united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

SMR/1220-20

Workshop on

Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

13 March - 14 April 2000

Miramare - Trieste, Italy

An introduction to the ENDF Formats

Robert. E. MacFarlane
Los Alamos National Laboratory
Los Alamos, USA

An Introduction to the ENDF Formats

The ENDF Evaluated Nuclear Data Formats are used all over the world to encode nuclear data evaluations for use in research and nuclear technology. For an introduction to the formats and how they are used in modern compilations of nuclear data, just follow the NEXT links. To browse through the pages in other orders, use the INDEX links.

If you have an operating version of NJOY 97 and the appropriate data files, you can work through a set of EXERCISES designed to illustrate some of the important features of the ENDF format. To do the exercises in order, just follow the NEXT links. To browse through the pages in other orders, use the INDEX links.

NEXT EXERCISES INDEX

---

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

Introduction to the ENDF Formats: Index

Jump directly to any page of the *Introduction to the ENDF Formats:*

Jump directly to any of the exercises:

The ENDF formats were originally developed for use in the US national nuclear data files called ENDF/B (the Evaluated Nuclear Data Files). These files went through various versions with names like ENDF/B-III, ENDF/B-IV, and ENDF/B-VI. The formats were upgraded with each version to handle new features, for example, the extension from the original upper limit of 15 MeV to 20 MeV, the addition of photon production information, the introduction of new resonance formats, or the addition of charged-particle data. As ENDF/B-VI was being prepared, it was noted that the ENDF formats were coming into wide use around the world, including the JEF files in Europe, the JENDL files in Japan, and the BROND files in Russia. It was decided to decouple the ENDF formats from the ENDF/B libraries in order to make this international use easier. Therefore, we now refer to the "ENDF-6 format" to distinguish it from the "ENDF/B-VI library."

Control over the ENDF formats has been retained by the US Cross Section Evaluation Working Group (CSEWG), and the format specifications are published through the National Nuclear Data Center at the Brookhaven National Laboratory.

NEXT INDEX

What's In A Name?

What's In A Name?

The ENDF formats were originally developed for use in the US national nuclear data files called ENDF/B (the Evaluated Nuclear Data Files). These files went through various versions with names like ENDF/B-III, ENDF/B-IV, and ENDF/B-VI. The formats were upgraded with each version to handle new features, for example, the extension from the original upper limit of 15 MeV to 20 MeV, the addition of photon production information, the introduction of new resonance formats, or the addition of charged-particle data. As ENDF/B-VI was being prepared, it was noted that the ENDF formats were coming into wide use around the world, including the JEF files in Europe, the JENDL files in Japan, and the BROND files in Russia. It was decided to decouple the ENDF formats from the ENDF/B libraries in order to make this international use easier. Therefore, we now refer to the "ENDF-6 format" to distinguish it from the "ENDF/B-VI library."

Control over the ENDF formats has been retained by the US Cross Section Evaluation Working Group (CSEWG), and the format specifications are published through the National Nuclear Data Center at the Brookhaven National Laboratory.

NEXT INDEX

What Are They For?

The uses of the ENDF formats have also evolved over the years. The first few versions were largely intended for thermal-reactor applications. ENDF/B-IV and ENDF/B-V shifted the emphasis toward fast-reactor and fusion applications. For ENDF/B-VI, additional extensions have been made for charged-particle and accelerator applications. In recent years, the ENDF system has also gained a role as a mode of publication and archiving of basic low-energy nuclear physics data. In general,

- ENDF-format libraries are computer-readable files of nuclear data that describe nuclear reaction cross sections, the distributions in energy and angle of reaction products, the various nuclei produced during nuclear reactions, the decay modes and product spectra resulting from the decay of radioactive nuclei, and the estimated errors in these quantities.

- ENDF-format libraries are intended to be used for a wide variety of applications that require calculations of the transport of neutrons, photons, and charged-particles through materials, the enumeration of the interactions of this radiation with the materials and their surroundings, and the time evolution of the radioactivity associated with the nuclear processes.

Examples of uses for ENDF-based libraries include fission and fusion reactor calculations, shielding and radiation protection calculations, criticality safety, nuclear weapons, nuclear physics research, medical radiotherapy, radioisotope therapy and diagnostics, accelerator design and operations, geological and environmental work, radioactive waste disposal calculations, and space travel calculations.

NEXT INDEX

Nuclear Data Evaluations

The answer to the question "What are they for?" has several implications and consequences. The work that is required to generate a file in ENDF format is called "nuclear data evaluation."

The requirement that the data be in a computer readable format puts strict limits on what an evaluator can do. Not every fact or physical effect can always be squeezed into the constraints of the format. But the evaluator has to do his or her best to get a good representation of reality. When these constraints are too limiting, we can try to extend the formats.

The fact that these evaluated data files are intended to be used for applications also has consequences. The data must be "complete" in some sense; for example, all energies must be represented, even when the data don't cover them all. Otherwise, particle transport calculations would be impossible. Modern evaluations are done by combining the experimental data with nuclear model code calculations to extend or interpolate the available data. In addition, the fact that these evaluated data files are intended to be used for applications adds factors of quality control, revision control, peer review, and data testing that might not be needed for other modes of publication.

NEXT INDEX

National Nuclear Data Organizations

The difficulty of modern nuclear data evaluation, together with the requirements for quality control, revision control, peer review, and data testing that result from the goal of using the data files for calculations that could have major impacts on public health and safety, has led to putting all modern nuclear data evaluation work under the control of a few national and international agencies, including:

- The Cross Section Evaluation Working Group (CSEWG), which handles the US ENDF/B libraries and the ENDF format. It is coordinated through the National Nuclear Data Center at the Brookhaven National Laboratory.
- The JEF and EFF Working Groups, now merged as the JEFF Working Group, which handles the Joint European File (JEF), the European Fusion File (EFF), and their forthcoming merger, JEFF. It is coordinated through the NEA Data Bank, a part of the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD).
- The Japanese Nuclear Data Committee (JNDC), which handles the Japanese Evaluated Nuclear Data Library (JENDL). It is coordinated through the Nuclear Data Center at the Japan Atomic Energy Research Institute (JAERI).

Each of these organizations has adopted the ENDF-6 format as the common method for publishing their nuclear data libraries, but each has been able to define its own procedures for using the formats, reviewing the evaluations, and testing the results.

NEXT INDEX

Basic Organization: MAT, MF MT

An ENDF-format nuclear data library has an hierarchical structure by tape, material, file, and section. Each of these levels has a characteristic numerical identifier:

- An ENDF "tape" is a file that contains one or more ENDF materials. We are fond of the word "tape" out of respect for the history of computing. As an example, Tape 511 was the ENDF/B-V Standards Tape.

- MAT labels an ENDF material. In older versions of ENDF/B, these numbers were assigned as the evaluations were completed, *e.g.*, MAT1301 is H-1 and MAT1395 is U-235 for ENDF/B-V. For ENDF/B-VI, CSEWG moved to MAT numbers computed from the target Z and A. The numbers step by threes to allow for isomers, and a last two digits of 25 point to the lightest of the common isotopes. Thus, 125 is H-1, 128 is H-2, 2625 is Fe-54, 6153 is Pm-148m, and 9228 is U-235. For ENDF/B-VI Tape and MAT numbers, see the Index to ENDF/B-VI Neutron Data.

- MF labels an ENDF file. "Files" are usually used to store different types of data, thus:
  - MF=1 contains descriptive and miscellaneous data,
  - MF=2 contains resonance parameter data,
  - MF=3 contains reaction cross sections vs energy,
  - MF=4 contains angular distributions,
  - MF=5 contains energy distributions,
  - MF=6 contains energy-angle distributions,
  - MF=7 contains thermal scattering data,
  - MF=8 contains radioactivity data
  - MF=9-10 contain nuclide production data,
  - MF=12-15 contain photon production data, and
  - MF=30-36 contain covariance data.

- MT labels an ENDF section. Sections are usually used to hold different reactions. For example, MT=1 is the total cross section, MT=2 is elastic scattering, MT=16 is the (n,2n) reaction., MT=18 is fission, and MT=102 is radiative capture. The ever increasing scope of use for the ENDF-format data has led to a continual increase in the number and types of reactions that can be represented: ENDF MT list. More discussion of the labeling of reactions will be found later in this presentation.

An ENDF tape contains one or more materials in increasing order by MAT. Each material contains several files in increasing order by MF. Each file contains several sections in increasing order by MT.

NEXT INDEX

ENDF MT Values

The ENDF format uses MT numbers to define reaction types, and some additional MT numbers are used for special sections, such as the descriptive data, or the resonance parameters. In the following tables, "z" stands for any of the particles, *i.e.*, n, p, d, t, He-3, a, or photonuclear gamma.

MT	Reaction	Description	Comments
1	(n,total)	Neutron total cross section. Sum of MT=2, 4, 5, 11, 16-18, 22-26, 28-37, 41-42, 44-45, and 102-117.	Redundant. Undefined for incident charged particles.
2	(z,z_0)	Elastic scattering cross section for incident particles.	
3	(z,nonelastic)	Nonelastic 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 MT=50-91.	Redundant. For incident neutrons, this is total inelastic scattering (MT=50 is undefined for neutrons).
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 particles 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; exclues all discrete reactions.	Redundant; to be used for derived files only.
27	(z,abs)	Absorption. Sum of MT=18 and MT=102-117.	Redundant. Rarely used.
101	(z,disap)	Disappearance. Sum of MT=102-117.	Redundant. Rarely used.

Neutron-Producing Continuum Reactions

MT	Reaction	Description	Comments
11	(z,2nd)	Production of two neutrons and a deuteron, plus a residual.	
16	(z,2n)	Production of two neutrons, plus a residual.	

17	(z,2n)	Production of three neutrons, plus a residual.	
18	(z,fission)	Total fission. Equal to the sum of MT=19, 20, 21, and 38, if present.	Redundant if MT=19 is present. Basic otherwise.
19	(z,f)	First-chance fission.	
20	(z,nf)	Second-chance fission.	
21	(z,2nf)	Third-chance fission.	
22	(z,na)	Production of a neutron and alpha particle, plus a residual.	
23	(z,n3a)	Production of a neutron and three alpha particles, plus a residual.	
24	(z,2na)	Production of two neutrons and an alpha particle, plus a residual.	
25	(z,3na)	Production of three neutrons and an alpha particle, plus a residual.	
28	(z,np)	Production of a neutron and a proton, plus a residual.	
29	(z,n2a)	Production of a neutron and two alpha particles, plus a residual.	
30	(z,2n2a)	Production of two neutrons and two alpha particles, plus a residual.	
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,nd2a)	Production of a neutron, a deuteron, and two alpha particles, plus a residual.	
36	(z,nt2a)	Production of a neutron, a triton, and two alpha particles, plus a residual.	
37	(z,4n)	Production of four neutrons, plus a residual.	
38	(z,3nf)	Fourth-change fission.	
41	(z,2np)	Production of two neutrons and a proton, plus a residual.	
42	(z,3np)	Production of three neutrons and a proton, plus a residual.	

44	(z,n2p)	Production of a neutron and two protons, plus a residual.	
45	(z,npa)	Production of a neutron, a proton, and an alpha particle, plus a residual.	

Neutron-Producing Discrete Reactions

MT	Reaction	Description	Comments
50	(z,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, leaving the residual nucleus in the first excited state.	
52	(z,n_2)	Production of a neutron, leaving the residual nucleus in the second excited state.	
	...		
90	(z,n_{40})	Production of a neutron, leaving the residual nucleus in the 40th excited state.	
91	(z,n_c)	Production of a neutron in the continuum not included in the above discrete representation.	

Reactions That Do Not Produce Neutrons

MT	Reaction	Description	Comments
102	(z,gamma)	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, and MT=600 is undefined (use MT=2).
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, and MT=650 is undefined (use MT=2).
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, and MT=700 is undefined (use MT=2).
106	(z,^{3}He)	Production of a He particles, plus a residual. Sum of MT=750-799, if they are present.	For incident ^{3}He particles, this is inelastic scattering, and MT=750 is undefined (use MT=2).
107	(z,a)	Production of an alpha particle, plus a residual. Sum of MT=800-849, if they are present.	For incident alphas, this is inelastic scattering, and MT=800 is undefined (use MT=2).
108	(z,2a)	Production of two alphas, plus a residual.	
109	(z,3a)	Production of three alphas, plus a residual.	
111	(z,2p)	Production of two protons, plus a residual.	
112	(z,pa)	Production of a proton and an alpha particle, plus a residual.	
113	(z,t2a)	Production of a triton and two alphas, plus a residual.	
114	(z,d2a)	Production of a deuteron and two alphas, plus a residual.	
115	(z,pd)	Production of a proton and a deuteron, plus a residual.	
116	(z,pt)	Production of a proton and a triton, plus a residual.	
117	(z,da)	Production of a deuteron and an alpha particle, plus a residual.	

Charged-Particle-Producing Discrete Reactions

MT	Reaction	Description	Comments
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, leaving the residual nucleus in the first excited state.	
602	(z,p_2)	Production of a proton, leaving the residual nucleus in the second excited state.	
	...		
648	(z,p_{48})	Production of a proton, leaving the residual nucleus in the 48th 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.	Not allowed for incident deuterons. Use MT=2.
651	(z,d_1)	Production of a deuteron, leaving the residual nucleus in the first excited state.	
	...		
698	(z,d_{48})	Production of a deuteron, leaving the residual nucleus in the 48th 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.	Not allowed for incident tritons. Use MT=2.
701	(z,t_1)	Production of a triton, leaving the residual nucleus in the first excited state.	
	...		
748	(z,t_{48})	Production of a triton, leaving the residual nucleus in the 48th excited state.	
749	(z,t_c)	Production of a triton in the continuum not included in the above discrete representation.	
750	$(z,^3He_0)$	Production of a ^{3}He particle, leaving the residual nucleus in the ground state.	Not allowed for incident ^{3}He particles. Use MT=2.

751	(z,$^3He_1$)	Production of a ^{3}He particle, leaving the residual nucleus in the first excited state.	
	...		
798	(z,$^3He_{48}$)	Production of a ^{3}He particle, leaving the residual nucleus in the 48th excited state.	
799	(z,^3He_c)	Production of a ^{3}He particle in the continuum not included in the above discrete representation.	
800	(z,a_0)	Production of an alpha particle, leaving the residual nucleus in the ground state.	Not allowed for incident alphas. Use MT=2.
801	(z,a_1)	Production of an alpha particle, leaving the residual nucleus in the first excited state.	
	...		
848	(z,a_{48})	Production of an alpha particle, leaving the residual nucleus in the 48th excited state.	
849	(z,a_c)	Production of an alpha particle in the continuum not included in the above discrete representation.	

NEXT INDEX

Reading An ENDF Tape

The keys to finding your way around on an ENDF tape are the MAT, MF, and MT numbers. On the ASCII versions of ENDF-format files, they appear in columns 67 to 75 of every "card" (we also use the term "card" out of respect for the history of computing--besides, some of us remember them real well!). The Fortran notation is I4,I2,I3. The MT value is zero to indicate the end of a section (SEND record), the MF value is zero to indicate the end of a file (FEND record), and the MAT number is zero to indicate the end of a material (MEND record). There is a special "tape ID" record at the beginning with the MAT value equal to the tape number, and a special tape-end record (TEND) with MAT=-1 at the end of the tape.

Here is an example of the skeletal structure for a typical ENDF tape (the 5-digit sequence numbers in columns 76 to 80 have been omitted for clarity):

```
tape id                                          7777 0  0
start of MF1, MT451 (description)                1111 1451
  ...
SEND record                                      1111 1  0
FEND record                                      1111 0  0
start of MF2, MT151 (resonances)                 1111 2151
 ...
SEND record                                      1111 2  0
FEND record                                      1111 0  0
start of MF3, MT1 (total cross section)          1111 3  1
  ...
SEND record                                      1111 3  0
start of MF3, MT2 (elastic cross section)        1111 3  2
  ...
FEND record                                      1111 0  0
MEND record                                         0 0  0
TEND record                                        -1 0  0
```

To find samples of this kind of structure, look at the "raw" ENDF files from ENDF/B-VI, JEF-2.2, or JENDL-3.2.

NEXT INDEX

Simple Cross Sections

Simple cross sections on ENDF files are examples of the general one-dimensional tabulation, or TAB1, record. As an example, here is the section for the (n,2n) reaction in natural silicon from ENDF/B-VI:

```
 1.400000+4 2.784400+1          0          0          0          01400 3 16
-8.473800+6-8.473800+6          0          0          1          121400 3 16
         12          2                                                1400 3 16
 8.778100+6 0.000000+0 1.000000+7 6.166000-3 1.100000+7 1.564000-21400 3 16
 1.200000+7 2.589000-2 1.300000+7 3.650000-2 1.400000+7 4.663000-21400 3 16
 1.500000+7 5.400000-2 1.600000+7 5.620000-2 1.700000+7 5.734000-21400 3 16
 1.800000+7 5.830000-2 1.900000+7 5.870000-2 2.000000+7 5.892000-21400 3 16
 0.000000+0 0.000000+0          0          0          0          01400 3  0
```

The first line is the HEAD record; it contains the ZA value (100*Z+A) and the AWR value (ratio of target mass to neutron mass). The second card starts the TAB1 record and contains the reaction Q value (-8.4738 MeV) and some counts. The third line contains some interpolation information. Finally, the rest of the record contains the tabulation given as energy, cross section pairs with energies in eV and cross sections in barns. Therefore, we can immediately read off the 14 MeV cross section of .04663 barns. The last line in the section is just the normal SEND record.

Note that this is an endothermic reaction (negative Q value), and it has a threshold energy of 8.7781 MeV. We can also compute the threshold from the Q value using

$$-Q*(AWR+1)/AWR,$$

which gives 8.778131 MeV. It is important to have the first energy point greater than or equal to the computed threshold in some applications, and NJOY checks this.

To fully understand this example, we need to have a more formal definition for the contents of a cross section record, more details on how Q values are used (why are there two values given?), and a description of how interpolation is used to define cross section values between the grid points given.

NEXT INDEX

Formal Specifications for File 3

The following is based on ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6.

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 data) 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). 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.

Formats

The following quantities are defined:

ZA,AWR
: standard material charge and mass parameters

QM
: is the 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 the masses of all other reaction products; that is, for

$$a+A \rightarrow b+c+...+B,$$
$$QM=[(m_a+m_A) - (m_b+m_c+...+m_B)] \times U,$$

where the mass unit U is 9.3150146e8 eV for masses given in AU, the standard C12-based mass units, or 9.395728e8 eV for masses given in neutron masses (AWR).

QI
: is the reaction Q value for the (lowest energy) state defined by the given MT value in a simple two-body reactions or a breakup reaction. It is 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).

LR
: complex or "breakup" reaction flag. Indicates that additional particles not specified by the MT number will be emitted.

NR,NP,EINT
: standard TAB1 parameters

S(E)
: cross section (barns) for a particular reaction (or 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/ EINT/ S(E)] TAB1
[MAT, 3, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

This standardized shorthand notation is used throughout the ENDF format manual to show what parameters appear in the various fields.

NEXT INDEX

ENDF Interpolation

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 gid points. Simple one-dimensional "graph paper" interpolation schemes and a special Gamow interpolation law for charged-particle cross sections are provided.

The function $y(x)$ 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 pairs given. The complete region over which x is defined is broken up into NR interpolation ranges. An interpolation range is defined as a range of the indendent variable x in which a specified interpolation scheme can be use; *i.e.*, the same scheme gives interpolated values of $y(x)$ for any value of x within this range. The definitions of the quantities in the interpolation table follow:

Parameter	Meaning
NP	Number of pairs x,y given
NR	Number of interpolation ranges given
INT(m)	interpolation scheme used in the m^{th} range
NBT(m)	pair index separating the m^{th} and $(m+1)^{th}$ ranges

The allowed interpolation schemes are

INT	Meaning
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	y obeys a Gamow charged-particle penetrability law

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 two different y values are given to make a discontinuity.

Examples of Interpolation Tables

The most common interpolation table in the ENDF/B files simply specifies that linear-linear interpolation is used throughout the range of x.

```
NR=1
NP=10

10     2
```

A more interesting example might be as follows:

```
NR=3
NP=10

2     2     6     5     10     1
```

which says that linear-linear interpolation is used between the first point (*e.g.*, the threshold) and the second point. Log-log interpolation is used between the second and fifth points, and histogram interpolation is used above the fifth point. For histogram interpolation, the value of x for the last point is used to define the end of the range of $y(x)$ and the y value is ignored.

Charged-Particle Cross Sections

A special one-dimensional interpolation law, INT=6, is defined for charged-particle cross sections. It is based on the limiting forms of the Coulomb penetrabilities for exothermic reactions at low energies and for endothermic reactions near the threshold. This scheme gives a concave upward energy dependence near the threshold that is quite different from the behavior of the neutron cross sections. At higher energies, non-exponential behavior will normally begin to appear, and linear-linear interpolation is more suitable. The formulas for INT=6 follow:

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

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

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

where E_1,σ_1 and E_2,σ_2 are two consecutive points in the cross-section tabulation. In these formulas, T=0 for exothermic reactions (Q>0). For endothermic reactions, T is the kinematic threshold.

NEXT INDEX

Interpolation Problems

The limitation to "graph paper" interpolation schemes causes some problems for reactions that are a sum of processes with different characteristic shapes. The classic example of this is the total cross section at low energies. At zero temperature, the elastic cross section tends to be constant for many materials, and it can be represented well using linear-linear interpolation. But the radiative capture cross section usually goes like $1/v$, and it is best described using log-log interpolation. Clearly, the sum of these two reactions will be OK at the grid points, but values intermediate between the grid points cannot be calculated with either linear-linear or log-log interpolation.

For this reason, summation cross sections, such as MT=1 (total cross sectin), MT=4 (total inelastic), and sometimes MT=18 (total fission), must not be considered fundamental. They must always be reconstructed from the sum of their parts.

In the NJOY Nuclear Data Processing System, linearization takes place in the RECONR module. A new energy grid is chosen iteratively that will represent each fundamental cross section, such as MT=2 and MT=102 as described above, to some desired accuracy (*e.g.*, 0.1%). The total cross section is then regenerated on the new grid by adding up the parts.

NEXT INDEX

Resonance Parameters

Except for the lightest isotopes, elastic, capture, fission, and sometimes inelastic cross sections show sharp peaks and valleys due to resonances. For the lighter isotopes, it is practical to include all the pointwise detail of the cross sections directly in File 3. Good examples of this approach include carbon, O-16, and Al-27 in the ENDF/B libraries.

For heavier isotopes, this approach would lead to very large files with tens of thousands of energy points. ENDF-format nuclear data evaluations combat this problem by using resonance cross section formulas to calculate the elastic, capture, and fission cross sections over a defined "resonance range." The parameters to use in these formulas are given in File 2 using MT=151. The ENDF-6 format allows the following options:

- Single-Level Breit-Wigner
- Multi-Level Breit-Wigner
- Reich-Moore
- Adler-Adler
- Hybrid R-Function
- Generalized R-Matrix

At higher energies and in heavier isotopes, the resonances get to be so closely spaced that they can no longer be resolved into separate peaks experimentally. In this "unresolved range," the ENDF format provide three ways to provide average resonance parameters to be used with statistical models from resonance theory to compute the cross sections:

- Energy-Independent Parameters
- Energy-Independent Parameters with Energy-Dependent Fission
- Energy-Dependent Parameters

The cross sections computed from the resonance formulas have to be combined with the cross sections given in File 3 to determine the evaluated cross sections. In most cases, the resonance energy range in File 3 for the resonance reactions (total, elastic, fission, capture) will either contain the value zero, or it will contain small positive and negative values to be added to the computed resonance cross sections as corrections. In a few unresolved cases, the unresolved resonance range in File 3 will contain the actual "infinitely dilute" cross section, which is to be multiplied by resonance shielding factors determined from the unresolved-resonance parameters.

NEXT INDEX

Single-Level Breit-Wigner Resonances

Earlier versions of the various evaluated data libraries made very heavy use of the Single-Level Breit-Wigner (SLBW) approach for the following reasons:

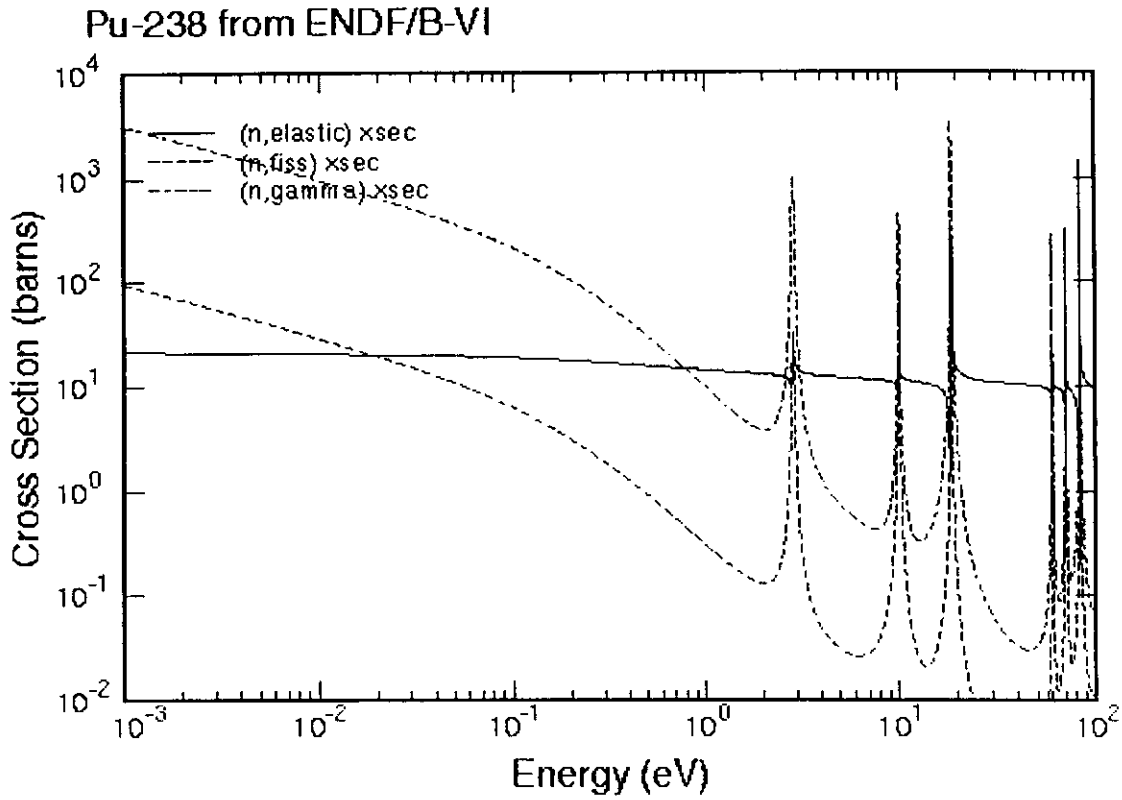
- it is easy to implement,
- it can use published resonance parameters,
- it can be Doppler broadened analytically, and
- it can be used analytically in reactor physics calculations.

However, it doesn't provide the best representation of the cross sections because of the neglect of multi-level and multi-channel effects--it can even produce unphysical negative cross sections for elastic scattering. Thus, some of the older files had corrections given as "File 3 backgrounds."

Here is an shortened example of the SLBW resonance parameters for Pu-238 from ENDF/B-VI:

```
 9.423800+4 2.360045+2          0          0          1          09434 2151
 9.423800+4 1.000000+0          0          1          2          09434 2151
 1.000000-5 2.000000+2          1          1          0          09434 2151
 0.000000+0 9.309000-1          0          0          1          09434 2151
 2.360045+2 0.000000+0          0          0         96         169434 2151
-1.000000+1 5.000000-1 6.217000-2 1.581000-2 4.500000-2 1.360000-39434 2151
-4.000000-1 5.000000-1 4.670000-2 3.400000-4 4.500000-2 1.360000-39434 2151
 2.855000+0 5.000000-1 3.808600-2 7.470000-5 3.680000-2 1.211000-39434 2151
 9.975000+0 5.000000-1 3.721300-2 2.084000-4 3.024000-2 6.765000-39434 2151
 1.856000+1 5.000000-1 4.249000-2 3.490000-3 3.739000-2 1.610000-39434 2151
 5.980000+1 5.000000-1 3.930000-2 1.550000-3 3.480000-2 2.950000-39434 2151
 ...
```

The third line says that the resonance range extends from 1e-5 to 200 eV. The fourth line says that the target spin is 0 and the scattering length is .9309. This translates into a potential scattering cross section of $4\pi a^2$ =10.89 barns. The parameters for 16 different resonances start on the sixth line: there is a negative-energy resonance at -10 eV with J=1/2, a total width of .06217 eV, a scattering width of .01581 eV, a capture width of .045 eV, and a fission width of .00136 eV. When these parameters are given to the RECONR module of the NJOY and Doppler broadened to 300K, the resulting cross sections are shown below:



NEXT INDEX

Multi-Level Breit-Wigner Resonances

Some materials in both old and new libraries use the MLBW representation because the interference effects are too strong for the simpler SLBW representation. MLBW has the advantage of always being positive definite also. However,

- it doesn't handle materials with multi-channel effects,
- it is much more expensive to process than SLBW,
- it doesn't lend itself to analytic Doppler broadening, and
- it doesn't work well using analytic reactor physics methods.

The multi-level Breit-Wigner parameters use the same format in File 2 as the SLBW representation.

NEXT INDEX

Reich-Moore Resonances

The Reich-Moore resonance representation (pronounced like "Rich-More") can handle both multi-level and multi-channel effects with good fidelity. No background corrections in File 3 are needed. Methods are now becoming available (the "multi-pole expansion") to allow analytic Doppler broadening and the direct use of Reich-Moore parameters in analytic reactor-physics methods. The Reich-Moore approach is used by the resonance analysis code SAMMY from ORNL, which is the current state of the art. Because of these factors, it has become the dominant choice for many of the new evaluations in ENDF/B-VI, including both fissionable isotopes with two fission channels like U-235, and nonfissionable materials like iron, copper, and lead.

```
 9.223501+4 2.330250+2          0          0          1          09228 2151
 9.223501+4 1.000000+0          0          1         12          09228 2151
 1.000000-5 4.000000+0          1          3          0          09228 2151
 3.500000+0 9.859600-1          0          0          1          39228 2151
 2.330200+2 9.859600-1          0          0        138         239228 2151
-1.000000+2 3.000000+0 1.145800-2 3.871290-2 1.229980-4 7.233640-29228 2151
-9.000000+1 4.000000+0 2.422100-6 3.680760-2 5.617020-2-2.168940-19228 2151
-4.297600+0 4.000000+0 7.164100-3 3.481860-2 3.192990-1-1.153500-19228 2151
-3.493400+0 3.000000+0 8.471500-8 3.780160-2-6.760010-3 1.298560-29228 2151
-1.504300+0 3.000000+0 8.519600-8 3.767610-2-7.010690-3 1.232090-29228 2151
-4.116100-1 3.000000+0 1.487500-4 2.984470-2-1.027260-3-1.554150-19228 2151
-1.942800-1 4.000000+0 5.044600-7 3.504170-2 1.989540-1-1.694210-39228 2151
 3.657500-5 4.000000+0 6.50520-11 2.984470-2-5.263430-4 9.645560-49228 2151
 2.819000-1 3.000000+0 4.439200-6 3.837130-2 1.065400-1-4.849860-39228 2151
 1.138900+0 4.000000+0 1.384200-5 4.069500-2-4.640000-6 1.093200-19228 2151
 2.036100+0 3.000000+0 9.358700-6 3.933000-2-7.736600-3-1.573500-39228 2151
 2.776700+0 4.000000+0 1.277200-6 3.887600-2 6.049200-2-4.250300-29228 2151
 3.156600+0 3.000000+0 2.432600-5 3.989600-2-7.995100-2 1.716100-29228 2151
 3.620800+0 4.000000+0 4.184000-5 3.764400-2-2.679600-2 2.849100-29228 2151
 4.850800+0 4.000000+0 7.560500-5 3.801700-2 4.666800-5-3.735100-39228 2151
 5.449700+0 4.000000+0 3.793200-5 3.920100-2-7.874000-2-3.612500-19228 2151
 6.209400+0 3.000000+0 1.654700-4 4.005100-2-1.079400-1 7.385900-29228 2151
 ...
```

In this case, the energy range being described is 1e-5 to 4.0 eV (other ranges are also given for higher energies up to 2.25 keV). The target spin is 3.5, and the scattering length of .98596 translates to a potential scattering cross section of 12.216 barns. The columns give resonance energy, J value, Γ_N, Γ_{gamma}, Γ_{FA}, and Γ_{FB}. The existence of two fission widths is part of the explanation for the great fidelity the the Reich-Moore fit to the experimental data for U-235. There is only one l value, l=0, for this case.

NEXT INDEX

Other Resonance Representations

Adler-Adler

The Adler-Adler representation can represent multi-channel effects, for example, the two fission channels found in even-odd fissile isotopes. It can also be Doppler broadened analytically. So far, it has only been used for one material, namely, U-233 in ENDF/B-VI. The Adler-Adler approach will probabably be entirely supplanted by the Reich-Moore representation.

Hybrid R-Function

This approach combines an R-function representation to give a full multi-level representation of elastic scattering with single-level Breit-Wigner resonance shapes in the other channels. This works well when the other channels are not strongly interacting, and it has the advantage of being able to treat charged-particle channels correctly. The hybrid approach has been used once in ENDF/B-VI.

Generalized R-Matrix

The Generalized R-Matrix approach is the ultimate representation. It can handle the full range of complexities in resonance cross sections for both light and heavy isotopes, including multi-level and multi-channel effects and charged-particle channels. However, this generality makes it very complex. There are currently no evaluations in this format, and no processing code can handle it. But the pressure is mounting to activate this generalized approach in the near future.

NEXT INDEX

Unresolved Resonances

At higher energies in the heavier isotopes, the resonances get so close together that they can no longer be resolved into separate lines. However, the fluctuations in the cross section in this energy range do lead to important effects, such as self shielding, in some applications (for example, fast breeder reactors). In ENDF-format evaluations, this "unresolved range" is handled by giving average values for the resonance spacing and the various partial widths, together with probability distributions for the spacing and partial widths. These unresolved resonance parameters are used three ways in practice:

- **Infinitely-dilute cross sections:** the cross sections that would be measured for a thin sample (which are equivalent to the cross sections that would act in a very dilute mixture) can be calculated using direct integrals over the probability distributions. These calculations are made with codes like RECENT and the RECONR module of NJOY.

- **Self-shielded effective cross sections:** effective cross sections for thicker targets or less dilute mixtures show self-shielding effects that can be computed *vs* temperature and background cross section. These calculations are made with the UNRESR module of NJOY.

- **Probability tables:** probability tables for the total cross section and the dependent elastic, fission, and capture cross sections can be used to sample for cross sections in continueous-energy Monte Carlo codes like MCNP. The probability table can be generated using the PURR module of NJOY.

NEXT INDEX

Formal Specifications for File 2

The following is based on ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6.

Resonance parameters for resolved and unresolved resonance ranges are given in File 2. It has only one section, with the reaction type number MT=151. 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. 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. 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 resonance range, the average effects of missed resonances, or competing cross sections. These backgrounds are to be added to the contributions computed from File 2. In the unresolved range, the File 3 section may optionally contain an "infinitely dilute" cross section. Self shielding factors are to be computed from File 2 and multiplied against the values in File 3. There must be double energy points corresponding to each resonance range boundary (except 1e-5 eV).

General Format for File 2

The following quantities are defined:

ZA,AWR
: standard material charge and mass parameters

NIS
: number of isotopes in the material (up to 10).

ZAI
: 1000*Z+A designation for an 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 (0=no, 1=yes).

NER
: number of resonance energy ranges for this isotope.

EL
: lower energy limit for an energy range.

EH
: upper energy limit for an energy range.

LRU
: flag indicating whether this enrgy range contains resolved or unresolved resonance parameters:
  - LRU=0, only the scattering radius is given (for information) and no resonance contributions are calculated for File 3.
  - 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 depend on the value of LRU):

- If LRU=1 (resolved parameters), then
  - LRF=1, single-level Breit-Wigner (SLBW);
  - LRF=2, multi-level Breit-Wigner (MLBW);
  - LRF=3, Reich-Moore (RM);
  - LRF=3, Adler-Adler (AA);
  - LRF=4, General R-matrix (GRM);
  - LRF=4, Hybrid R-function (HRF);
- If LRU=2 (unresolved parameters), then
  - LRF=1, only average fission widths are energy dependent;
  - LRF=2, all parameters are energy dependent.

NRO

flag designating possible energy dependence of the scattering radius (0=no, 1=yes).

NAPS

flag controlling the use of the two radii, the channel radius a and the scattering radius AP.

- If NRO=0 (AP energy independent), then
  - NAPS=0: calculate a from AWRI and read AP. Use a in the penetrabilities and shift factors, but use AP in the hard-sphere phase shifts.
  - NAPS=1: read AP and use it in the penetrabilities, shift factors, and phase shifts.
- If NRO=1 (AP energy dependent), then
  - NAPS=0: calculate a from AWRI and read AP(E). Use a in the penetrabilities and shift factors, but use AP(E) in the hard-sphere phase shifts.
  - NAPS=1: read AP(E) and use it in the penetrabilities, shift factors, and phase shifts.
  - NAPS=2: read AP(E) and use it in the phase shifts. In addition, read the constant AP from the range card and use it for penetrabilities and shift factors.

The structure of a section for the special case, in which just a scattering radius is specified (no resolved or unresolved resonance 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, 1, 0] HEAD
[MAT, 2, 151/ ZA, 1., 0, 0, 1, 0] CONT
[MAT, 2, 151/ EL, EH, 0, 0, 0, 0] CONT
[MAT, 2, 151/ SPI, AP, 0, 0, 0, 0] CONT
[MAT, 2, 0/ 0., 0., 0, 0, 0, 0] SEND
```

If resonance parameters are given, the structure of a section is

```
[MAT, 2, 151/ ZA, AWR, 0, 0, NIS, 0] HEAD
[MAT, 2, 151/ ZAI, ABN, 0, LFW, NER, 0] CONT
[MAT, 2, 151/ EL, EH, LRU, LRF, NRO, NAPS] CONT
   subsection for the first energy range
   of the first isotope
[MAT, 2, 151/ EL, EH, LRU, LRF, NRO, NAPS] CONT
   subsection for the second energy range
   of the first isotope
 ...
[MAT, 2, 151/ ZAI, ABN, 0, LFW, NER, 0] CONT
```

```
[MAT, 2, 151/ EL, EH, LRU, LRF, NRO, NAPS] CONT
   subsection for the first energy range
   of the second isotope
 ...
[MAT, 2, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

If NRO is not equal to zero, at TAB1 record giving AP(E) is inserted just after the energy range card.

More information on the formats and methods used for the various resonance representations will be found on the following pages:

- Single-Level Breit-Wigner
- Multi-Level Breit-Wigner
- Reich-Moore
- Adler-Adler
- Hybrid R-Function
- Generalized R-Matrix

NEXT INDEX

SLBW Resonance Format

The single-level Breit-Wigner equations can be written in the following form (which is the form used in NJOY, not the form from ENDF-102):

$$\begin{aligned}
\sigma_n &= \sigma_p \\
&\quad + \sum_\ell \sum_r \sigma_{mr} \left\{ \left[\cos 2\phi_\ell - (1 - \frac{\Gamma_{nr}}{\Gamma_r}) \right] \psi(\theta, x) \right. \\
&\quad \left. + \sin 2\phi_\ell \chi(\theta, x) \right\} , \\
\sigma_f &= \sum_\ell \sum_r \sigma_{mr} \frac{\Gamma_{fr}}{\Gamma_r} \psi(\theta, x) , \\
\sigma_\gamma &= \sum_\ell \sum_r \sigma_{mr} \frac{\Gamma_{\gamma r}}{\Gamma_r} \psi(\theta, x) , \\
\sigma_p &= \sum_\ell \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \theta_\ell ,
\end{aligned}$$

where

$$\sigma_{mr} = \frac{4\pi}{k^2} g_J \frac{\Gamma_{nr}}{\Gamma_r} ,$$

$$g_J = \frac{2J + 1}{4I + 2} ,$$

$$k = (2.196771 \times 10^{-3}) \frac{A}{A + 1} \sqrt{E} .$$

The resonance energies, J values, total widths, and partial widths are all given in the ENDF file; see ER, AJ, GT, GN, GG, and GF below. The actual resonance energy is different from the nominal E_r value due to the "shift factors" S. The actual neutron width is different from GN due to the "penetrabilities" P. These two quantities are shown in the following:

$$\Gamma_{nr}(E) = \frac{P_\ell(E)\Gamma_{nr}}{P_\ell(|E_r|)} .$$

$$\begin{aligned}
P_0 &= \rho . \\
P_1 &= \frac{\rho^3}{1+\rho^2} . \\
P_2 &= \frac{\rho^5}{9+3\rho^2+\rho^4} . \\
P_3 &= \frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6} . \\
P_4 &= \frac{\rho^9}{11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8} .
\end{aligned}$$

$$E_r' = E_r + \frac{S_\ell(|E_r|) - S_\ell(E)}{2(P_\ell(|E_r|)} \Gamma_{nr}(|E_r|) .$$

$$\begin{aligned}
S_0 &= 0 . \\
S_1 &= -\frac{1}{1+\rho^2} . \\
S_2 &= -\frac{18+3\rho^2}{9+3\rho^2+\rho^4} . \\
S_3 &= -\frac{675+90\rho^2+6\rho^4}{225+45\rho^2+6\rho^4+\rho^6} . \\
S_4 &= -\frac{44100+4725\rho^2+270\rho^4+10\rho^6}{11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8} .
\end{aligned}$$

The phase shifts in the SLBW formulas are given by

$$\begin{aligned}
\phi_0 &= \hat{\rho} . \\
\phi_1 &= \hat{\rho} - \tan^{-1}\hat{\rho} . \\
\phi_2 &= \hat{\rho} - \tan^{-1}\frac{3\hat{\rho}}{3-\hat{\rho}^2} . \\
\phi_3 &= \hat{\rho} - \tan^{-1}\frac{15\hat{\rho}-\hat{\rho}^2}{15-6\hat{\rho}^2} . \\
\phi_4 &= \hat{\rho} - \tan^{-1}\frac{105\hat{\rho}-10\hat{\rho}^3}{105-45\hat{\rho}^2+\hat{\rho}^4} .
\end{aligned}$$

These quantities depend on *rho=k*a* and *rho-hat=k*a-hat*. There are several options for choosing the two characteristic lengths *a* and *a-hat*. The most common is to use AP from the file for the "scattering radius" *a-hat* and to compute the "channel radius" *a* based on the nuclear size, $0.123*\mathrm{AWRI}^{1/3}+0.08$. Other options allow for using the scattering radius for *a* or for having an energy-dependent scattering radius.

At zero temperature, the resonance shapes in the SLBW formulas are given by

$$\psi = \frac{1}{1+x^2},$$
$$\chi = \frac{x}{1+x^2},$$
$$x = \frac{2(E-E_r')}{\Gamma_r}.$$

but for higher temperatures, we can use

$$\theta = \frac{\Gamma_r}{\sqrt{\frac{4kTE}{A}}},$$

$$\psi = \frac{\sqrt{\pi}}{2}\theta\,\mathrm{Re}W\left(\frac{\theta x}{2},\frac{\theta}{2}\right),$$

$$\chi = \frac{\sqrt{\pi}}{2}\theta\,\mathrm{Im}W\left(\frac{\theta x}{2},\frac{\theta}{2}\right),$$

$$W(x,y) = e^{-z^2}\,\mathrm{erfc}(-iz) = \frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{z-t}\,dt.$$

This is a very fast way to generate Doppler-broadened cross sections from SLBW resonances, but the use of the BROADR module of NJOY is more general, and the psi-chi option of RECONR is rarely used.

The following quantities are defined for SLBW subsections:

SPI
spin *I* of the target nucleus.

AP
scattering radius in units of 10^{-12} cm.

NLS
number of l values (neutron orbital angular momentum) in this energy region. A set of resonances is given for each l.

AWRI
ratio of the mass of a praticular 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. Could be used for competition with discrete inelastic scattering, but this is not implemented in NJOY. QX will be zero unless LRX is nonzero.

L

value of l.

LRX

flag indicating whether this energy range contains a competitive width. Currently not implemented in NJOY.

NRS

number of resolved resonances for the current l value. (NRS<=600)

ER

resonance energy (in the laboratory system).

AJ

floating-point value for J (the total angular momentum of the resonance).

GT

resonance total width evaluated at the resonance energy ER.

GN

neutron width evaluated at the resonance energy ER.

GG

radiation width, a constant.

GF

fission width, a constant.

The structure of a subsection of SLBW data follows:

```
[MAT,2,151/0.,0.,0,0,NR,NP/Eint/AP(E)] TAB1  if NRO is not zero
[MAT,2,151/SPI,AP,0,0,NLS,0] CONT
[MAT,2,151/AWRI,QX,L,LRX,6*NRS,NRS/
           ER_1,AJ_1,GT_1,GN_1,GG_1,GF_1,
           ER_2,AJ_2,GT_2,GN_2,GG_2,GF_2,
             ... for NRS resonances ...    ] LIST
   ... repeat LIST for NLS l values ...
```

NEXT INDEX

Particle Distributions in Energy and Angle

In order to follow the transport of nuclear radiation through a material, it is important to know which secondary products are produced, the yield of each product, and how each product is distributed in energy and angle. The capabilities of the ENDF-format to represent this information about the products has evolved from fairly simple representations using Files 4 and 5 to the current rather complete capabilities found in File 6. In general, the cross section (in barns/steradian) for producing a particle can be written

$$\sigma(\mu,E,E') = \sigma(E)\, y_i(E)\, f_i(\mu,E,E') / 2\pi$$
$$\int dE' \int d\mu\, f_i(\mu,E,E') = 1$$

in terms of a cross section $\sigma(E)$, a yield $y(E)$, and a normalized distribution in initial energy E, final energy E', and cosine μ.

The cross section is always given in File 3.

The yield may be implicit as determined by the MT number, or in File 6, it may be given explicitly as integers for simple reactions or in noninteger form for the complex summation reaction MT=5.

The distributions may be represented using three different approaches:

- For simple two-body reactions, E' can always be computed from kinematics, and it is only necessary to give $f(E,\mu)$. The function is given using File 4 or a special "law" in File 6. This option is used for elastic scattering (MT=2), neutron discrete-levels (MT=51-90), or neutron and particle discrete reactions (MT=50-90, 600-648, 650-698, etc.).

- For older evaluations (incident neutrons), it is often assumed that the secondary-neutron distribution can be represented as a product of an angular distribution and an energy distribution, *i.e.*, $f(E,\mu)*g(E,E')$. The angular distribution is given in File 4 and the secondary-energy distribution is given in File 5. This approach is often used for MT=16, 18, or 91.

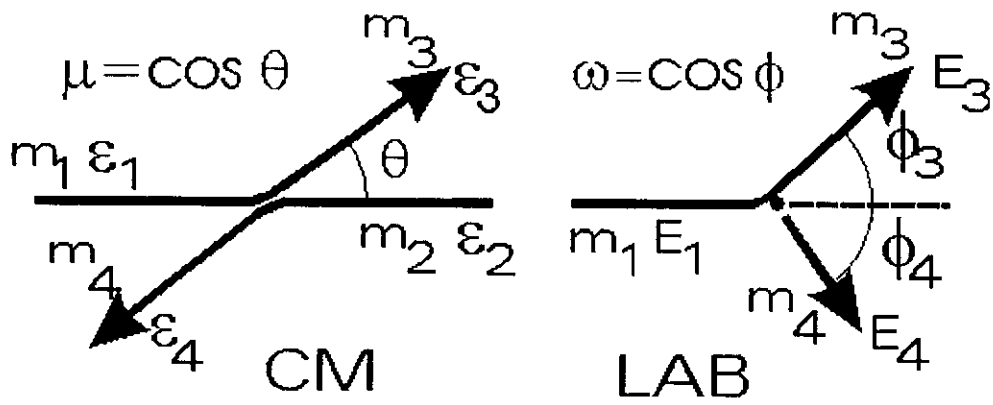
- For newer evaluations, the distributions are often given as fully coupled energy-angle distributions in File 6 using one of the several "laws" offered there. The use of File 6 is required for incident charged particles.

The File 5 representation is always used for fission in ENDF files. The neutrons are assumed to be emitted isotropically in the laboratory reference frame.

NEXT INDEX

Two-Body Reactions

Two-body reactions, such as elastic scattering, neutron inelastic scattering to a level, or (p,n) to a discrete level, obey simple kinematical formulas that couple the outgoing energy E', the incident energy E, and the scattering cosine μ. The parameters for two-body collisions are shown below in both center-of-mass and laboratory reference frames:



The non-relativistic kinematical formulas can now be written as follows:

$$A = \frac{m_2}{m_1}$$

$$A' = \frac{m_3}{m_1}$$

$$\beta = \sqrt{\frac{A(A+1-A')}{A'}\left[1+\frac{1+A}{A}\frac{Q}{E_1}\right]}$$

$$\gamma = \frac{A'}{A+1-A'}\beta$$

$$\frac{\varepsilon_3}{\varepsilon_1} = \frac{A'}{A^2}\beta^2$$

$$\varepsilon_1 = \left(\frac{A}{A+1}\right)^2 E_1$$

$$\mu_3 = \mu$$

$$\frac{\varepsilon_4}{\varepsilon_1} = \frac{A'}{A+1-A'}\frac{\varepsilon_3}{\varepsilon_1}$$

$$\mu_4 = \mu$$

$$\frac{E_3}{E_1} = \frac{A'}{(1+A)^2}(\beta^2 + 1 + 2\beta\mu)$$

$$\omega_3 = \frac{1+\beta\mu}{\sqrt{\beta^2+1+2\beta\mu}}$$

$$\frac{E_4}{E_1} = \frac{A+1-A'}{(1+A)^2}(\gamma^2 + 1 - 2\gamma\mu)$$

$$\omega_4 = \frac{1-\gamma\mu}{\sqrt{\gamma^2+1-2\gamma\mu}}$$

If the incident and scattered particles are the same, $A'=1$, and these formulas reduce to the more familiar set often given for neutron scattering. The elastic reaction corresponds to $A'=1$ and $Q=0$.

Note that the energy-angle distribution of the emitted particle and the full energy-angle distribution of the recoil nucleus are completely determined by A, A', Q, and the angular distribution $f(E,\mu)$.

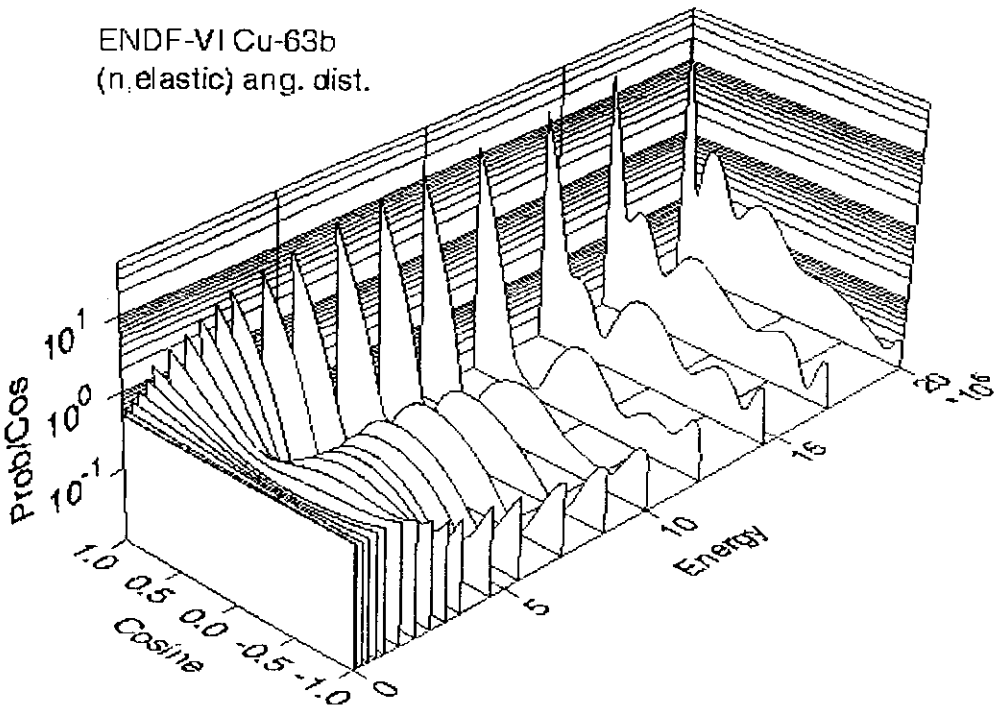
NEXT INDEX

Angular Distributions

The angular distributions for two-body scattering reactions are given in either File 4 or a special "law" of File 6. The most common way of representing them uses Legendre coefficients:

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

At low energies for elastic scattering, the angular distribution will be isotropic in the center of mass reference frame. As the energy increases, the scattering typically becomes more and more forward peaked, and higher and higher Legendre orders will be needed. If the energy goes through a resonance, dramatic swings from forward scattering to backward scattering may be seen. The following figure is typical:



At the highest energies, the scattering is basically the diffraction of a wave around a hard sphere, and the results are similar to diffraction patterns for light. The forward peak is like the bright central spot in a diffraction pattern, and the oscillations at larger angles are analogous to the fringes seen for light.

The following is an example of a section of File 4 for elastic scattering (^{63}Cu from ENDF/B-VI). The "1" in the fourth position of the first card indicates that the data are in the center-of-mass system. Cards 5 and 6 indicate that the scattering is isotropic at 1e-5 eV (the P_1 coefficient is zero). Cards 9 and 10 show anisotropy beginning to show up at 10 keV. The anisotropy gradually increases with energy until a Legendre order of 14 is needed to represent the angular distribution at 20 MeV.

```
2.906300+4 6.238900+1          0          1          0          02925 4  2
0.000000+0 6.238900+1          0          2          0          02925 4  2
0.000000+0 0.000000+0          0          0          1          222925 4  2
        22          2                                            2925 4  2
0.000000+0 1.000000-5          0          0          1          02925 4  2
0.000000+0                                                       2925 4  2
0.000000+0 2.530000-2          0          0          1          02925 4  2
0.000000+0                                                       2925 4  2
0.000000+0 1.000000+4          0          0          2          02925 4  2
3.214700-3 1.190800-4                                            2925 4  2
0.000000+0 1.000000+5          0          0          4          02925 4  2
3.619500-2 3.845600-3 3.661300-5 0.000000+0                      2925 4  2
0.000000+0 3.000000+5          0          0          4          02925 4  2
7.500000-2 1.800000-2 4.000000-4 0.000000+0                      2925 4  2
0.000000+0 5.000000+5          0          0          4          02925 4  2
1.200000-1 5.500000-2 2.550000-3 1.200000-4                      2925 4  2
0.000000+0 7.500000+5          0          0          4          02925 4  2
1.730000-1 1.070000-1 1.300000-2 2.730000-3                      2925 4  2
0.000000+0 1.000000+6          0          0          6          02925 4  2
2.258400-1 1.602700-1 3.980500-2 1.286300-2 1.560800-5 0.000000+02925 4  2
0.000000+0 1.500000+6          0          0          6          02925 4  2
2.738500-1 2.188700-1 9.602200-2 3.370000-2 1.499300-4 0.000000+02925 4  2
...
0.000000+0 2.000000+7          0          0         14          02925 4  2
8.105400-1 6.500300-1 5.507300-1 4.828500-1 4.177800-1 3.523300-12925 4  2
2.899200-1 2.378900-1 1.840200-1 1.207600-1 6.096100-2 2.102800-22925 4  2
4.210300-3 0.000000+0                                            2925 4  2
                                                                 2925 4  0
```

NEXT INDEX

Formal Specifications for File 4

The following is based on ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6.

File 4 is used to describe the angular distribution of emitted particles. It is used for reactions with incident neutrons only; see File 6 for for other projectiles. Angular distributions should be given for elastically scattered neutrons and for the neutrons resulting from discrete level excitation due to inelastic scattering. File 4 can also be given for particles resulting from (n,n'continuum), (n,2n), and other continuum reactions, but in these cases only the integral over all final energies is provided. There is normally coupling between the secondary energy and angle in these cases, and File 6 is preferred. 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).

In some cases, it may be possible to compute the angular distributions in the resolved range from resonance parameters. In such cases, the computed distributions may be preferable to the distributions from File 4, which will be a smoothed average when the resonances are close together.

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 can be expressed as normalized probability distributions or as Legendre expansions of the probability distributions:

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

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

where $f(\mu,E)d\mu$ is the probability that a particles 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)$^{-1}$. In addition,

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 from File 3 for this MT,

l
: order of the Legendre polynomial,

$\sigma(\mu,E)$
: differential scattering cross section in units of barns per steradian, and

a_l
: the lth Legendre polynomial coefficient, and it is understood that a_0=1.0 (only l values of 1, 2, ..., NL are given).

The angular distributions may be given in either the center-of-mass (CM) or laboratory (LAB) system.

Formats

File 4 is divided into sections, each containing data for a particular reaction type (MT number), and ordered by increasing MT number. Each section always starts with a HEAD record and ends with a SEND record. The following quantities are defined:

ZA,AWR
: standard material charge and mass parameters

LTT
: flag to specify the representation used:
  - LTT=0, all angular distributions are isotropic,
  - LTT=1, the data are given as Legendre expansion coefficents, a_l, or
  - LTT=2, the data are given as tabulated normalized probability distributions, $f(\mu,E)$.

LI
: flag to specify whether all the angular distributions are isotropic:
  - LI=0, not all isotropic, or
  - LI=1, all isotropic.

LCT
: flag to specify the frame of reference used:
  - LCT=1, the data are given in the LAB system, or
  - LCT=2, the data are given in the CM system.

LVT
: an obsolete flag, now always zero.

NE
: number of incident energy points at which angular distributions are given (up to 1200).

NL
: higher order Legendre polynomial coefficient that is given at each energy (up to 64).

NK
: obsolete parameter. Now always zero.

NM
: maximum order Legendre polynomial that will be required to describe the angular distributions of elastic scattering in either the center-of-mass or the laboratory system. NM should be an even number.

NP
: number of angular points (cosines) used to give the tabulated probability distributions for each energy.

The structure of a section depends on the values of LTT.

Legendre Polynomial Coefficients

```
[MAT, 4, MT/ ZA, AWR, LVT, LTT, 0, 0] HEAD   LVT=0, LTT=1
[MAT, 4, MT/ 0., AWR, LI, LCT, 0, 0] CONT   LI=0
[MAT, 4, MT/ 0., 0., 0, 0, NR, NE/ Eint] TAB2
[MAT, 4, MT/ 0., 0., 0, 0, NL, 0/ a_1(E_1)] LIST
[MAT, 4, MT/ 0., 0., 0, 0, NL, 0/ a_2(E_2)] LIST
 ...
[MAT, 4, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

Tabulated Probability Distributions

```
[MAT, 4, MT/ ZA, AWR, LVT, LTT, 0, 0] HEAD   LVT=0, LTT=2
[MAT, 4, MT/ 0., AWR, LI, LCT, 0, 0] CONT   LI=0
[MAT, 4, MT/ 0., 0., 0, 0, NR, NE/ Eint] TAB2
[MAT, 4, MT/ 0., 0., 0, 0, NR, NP/ muint/ f(mu,E_1)] TAB1
[MAT, 4, MT/ 0., 0., 0, 0, NR, NP/ muint/ f(mu,E_1)] TAB1
 ...
[MAT, 4, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

All Angular Distributions are Isotropic

```
[MAT, 4, MT/ ZA, AWR, LVT, LTT, 0, 0] HEAD   LVT=0, LTT=0
[MAT, 4, MT/ 0., AWR, LI, LCT, 0, 0] CONT   LI=1
[MAT, 4, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

Procedures

The angular distributions for two-body reactions should be given in the CM system (LCT=2). It is recommended that other reactions (such as continuum inelastic, fission, etc.) should be given in the LAB system.

For Legendre polynomial expansions, a linear-linear interpolation scheme (INT=2) should be used for the incident energy.

For tabulated distributions, the cosine interval should span the entire range -1 to +1. The interpolation scheme for incident energy E should be linear-linear (INT=2) and the interpolation scheme for the cosine should be log-linear (INT=4).

NEXT INDEX

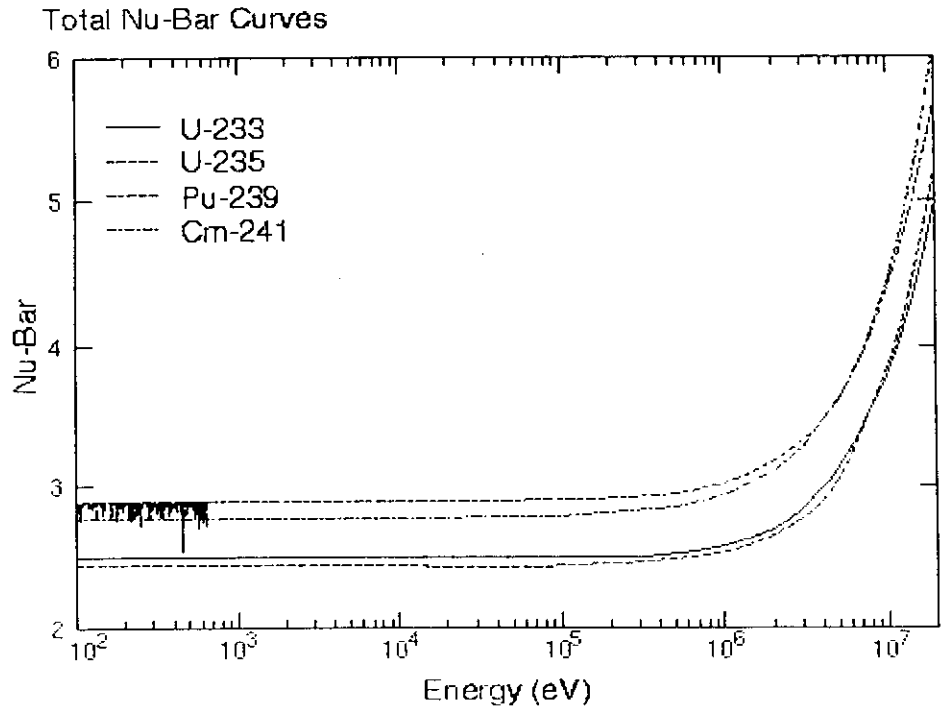
Fission Neutron Yields

The number of neutrons produced in a fission reaction is highly important for fission reactors, explosive fission devices, and the safe storage and processing of fissionable materials. It is an energy-dependent quantity, and it has both prompt and delayed components. Fission neutron yields, or "nu-bar's," are given in three special sections of File 1:

- MT=452, total neutrons per fission,
- MT=456, prompt neutrons per fission, and
- MT=455, delayed neutrons per fission and time constants.

Upon fission, the excited nucleus formed by the target and the projectile breaks up into two roughly equal "fission fragments" and a number of additional neutrons (1, 2, 3, 4, ...). It is the average over all these possible break-up modes that gives the "prompt" nu-bar (*e.g.*, 2.5). Some of the excited fission fragments emit additional neutrons as they decay over the next second or so; these are called "delayed neutrons."

Prompt nu-bar tends to be constant at low energies, and then it gradually increases as the energy increases. In earlier times, this increasing trend was often represented as a simple polynomial (approximately linear) in energy *E*. More detailed analysis shows more structure associated with second- and third-chance fission processes. Some evaluations even have structure at very low energies. Therefore, most modern evaluations use a detailed tabulated function to represent the energy dependence of the fission nu-bar. The following figure shows a few examples:



The following example is U-233 from ENDF/V-VI. The "2" in the fourth field on the first line says that the nu-bar data are given in tabulated form. The actual tabulation of total nu-bar *vs* energy starts on line 4.

```
9.223300+4 2.310430+2          0          2          0          09222 1452
0.000000+0 0.000000+0          0          0          1         109222 1452
        10          2                                           9222 1452
1.000000-5 2.494700+0 2.530000-2 2.494700+0 3.200000+5 2.494000+09222 1452
2.000000+6 2.687400+0 4.500000+6 3.052000+0 6.000000+6 3.268000+09222 1452
6.500000+6 3.340900+0 1.400000+7 4.270400+0 1.500000+7 4.393800+09222 1452
2.000000+7 5.013500+0                                          9222 1452
                                                               9222 1  0
```

The formats for prompt nu-bar and total nu-bar are the same. The format for delayed nu-bar has an additional LIST record giving the decay constants that are used to describe the time history of delayed neutron emission. This will be discussed later.

NEXT INDEX

Formal Specifications for File 1 Fission Nu-bars

The following is based on ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6.

This page describes MT=452, 456, and 455 from File 1.

Number of Neutrons per Fission, nu-bar (MT=452)

If the material fissions, then a section specifying the average *total* number of neutrons per fission, nu-bar (MT=452), must be given. This format applies to both particle-induced and spontaneous fission, each in its designated sublibrary. Values of nu-bar may be tabulated a function of energy or represented by coefficients provided for the following polynomial expansion of nu-bar*(E)*:

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

where

nu-bar(E)
: the average total (prompt plus delayed) number of neutrons per fission produced by neutrons of incident energy E (eV),

C_n
: the n^{th} 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.

Formats

The structure of this section depends on whether the data are given in tabulated form or as a polynomial expansion. The following quantities are defined:

ZA,AWR
: standard material charge and mass parameters

LNU
: flag to specify the representation used:
  - LNU=1, polynomial representation has been used, or
  - LNU=2, tabulated representation.

NC
: count of the number of terms used in the polynomial expansion. Up to 4.

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

NR
: [illegible]

number of interpolation ranges used to tabulate values of nu-bar(*E*).

NP

total number of energy points used to tabulate nu-bar>*(E)*.

nu-bar*(E)*

average total number of neutrons per fission.

If LNU=1, the structure of a section is

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

If LNU=2, the structure of the section is

```
[MAT, 1, 452/ ZA, AWR, 0, LNU, 0, 0] HEAD   LNU=2
[MAT, 1, 452/ 0., 0., 0, 0, NR, NP/ Eint/ nu-bar(E)] TAB1
[MAT, 1, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

For spontaneous fission, the polynomial representation (LNU=1) is used with NC=1. There is no energy dependence.

The polynomial form for particle-induced nu-bar is only used when neither prompt nor delayed nu-bar values are given.

Delayed Neutron Data, nu-bar-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, nu-bar-d, is given, along with the decay constants $lambda_i$ for each precursor family. The fraction of delayed neutrons generated for each family is given in MT=455 of File 5. The energy distribution 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), just as for MT=452. For spontaneous fission, the polynomial representation (LNU=1) is used with NC=1, just as for MT=452.

Formats

The following quantities are defined:

ZA,AWR

standard material charge and mass parameters

LNU

flag to specify the representation used:

- LNU=1, polynomial representation has been used, or
- LNU=2, tabulated representation.

NC

count of the number of terms used in the polynomial expansion. If used, it is 1.

NR

number of interpolation ranges used to tabulate values of nu-bar-d*(E)*.

NP

total number of energy points used to tabulate nu-bar-d>*(E)*.

nu-bar-d*(E)*

average total number of delayed neutrons per fission.

NNF

number of precursor families considered.

***lambda*$_i$**

decay constant (sec^{-1}) for the i^{th} precursor.

The structure when values of nu-bar-d are tabulated (LNU=2) is:

```
[MAT, 1, 455/ ZA, AWR, 0, LNU, 0, 0] HEAD   LNU=2
[MAT, 1, 455/ 0., 0., 0, 0, NNF, 0/ lambda1, lambda2, ...] LIST
[MAT, 1, 455/ 0., 0., 0, 0, NR, NP/ Eint/ nu-bar-d(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, 455/ ZA, AWR, 0, LNU, 0, 0] HEAD   LNU=1
[MAT, 1, 455/ 0., 0., 0, 0, NNF, 0/ lambda1, lambda2, ...] LIST
[MAT, 1, 455/ 0., 0., 0, 0, NC, 0/ nu-bar-d] TAB1  NC=1
[MAT, 1, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

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

Number of Prompt Neutrons per Fission, nu-bar-p (MT=456)

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

The following quantities are defined:

ZA,AWR

standard material charge and mass parameters

LNU

flag to specify the representation used:

- LNU=1, polynomial representation has been used, or
- LNU=2, tabulated representation.

NC

count of the number of terms used in the polynomial expansion. If used, it is 1.

NR

number of interpolation ranges used to tabulate values of nu-bar*(E)*.

NP

total number of energy points used to tabulate nu-bar-p>*(E)*.

nu-bar-p*(E)*

average number of prompt neutrons per fission.

If LNU=2, 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, NR, NP/ Eint/ nu-bar-p(E)] TAB1
[MAT, 1, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

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

```
[MAT, 1, 456/ ZA, AWR, 0, LNU, 0, 0] HEAD   LNU=1
```

```
[MAT, 1, 456/ 0., 0., 0, 0, NC, 0/ nu-bar-p] LIST  NC=1
[MAT, 1, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

For spontaneous fission, the polynomial representation (LNU=1) is used with NC=1. There is no energy dependence.

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

NEXT INDEX

Simple Emission Spectra

In many ENDF-format evaluations, the spectra of neutrons emitted in a reaction are given as independent of angle using File 5. This is reasonable in some cases, but at higher neutron energies there is often a strong correlation between the energy distribution and the angle of emission. Correlated energy distributions can be described using File 6.

File 5 allows for several different representations of the spectra of outgoing neutrons:

LF=1, Arbitrary tabulation function: A set of incident energies is given, and a normalized tabulated distribution is given at each incident energy. This option is very general, and it is the modern choice for detailed fission spectra, such as those produced with the Los Alamos Standard Model.

LF=5, General evaporation spectrum: Here a temperature-like quantity θ is tabulated against incident energy E, and a single spectrum is given as a function of E'/θ. The only current application for this law is to give six different delayed-neutron spectra for six time groups, and θ is just set to one. See MF=5, MT=455 in fissionable materials.

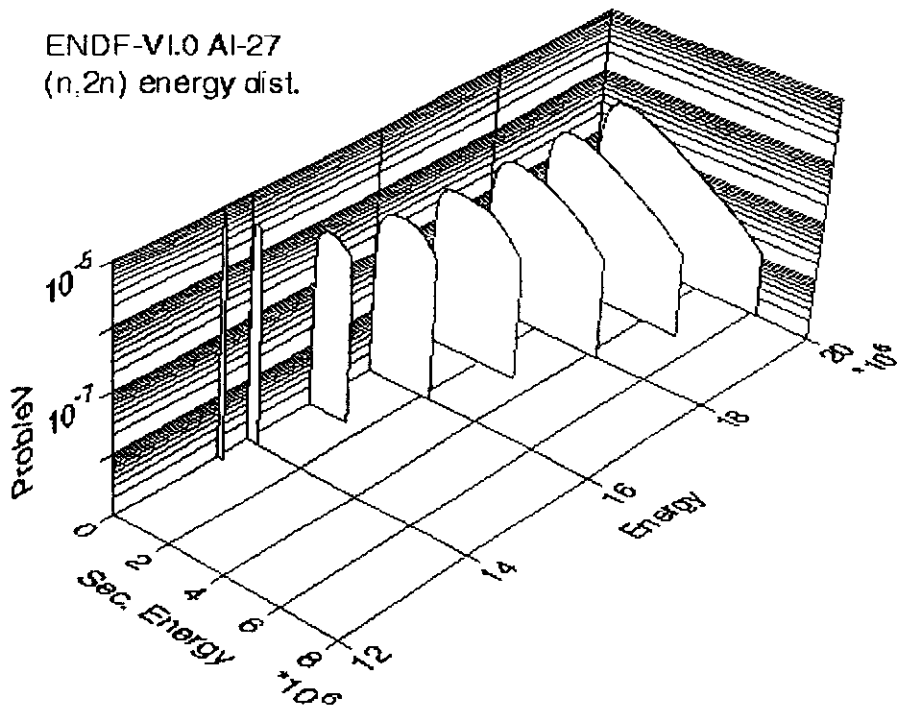
LF=7, Simple Maxwellian fission spectrum: This is a fairly old model for the distribution of neutrons emitted by fission, but it is still in fairly wide use. The effective temperature θ is tabulated against the incident energy E, and the range of final energies allowed is from zero to E-U.

LF=9, Evaporation spectrum: This is the kind of shape that would be expected if the the compound nucleus during a reaction had lots of time to come into equilibrium before the neutron was emitted, and it may not be a bad approximation for fairly low incident energies (a few MeV). At higher energies, preequilibrium emission begins to change the shape away from the evaporation form, but this is also the region where energy-angle correlation begins to be important. Once again, the effective temperature of the compound system θ is tabulated against the incident energy E, and the range of final energies allowed is from zero to E-U.

LF=11, Energy-dependent Watt spectrum: The Watt spectrum is a more sophisticated representation of fission than the simple Maxwellian law described above. Two functions $a(E)$ and $b(E)$ are tabulated in File 5, and the range of final energies allowed is from zero to E-U.

LF=12, Madland-Nix fission spectrum: This is another sophisticated fission model based on two constants EFL and EFM, the average kinetic energies of the light and heavy fragments, respectively, and a temperature-like quantity TM that is given as a function of incident energy E.

The following is an example of a tabulated distribution (LF=1) from File 5 for the ^{27}Al(n,2n) reaction from ENDF/B-VI Release 0:


ENDF-VI.0 Al-27
(n,2n) energy dist.
Prob/eV
10^{-5}
10^{-7}
0
2
4
6
8
10
12
Sec. Energy
*10^6
14
16
18
20
Energy
*10^6

NEXT INDEX

Formal Specifications for File 5

The following is based on ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6.

File 5 is used to describe the energy distribution of a secondary particle expressed as normalized probability distributions. File 5 is used for incident neutron reactions and spontaneous fission only; reactions induced by charged particles will be represented in File 6. Energy distributions for two-body reactions, such as elastic scattering (MT=2), discrete inelastic levels (MT=51-90), or charged-particle levels (MT=600 series) can be computed directly from the angular distributions in File 4, and those reactions will not appear in File 5. Reactions with appreciable energy-angle correlation are best represented using File 6.

The representation provided by File 5, except possibly for fission, is inadequate for modern evaluations, and it is gradually being supplanted by File 6.

The distributions given in File 5 are normalized so that

$$\int p(E \rightarrow E')\, dE' = 1$$

and they can be broken down into partial energy distributions of the form

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

where the p_k are the fractional probabilities for each of the partial distributions f_k at energy E. The partial distributions can be represented using one of six different distribution laws, as described below.

Secondary Energy Distribution Laws

LF=1, Arbitrary tabulation function: A set of incident energies is given, and a normalized tabulated distribution $g(E,E')$ is given at each incident energy E.

LF=5, General evaporation spectrum: A temperature-like quantity θ is tabulated against incident energy E, and a single spectrum is tabulated as a function of $E'/\theta(E)$.

LF=7, Simple Maxwellian fission spectrum: The effective temperature θ is tabulated against the incident energy E, and the spectrum is given by

$$g(E,E') = \frac{\sqrt{E'}}{I}\exp\left(-\frac{E'}{\theta(E)}\right),$$
$$I = \theta^{3/2}\left[\sqrt{\frac{\pi}{4}}\,\mathrm{erf}(x) - xe^{-x}\right].$$
$$x = \frac{E-U}{\theta}.$$

The constant U is introduced to define the range of final energies allowed (zero to E-U).

LF=9, Evaporation spectrum: The effective temperature θ is tabulated against the incident energy E, and the spectrum of emitted particles is given by

$$g(E,E') = \frac{E'}{I}\exp\left(-\frac{E'}{\theta(E)}\right),$$
$$I = \theta^2\left[1 - e^{-x}(1+x)\right].$$
$$x = \frac{E-U}{\theta}.$$

The range of final energies allowed is from zero to E-U.

LF=11, Energy-dependent Watt spectrum: Two functions $a(E)$ and $b(E)$ are tabulated, and the spectrum is calculated using

$$g(E,E') = \frac{e^{-E'/a}}{I}\sinh\left(\sqrt{bE'}\right),$$
$$I = \frac{1}{2}\sqrt{\frac{\pi a^3 b}{4}}\,e^{x_0}\left[\mathrm{erf}\left(\sqrt{x}-\sqrt{x_0}\right) + \mathrm{erf}\left(\sqrt{x}+\sqrt{x_0}\right)\right] - ae^{-x}\sinh(ab,x).$$
$$x = \frac{E-U}{a}.$$
$$x_0 = \frac{ab}{4}.$$

The range of final energies allowed is from zero to E-U.

LF=12, Madland-Nix fission spectrum: Two constants EFL and EFH, the average kinetic energies of the light and heavy fragments, respectively, and a temperature-like quantity TM(E) are tabulated, and the spectrum is computed using

$$g(E,E') = \frac{1}{2}[G(E',E_{fl}) + G(E',E_{fh})] ,$$

$$G(E',E_f) = \frac{1}{3\sqrt{E_f T_m}}\left[u_2^{3/2}E_1(u_2) - u_1^{3/2}E_1(u_1) + \gamma(3/2,u_2) - \gamma(3/2,u_1)\right] ,$$

$$u_1 = (\sqrt{E'} - \sqrt{E_f})^2/T_m ,$$
$$u_2 = (\sqrt{E'} + \sqrt{E_f})^2/T_m ,$$

where E_1 and γ are the standard exponential integral and gamma functions.

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. A section may be divided up into several subsections, each containing the data for one partial energy distribution. The structure of a subsection depends on the value of LF. The following quantities are defined:

NK
: number of partial distributions.

U
: constant that defines the upper energy limit for the secondary particle; the energy can vary from 0 to *E-U*.

θ
: effective temperature used to parameterize the secondary energy distribution for LF=5, 7, or 9.

LF
: flag specifying the distribution law for this subsection.

$p_k(E)$
: fraction of the distribution that can be described by the partial distribution in this subsection.

$f_k(E)$
: partial distribution in this subsection.

a,b
: energy-dependent parameters used in the Watt spectrum,

EFL,EFH
: constant parameters used in the Madland-Nix spectrum,

TM
: energy-dependent parameter used in the Madland-Nix spectrum,

The structure of a section of File 5 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, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The structure of a subsection depends on the value of LF. The formats for the various values of LF are given below.

LF=1, Arbitrary tabulated function

```
[MAT, 5, MT/ ZA, AWR, 0, LF, NR, NP/ Eint/ p(E)] TAB1 LF=1
[MAT, 5, MT/ 0., 0., 0, 0, NR, NE/ Eint] TAB2
[MAT, 5, MT/ 0., 0., 0, 0, NR, NF/ E'int/ g(E1,E')] TAB1
[MAT, 5, MT/ 0., 0., 0, 0, NR, NF/ E'int/ g(E2,E')] TAB1
 ...continue for NE TAB1 records....
```

Note that the incident energy mesh for $p_k(E)$ doesn't have to the same as the E mesh used to specify the energy distributions. The interpolation scheme used between incident energy point E and secondary energy points E' should be linear-linear.

LF=5, General evaporation spectrum

```
[MAT, 5, MT/ U, 0.0, 0, LF, NR, NP/ Eint/ p(E)] TAB1 LF=5
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint/ theta(E)] TAB1
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NF/ xint/ g(x)] TAB1 x=E'/theta(E)
```

LF=7, Simple Maxwellian fission spectrum

```
[MAT, 5, MT/ U, 0.0, 0, LF, NR, NP/ Eint/ p(E)] TAB1 LF=7
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint/ theta(E)] TAB1
```

LF=9, Evaporation spectrum

```
[MAT, 5, MT/ U, 0.0, 0, LF, NR, NP/ Eint/ p(E)] TAB1 LF=9
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint/ theta(E)] TAB1
```

LF=11, Energy-dependent Watt spectrum

```
[MAT, 5, MT/ U, 0.0, 0, LF, NR, NP/ Eint/ p(E)] TAB1 LF=11
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint/ a(E)] TAB1
[MAT, 5, MT/ 0.0, 0.0, 0, 0, NR, NE/ Eint/ b(E)] TAB1
```

LF=12, Madland-Nix fission spectrum

```
[MAT, 5, MT/ U, 0.0, 0, LF, NR, NP/ Eint/ p(E)] TAB1 LF=12
[MAT, 5, MT/ EFL, EFH, 0, 0, NR, NE/ Eint/ TM(E)] TAB1
```

NEXT INDEX

Energy-Angle Distributions

The old-fashioned approach of representing an energy-angle distribution as a product of an angular distribution (MF=4) and a secondary energy distribution (MF=5) is no longer adequate for modern evaluations. For incident energies larger than a few MeV, preequilibrium effects begin to appear, which lead to a coupling between the emission angle and the emission energy. In addition, it is sometimes necessary to have detailed information about the emission of other particles than neutrons, for example, the protons from an (n,n'p) reaction. The combination of File 4 and File 5 only allows one particle to be represented. Most modern evaluations are made with the help of a nuclear model code, such as GNASH, to complete the ranges of energy and angle that are not available from experiment. These codes follow all reaction channels and emitted particles, and it is important to have a way to include all the code results into the ENDF format. It was these kinds of arguments that led to the development of File 6 as introduced for the ENDF-6 format.

A section of File 6 is divided into subsections, one for each product. The products can include neutrons and light charged particles ordered by ZA, followed by residual nuclei ordered by ZA, followed by photons, followed by electrons:

```
[MAT, 6, MT/ ZA, AWR, 0, LCT, NK, 0] HEAD
[MAT, 6, MT/ ZAP, AWP, LIP, LAW, NR, NP/ Eint/ Y(E)] TAB1
    law-dependent data for product 1
    ---------------------------------
    repeat TAB1 and law-dependent data
    for the rest of the NK products
    ---------------------------------
[MAT, 6, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The individual products are identified by ZAP, AWP, and LIP (to allow for isomers). The different representations allowed in a subsection are defined by the value of LAW:

- LAW=0, Unknown distribution.;
- LAW=1, Energy-angle distribution.;
- LAW=2, Two-body angular distribution.;
- LAW=3, Isotropic two-body distribution;
- LAW=4, Recoil distribution for a two-body reaction;
- LAW=5, Charged-particle elastic scattering;
- LAW=6, N-body phase-space distribution; and
- LAW=7, Laboratory angle-energy law.

NEXT INDEX

Kalbach Distributions

File 6 with LAW=1 provides for an especially elegant and compact representation of coupled energy-angle distributions for neutrons and charged particles developed by Kalbach based on systematics. The general shape of the function was later shown to come directly out of preequilibrium theory by Chadwick. The Kalbach distribution for a reaction of the form

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

can represented by

$$f(\mu_b, E_a, E_b) = f_0(E_a, E_b)\left\{\frac{a}{\sinh(a)}[\cosh(a\mu_b) + r\sinh(a\mu_b)]\right\}$$

where $r(E_a, E_b)$ is the precompound fraction as given by the evaluator, and $a(E_a, E_b)$ is a simple parameterized function that depends on emission energy, incident energy, and particle type.

Note that if r and a are small, the distributions are basically isotropic. This corresponds to emission from a well equilibrated compound system. As r increases, the distribution becomes more forward peaked. Because r tends to increase with the emission energy, we see forward peaking for high particle energies and isotropy for low particle energies. This is the effect that cannot be represented using the combination of File 4 and File 5.

The following is an example taken from the ENDF/B-VI evaluation for ^{27}Al. It shows the (n,2n) neutron emission distribution for an incident energy of 40 MeV. Each line contains two triplets: E', $f(E,E')$, and $r(E,E')$. Note the increase in r with increasing E'.

```
0.000000+0 4.000000+7          0          1        198         661325 6 16
0.000000+0 1.463653-8 2.774204-4 3.609812+4 2.663865-8 2.908748-41325 6 16
7.219623+4 3.562323-8 3.043292-4 1.203271+5 4.369308-8 3.222684-41325 6 16
1.684579+5 5.047795-8 3.402077-4 2.165887+5 5.644923-8 3.581469-41325 6 16
...
4.091120+6 5.029411-8 8.229791-3 4.572428+6 4.580329-8 1.160481-21325 6 16
5.053736+6 4.182685-8 1.619895-2 5.535044+6 3.824886-8 2.245802-21325 6 16
6.016353+6 3.515369-8 3.071985-2 6.497661+6 3.237198-8 4.158862-21325 6 16
6.978969+6 2.981761-8 5.597233-2 7.460277+6 2.765722-8 7.438953-21325 6 16
7.941585+6 2.592982-8 9.753015-2 8.422894+6 2.461467-8 1.260132-11325 6 16
8.904202+6 2.364081-8 1.603900-1 9.385510+6 2.298213-8 2.006077-11325 6 16
9.866818+6 2.272568-8 2.456513-1 1.034813+7 2.276480-8 2.963706-11325 6 16
1.082943+7 2.312538-8 3.510374-1 1.131074+7 2.376400-8 4.081861-11325 6 16
1.179205+7 2.465185-8 4.658113-1 1.227336+7 2.581909-8 5.226821-11325 6 16
1.275467+7 2.726533-8 5.776199-1 1.323598+7 2.899395-8 6.296106-11325 6 16
1.371728+7 3.098722-8 6.779314-1 1.419859+7 3.324436-8 7.218539-11325 6 16
1.467990+7 3.557207-8 7.621944-1 1.516121+7 3.833738-8 7.979111-11325 6 16
...
2.430606+7 1.964407-9 9.958412-1 2.478737+7 0.000000+0 0.000000+01325 6 16
```

The Kalbach representation is used in many of the Los Alamos evaluations in ENDF/B-VI, and it is an important factor in the new high-energy libraries to 150 MeV now being constructed for accelerator applications at several laboratories in the world.

NEXT INDEX

---

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

Formal Specifications for File 6

The following is based on ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6.

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 in normalized form as shown by the following equations:

$$\sigma(\mu,E,E') = \sigma(E)\, y_i(E)\, f_i(\mu,E,E') / 2\pi$$

$$\int dE' \int d\mu\, f_i(\mu,E,E') = 1$$

In these equations, 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)$^{-1}$.

This representation ignores most correlations between products and most sequential reactions; that is, the distributions given here are those that 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, or "LAWS", as shown in the following table:

LAW	Meaning
0	unknown distribution
1	continuum energy-angle distribution
2	two-body reaction angular distribution
3	isotropic two-body distribution
4	recoil distribution of a two-body reaction
5	charged-particle elastic scattering
6	n-body phase-space distribution
7	laboratory angle-energy law

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.

NK number of subsections in the 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).

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.

AWP
product mass in neutron units.

LIP product modifier flag.

LAW
distinguishes between different representations for the distribution function f_i: see table above.

NR,NP,EINT
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/ EINT/ Y_1(E)] TAB1
             [LAW-dependent structure for product 1]
             --------------------------
             repeat TAB1 and LAW-dependent structures
             for the rest of the NK subsections
             --------------------------
[MAT, 6, MT/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

File 6 should have a subsection for **every** product of the reaction or sum of reactions being described except for MT=3, 4, or 103-107 when they are bing 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 in the following pages:

NEXT INDEX

File 6 - 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.

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

File 6 - Continuum Energy-Angle Distributions

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 with 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 that selects the angular representation to be used:
LANG=1, Legendre coefficients are used;
LANG=2, Kalbach systematics is 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, histogram;
LEP=2, linear-linear, etc.

NR,NE,EINT
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=22-25 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 entries in the list of NEP energies are discrete, and the remaining NEP-ND entries are to be used with LEP to describe a continuous distribution. Discrete primary photons should be flagged with negative energies. ND can be zero, and it must be less than or equal to NEP.

NA
number of angular parameters:
use NA=0 for isotropic distributions (note that all options are identical if NA=0);
use NA=1 with LANG=2 (Kalbach).

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/
             EP1, B0(E1,EP1), B1(E1,EP1), ... BNA(E1,EP1),
             EP2, B0(E1,EP2), ...
             EPNEP, B0(E1,EPNEP), ... BNA(E1,EPNEP)] LIST
             --------------------
             continue with LIST records for the
             rest of the incident energies
```

---

where the contents of the B0, B1, *etc.* entries depends on LANG (see below).

LANG =1 -- Legendre Coefficients

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

$$f_i(\mu,E,E') = \sum_{\ell=0}^{\mathrm{NA}} \frac{2\ell+1}{2} f_\ell(E,E') P_\ell(\mu)$$

where NA is the number of angular parameters, i denotes the product being described, E is the incident energy, E' is the energy of the product emitted with cosine μ, f_i is the normalized distribution with units (eV-unit cosine)$^{-1}$, $f_l(E,E')$ are the Legendre coefficients, and $P_l(\mu)$ are the Legendre polynomials. 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 B0, f_1 in B1, *etc.* Therefore, an isotropic distribution would go like this

```
EP1, f0(E,EP1), EP2, f0(E,EP2), EP3, f0(E,EP3),
EP4, f0(E,EP4), ...,
```

a P_1 distribution would go like this

```
EP1, f0(E,EP1), f1(E,EP1), EP2, f0(E,EP2), f1(E,EP2),
EP3, ...,
```

and so on.

LANG=2 -- Kalbach Systematics

For LANG=2, the angular distribution is represented by using Kalbach-Mann systematics in the extended form developed by Kalbach in 1987. This formulation addresses reactions of the form

A + a -> C -> B + b

where

A is the target,
a is the incident particle,
C is the compound system,
b is the emitted particle, and
B is the residual nucleus.

The following quantities are defined:

E_a energy of the incident projectile **a** in the laboratory system (normally called

E),

eps_a entrance channel energy, the sum of the kinetic energy of the incident projectile **a** and the target particle **A** in the center-of-mass system,

eps_b emission channel energy, the sum of the kinetic energy of the emitted particle **b** and the residual nucleus **B** in the center-of-mass system,

E_b energy of the emitted particle in the center-of-mass system (normally called E'), and

μ_b cosine of the emission angle of particle **b** in the center-of-mass system.

These energies are related as follows:

$$\varepsilon_a = E_a \times \frac{\mathrm{AWR}_A}{\mathrm{AWR}_A + \mathrm{AWR}_a}$$

$$E_b = \varepsilon_b \times \frac{\mathrm{AWR}_B}{\mathrm{AWR}_B + \mathrm{AWR}_b}$$

*It is **required** that LCT=2 with LANG=2.*

The Kalbach distribution is represented by

$$f(\mu_b, E_a, E_b) = f_0(E_a, E_b)\left\{\frac{a}{\sinh(a)}[\cosh(a\mu_b) + r\sinh(a\mu_b)]\right\}$$

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 (see below).

The center-of-mass energies and angles E_b and μ_b are transformed into the laboratory system using the expressions

$$E_{b,lab} = E_b + \frac{\mathrm{AWR}_a \mathrm{AWR}_b}{(\mathrm{AWR}_A + \mathrm{AWR}_a)^2} E_a + 2\frac{\sqrt{\mathrm{AWR}_a}\sqrt{\mathrm{AWR}_b}}{\mathrm{AWR}_A + \mathrm{AWR}_a}\sqrt{E_a E_b}\,\mu_b$$

$$\mu_{b,lab} = \sqrt{\frac{E_b}{E_{b,lab}}}\,\mu_b + \frac{\sqrt{\mathrm{AWR}_a}\sqrt{\mathrm{AWR}_b}}{\mathrm{AWR}_A + \mathrm{AWR}_a}\sqrt{\frac{E_a}{E_{b,lab}}}$$

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 Kalbach *slope parameter*, $a(E_a, E_b)$, is

$$a(E_a, E_b) = C_1 X_1 + C_2 X_1^2 + C_3 M_a m_b X_3^4$$

where

$$e_a = eps_a + S_a \qquad e_b = eps_b + S_b$$

$$R_1 = \min(e_a, E_{t1}) \qquad R_3 = \min(e_a, E_{t3})$$

$$X_1 = R_1 e_b / e_a \qquad X_3 = R_3 e_b / e_a$$

$$C_1 = 0.04/\text{MeV} \qquad C_2 = 1.8\text{x}10^{-6}/\text{MeV}$$

$$C_3 = 6.7\text{x}10^{-7}/\text{MeV}$$

$$E_{t1} = 130 \text{ MeV} \qquad E_{t3} = 41 \text{ MeV}$$

$$M_n = 1 \qquad M_p = 1$$

$$M_d = 1 \qquad M_{alpha} = 0$$

$$m_n = 1/2 \qquad m_p = 1$$

$$m_d = 1 \qquad m_t = 1$$

$$m_{3He} = 1 \qquad m_{alpha} = 2$$

The quantities S_a and S_b are the separation energies for the incident and emitted particles, respectively, neglecting pairing and other effects. The formulas for the separation energies are:

$$\begin{aligned} S_a &= 15.68[A_C - A_A] - 28.07\left[\frac{(N_C - Z_C)^2}{A_C} - \frac{(N_A - Z_A)^2}{A_A}\right] \\ &- 18.56[A_C^{2/3} - A_A^{2/3}] + 33.22\left[\frac{(N_C - Z_C)^2}{A_C^{4/3}} - \frac{(N_A - Z_A)^2}{A_A^{4/3}}\right] \\ &- 0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_A^2}{A_A^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_A^2}{A_A}\right] - I_a \end{aligned}$$

$$\begin{aligned} S_b &= 15.68[A_C - A_B] - 28.07\left[\frac{(N_C - Z_C)^2}{A_C} - \frac{(N_B - Z_B)^2}{A_B}\right] \\ &- 18.56[A_C^{2/3} - A_B^{2/3}] + 33.22\left[\frac{(N_C - Z_C)^2}{A_C^{4/3}} - \frac{(N_B - Z_B)^2}{A_B^{4/3}}\right] \\ &- 0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_B^2}{A_B^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_B^2}{A_B}\right] - I_b \end{aligned}$$

where S_a and S_b are the separation energies in MeV; the subscripts A, B, and C refer to the target nucleus, the residual nucleus, and the compound nucleus as before; the quantities N, Z, and A are the neutron, proton, and mass numbers of the nuclei; and I_a and I_b are the energies required to break the incident and emitted particles into their constituent nucleons as taken from the following table:

a or b	I_a or I_b (MeV)
n	0.0
p	0.0
d	2.22
t	8.48
^{3}He	7.72
alpha	28.3

The parameter $f_0(E_a,E_b)$ has the same meaning as f_0 in the first equation of this page; 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 the f_0 and r are stored in the positions of B0 and B1, respectively. Therefore, a particular distribution goes as follows:

```
EP1, f0(E,EP1), r(E,EP1), EP2, f0(E,EP2), r(E,EP2),
EP3, ...,
```

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, the same S_b would be used for all reactions, for example both (z,n') and (z,2n).

LANG=11-15 -- Tabulated Angular Distribution

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 (never use log interpolation with the cosine!). The cosine grid of NA/2 μ values must span the entrie angular range open to the particle for this E and E', and the integral of $f(\mu)$ over all angles must give the total emission probability for the E and E' (that is, it must equal f_0 as defined above). The value of f below the first μ value or above the last μ value is zero. The tabulation is stored in the angular parameters as follows:

$$B0 = f_0,$$

$$B1 = \mu_1,$$

$$B2 = 0.5 * f_1(\mu_1)/f_0,$$

$$B3 = \mu_2,$$

$$\ldots,$$

$$BNA = 0.5 * f_{NA/2}(\mu_{NA/2})/f_0.$$

In order to make things line up neatly, the preferred values for NA are 4, 10, 16, 22, *etc.* As an example, a simple distribution with NA=4 might look like this:

```
EP1, f0(E,EP1), -1.0, 0.5, 1.0, 0.5,
EP2, f0(E,EP2), -1.0, 0.4, 1.0, 0.6,
EP3, ....
```

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.

File 6 - 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

$$p_i(\mu,E) = \int dE' f_i(\mu,E,E')$$
$$= 0.5 + \sum_{\ell=1}^{NL} \frac{2\ell+1}{2} a_\ell(E) P_\ell(\mu)$$

where the P_l are the Legendre polynomials with the maximum order NL. Note that the angular distribution p_i is normalized.

The following quantities are defined for LAW=2:

LANG
flag that indicates the representation:
LANG=0, Legendre expansion;
LANG=12, tabulation with $p_i(\mu)$ linear in μ;
LANG=14, tabulation with $\ln p_i(\mu)$ linear in μ.

NR,NE,EINT
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.

AL
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/ EINT] TAB2
[MAT, 6, MT/ 0.0, E1, LANG, 0, NW, NL/ AL(E1)] LIST
             --------------------
             continue with LIST records for the
             rest of the incident energies
             --------------------
```

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

---

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

File 6 - 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.

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

File 6 - Discrete Two-Body Recoils (LAW=4)

If the recoil nucleus of a two-boy 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.

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

File 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.

We define the following parameters:

$\sigma_{cd}(\mu,E)$
: 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, 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$^{-1/2}$)

eta
: dimensionless Coulomb parameter

The Coulomb cross sections can now be written as follows:

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

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

$$k = \frac{\mu V}{\hbar} = \frac{A}{1+A}[(4.78453\times10^{-6})m_1E]^{1/2}$$

$$\eta = \frac{Z_1Z_2e^2}{\hbar V} = Z_1Z_2[(2.48058\times10^{-4})m_1/E]^{1/2}$$

Note that $A=1$ and $Z_1 = Z_2$ for identical particles. In the equation for k, μ is the reduced mass. The symbol V represents the relative velocity. The constants in the last two equations are reduced to numerical form with our choice of units for the

user's convenience.

The net elastic scattering cross sections for distinguishable and identical particles are as follow:

$$\begin{aligned}\sigma_{ed}(\mu,E) &= \sigma_{cd}(\mu,E) \\ &- \frac{2\eta}{1-\mu}\mathrm{Re}\left\{\exp\left(i\eta\ln\frac{1-\mu}{2}\right)\sum_{\ell=0}^{\mathrm{NL}}\frac{2\ell+1}{2}a_\ell(E)P_\ell(\mu)\right\} \\ &+ \sum_{\ell=0}^{\mathrm{NL}}\frac{2\ell+1}{2}b_\ell(E)P_\ell(\mu)\end{aligned}$$

$$\begin{aligned}\sigma_{ei}(\mu,E) &= \sigma_{ci}(\mu,E) \\ &- \frac{2\eta}{1-\mu^2}\mathrm{Re}\left\{\sum_{\ell=0}^{\mathrm{NL}}\left[(1+\mu)\exp\left(i\eta\ln\frac{1-\mu}{2}\right)\right.\right. \\ &+ \left.\left.(-1)^\ell(1-\mu)\exp\left(i\eta\ln\frac{1+\mu}{2}\right)\right]\frac{2\ell+1}{2}a_\ell(E)P_\ell(\mu)\right\} \\ &+ \sum_{\ell=0}^{\mathrm{NL}}\frac{4\ell+1}{2}b_\ell(E)P_{2\ell}(\mu)\end{aligned}$$

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 the following holds:

$$\sigma_{ei}(-\mu,E) = \sigma_{ei}(\mu,E)$$

The three terms in the equations for the net elastic cross section 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 section*** representation:

$$\sigma_{Rd}(\mu,E) = (1-\mu)[\sigma_{ed}(\mu,E) - \sigma_{cd}(\mu,E)]$$
$$\sigma_{Ri}(\mu,E) = (1-\mu^2)[\sigma_{ei}(\mu,E) - \sigma_{ci}(\mu,E)]$$

The σ_R can be given as Legendre expansions in the forms

$$\sigma_{Rd}(\mu,E) = \sum_{\ell=0}^{NL} \frac{2\ell+1}{2} c_{\ell d}(E)\, P_\ell(\mu)$$

$$\sigma_{Ri}(\mu,E) = \sum_{\ell=0}^{NL} \frac{4\ell+1}{2} c_{\ell i}(E)\, P_\ell(\mu)$$

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 due to the large magnitude of the Coulomb term.

It is also possible to represent experimental data using the ***nuclear plus interference*** representation. The cross section for File 3 and the angular distribution for File 6 are defined as follows:

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

$$p_{NI}(\mu,E) = \begin{cases} \dfrac{\sigma_e(\mu,E) - \sigma_c(\mu,E)}{\sigma_{NI}(E)}, & \mu_{min} \le \mu \le \mu_{max} \\ 0, & \text{otherwise} \end{cases}$$

where μ_{min} is -1 for distinguishable 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 one of the first two equations on the page, depending on whether distinguishable or identical particles are being considered.

The following quantities are defined for LAW=5:

SPI
spin of the particle. Used for identical particles (SPI = 0, 1/2, 1, *etc.*).

LIDP
flag that indicates that the particles are identical when LIDP=1; otherwise, LIDP=0.

LTP
flag that indicates the representation:
LTP=1, nuclear amplitude expansion;
LTP=2, residual cross section expansion as Legendre coefficients;
LTP=12, nuclear plus interference distribution with $\ln p_{NI}$ linear in μ; and
LTP=14, nuclear plus interference distribution with p_{NI} linear in μ.

NR,NE,EINT
standard TAB2 parameters

NL
for LTP<3, NL is the highest Legendre order of nuclear partial waves used; and
for LTP>2, NL is the number of cosine tabulated.

NW

number of parameters given in the LIST record:
for LTP=1 and LIDP=0, use NW=4*NL+3;
for LTP=1 and LIDP=1, use NW=3*NL+3;
for LTP=2, use NW=NL+1; and
for LTP>2, use NW=2*NL.

AL(E)
coefficients a_i, b_i, or c_i in barns/sr as described below, 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/ AL(E)] 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
$b_0, b_1, \ldots b_{2*NL}, Ra_0, Ia_0, Ra_1, Ia_1, \ldots Ia_{NL}$;
LTP=1 and LIDP=1
$b_0, b_1, \ldots b_{NL}, Ra_0, Ia_0, Ra_1, Ia_1, \ldots Ia_{NL}$;
LTP=2
$c_0, c_1, \ldots c_{NL}$; and
LTP>2
$\mu_1, p_{NI}(\mu_1), \ldots \mu_{NL}, p_{NI}(\mu_{NL})$,

File 6 - 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 distributions are described by the following formulas:

$$P_i^{CM}(\mu,E,E') = C_n\sqrt{E'}\left(E_i^{\max} - E'\right)^{3n/2-4}$$

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

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

$$E_a = \frac{m_T}{m_P + m_T}E + Q$$

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

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

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

where

E
: is the projectile energy in the laboratory;

E',μ
: are the energy and cosine for the outgoing particle, both in the lab or CM, depending on LCT;

E_i^{max}
: is the maximum possible CM energy for particle i;

E_{CM}
: is the energy of the CM motion in the laboratory;

E_a
: is the energy available in the CM for a one-step reaction;

M
: is the total mass of the n particles being treated by this law;

m_i
: is the mass of the particle being described in this section of File 6;

m_P
: is the projectile mass;

m_T
: is the target mass; and

Q
is the reaction QI values from File 3.

Note that *M* may be less than the total mass of products for reaction like

$$\alpha + {}^{9}\mathrm{Be} \rightarrow n + 3\alpha$$

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 the E_i^{max} can be determined without having to process the other subsections of this section.

The following quantities are defined for LAW=6:

APSX
total mass in neutron units of the n particles being treated by the law; and
NPSX
number of particles distributed according to the phase-space law.

Only a CONT record is given for a LAW=6 subsection:

```
[MAT, 6, MT/ APSX, 0.0, 0, 0, 0, NPSX] CONT
```

File 6 - 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,EINT
normal TAB2 parameters for incident energy E;
NRM,NMU,MUINT
normal TAB2 parameters for emission cosine MU; and
NRP,NEP,EPINT
normal TAB1 parameters for secondary energy EP.

The structure of a subsection is:

```
[MAT, 6, MT/ 0.0, 0.0, 0, 0, NR, NE/ EINT] TAB2
[MAT, 6, MT/ 0.0, E1, 0, 0, NRM, NMU/ MUINT] TAB2
[MAT, 6, MT/ 0.0, MU1, 0, 0, NRP, NEP/ EPINT/
             EP1, f(E1,EP1,MU1), EP2, f(E1,EP2,MU1), ...
             EPNEP, f(E1,EPNEP,MU1)] TAB1
             ----------------------------
             continue with TAB1 structures for
             the rest of the NMU emission cosines
             ----------------------------
             continue with TAB2/TAB1 structures for
             the rest of the NE incident energies
             ----------------------------
```

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.

Coming Attractions

This online course on the ENDF formats is not yet complete. We have to provide pages on the other resonance parameters beside SLBW. Soon, we hope to provide a detailed discussion of the complex formats used to describe photon production. Further down the line, you can expect discussions of photoatomic interactions, radionuclide production, fission yields, covariances, and so on.

Even though the course in not complete, we hope that it has served as an suitable introduction for you. Please check back occasionally to see how we are doing.

INDEX

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*