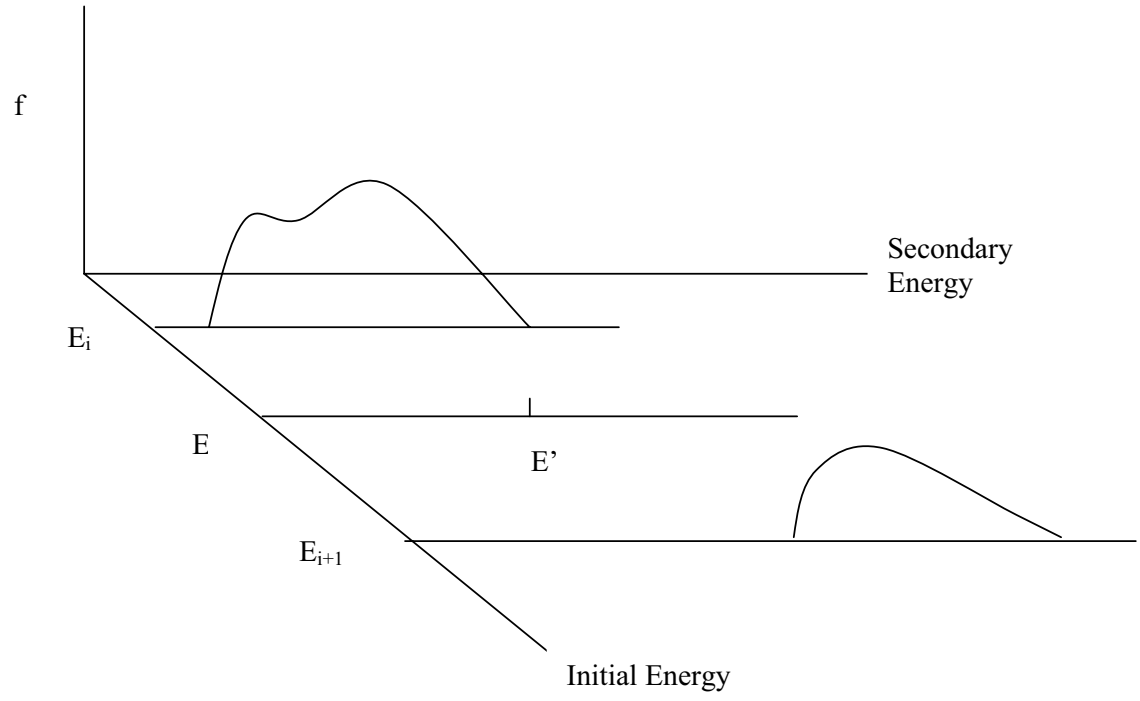
Figure 0.1
Interpolation of a Tabulated One-dimensional Function
Illustrated for the Case NP=10, NR=3



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 initial energy and there 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:

$$f(E, E') = f(E_i, E') + \frac{E - E_i}{E_{i+1} - E_i}[f(E, E') - f(E_i, E')] \tag{0.4}$$

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

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

$$x \equiv \frac{E' - E'_i(1)}{E'_i(N) - E'_i(1)} \tag{0.5}$$

In this case, $E'_i(1)$ is the energy of the first sink energy in the panel at E_i and $E'_i(N)$ is the last point. An exactly analogous equation is used to define the value of x at E_{i+1} and at E. From here, the interpolation is made using an expression such as shown in 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.,

$$\int dE'\ f(E') = \int dx\ g(x) \tag{0.6}$$

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

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

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

$$E'_{high}(E) = E'_i(N) + \frac{E - E_i}{E_{i+1} - E_i}[E'_{i+1}(M) - E'_i(N)] \tag{0.8}$$

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

$$E'_i(E') = E'_i(1) + \frac{E' - E'_{low}}{E'_{high} - E'_{low}}[E'_i(N) - E'_i(1)] \tag{0.9}$$

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.

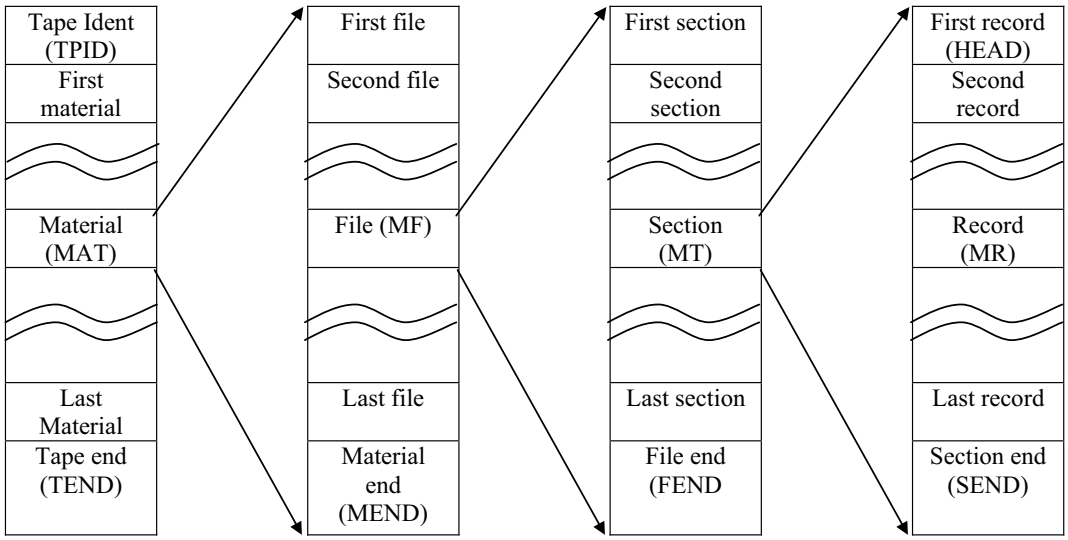
0.7.1. Structure of an ENDF Data Tape

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 six possible types, denoted by TEXT, CONT, LIST, TAB1, TAB2, and INTG. The CONT record has six special cases called DIR, HEAD, SEND, FEND, MEND, and TEND. The TEXT record has the special case TPID. Every record contains the basic control numbers MAT, MF, and MT, as well as 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.

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] SEND[14]
[MAT, 0,    0/  0.0,  0.0,   0,   0,   0,   0] FEND
[  0, 0,    0/  0.0,  0.0,   0,   0,   0,   0] MEND
```

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

[14] The SEND record has the sequence number 99999.

```
[ -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 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.

0.7.9 INTG records

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

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

where II and JJ are position locators, and KIJ is an array of dimension 18.

The INTG record can be read with the following FORTRAN statements:

```
   DIMENSION KIJ(18)
   READ (LIB,10) II, JJ, KIJ, MAT, MF, MT, NS
10 FORMAT (2I5, 1X, 18I3, 1X,  I4, I2, I3, I5)
```

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

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.