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ENDF/B-5 Formats Manual

Revised update pages of Nov. 1983

Reprint of
B.A. Magurno, "BNL-NCS-50496 [ENDF-102]
2nd Edition Revised, Nov. 1983"

Abstract: The ENDF-5 Format, originally the format of the US Evaluated Nuclear Data File ENDF/B-5, was internationally recommended for the computer storage, processing and exchange of evaluated neutron nuclear data. The pages included in this document serve as an update to the original ENDF-5 Formats Manual BNL-NCS-50496 [ENDF-102] 2nd Edition, October 1979.

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ENDF-Format, cross-references

ENDF-4 Format:

D. Garber et al., "BNL-NCS-50496 [ENDF-102], Oct. 1975"
Reprint as IAEA-NDS-74.

ENDF-5 Format:

R. Kinsey, "BNL-NCS-50496 [ENDF-102] 2nd Edition, Oct. 1979"
Microfiche as IAEA-NDS-10/102.

This was updated by
B.A. Magurno, "BNL-NCS-50496 [ENDF-102] 2nd Edition Revised,
Nov. 1983. The update pages are available as IAEA-NDS-73.

The current version of the Manual, including the 1979 Manual
plus the 1983 revision, is available as IAEA-NDS-75.

Note: The formats should be called ENDF-4 and ENDF-5.

The terms ENDF/B-4 and ENDF/B-5 should be reserved for the
US data libraries.

One may have, for example, a material from the ENDF/B-4 library
in ENDF-5 format.

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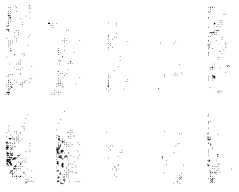
ENDF-102

DATA FORMATS AND PROCEDURES FOR THE EVALUATED NUCLEAR DATA FILE, ENDF/B-V

Edited by R. Kinsey
OCTOBER 1979
Revised by B.A. Magurno
NOVEMBER 1983



NATIONAL NUCLEAR DATA CENTER

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BNL 8381, ENDF — Evaluated Nuclear Data File Description and Specifications, June 1964, H.C. Honeck.

BNL 50066, ENDF 102, Vol. 1 — ENDF/B — Specifications for an Evaluated Nuclear Data File for Reactor Applications, May 1966, H.C. Honeck; Rev. July 1967, S. Pearlstein; Rev. Oct. 1970, M.K. Drake, Editor.

LA 4549, ENDF 102, Vol. II — ENDF Formats and Procedures for Photon Production and Interaction Data, Oct. 1970, D.J. Dudziak.

BNL-NCS-50496, ENDF 102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF, Oct. 1975, D. Garber, C. Dunford, and S. Pearlstein, Editors.

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

As in the previous edition, it brings under one cover both the neutron and photon formats and in addition includes the new data covariance formats.

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DATA FORMATS AND PROCEDURES

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Each file is divided into sections, each containing the data for a particular reaction type. The various reaction types are identified by the symbol MT. The definitions for allowed reaction types (MT numbers) are given in Appendix B.

The first record of each section contains a ZA number that identifies the specific material. ZA is the (Z,A) designation (charge, mass). ZA for a specific material is constructed by

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

where Z is the atomic number and A is the mass number for the material. For example, ZA = 92238.0 for ^{238}U. If the material is an element containing two or more naturally occurring isotopes, A, in the above equation, is taken to be 0.0. The ZA designators for materials that are molecules or common mixtures have been assigned certain values. These designators are given in Appendix C.

The first record of each section also contains a quantity that is proportional to the nuclear mass of the material. This quantity symbol AWR, is defined as the ratio of the nuclear mass of the material (isotope, element, molecule, or mixture) to that of the neutron. The mass of a neutron is taken to be 1.008665 (in the carbon-12 system).

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

Parameters	Units
energies	electron volts
angles	dimensionless cosines of the angle
cross sections	barns
temperatures	°Kelvin
mass	in units of the neutron mass
angular distributions	probability per unit cosine

energy distributions	probability per electron volt
energy-angle distributions	probability per unit cosine per electron volt
half life	seconds

0.4.2. Structure of an ENDF Data Tape

The structure of an ENDF data tape is illustrated schematically in Figure 0.4.2-1. The structure of the tape is the same whether it is a BCD card image tape or binary tape.

The tape contains a single record at the beginning that identifies the tape (TPID), and a single record at the end (TEND) that signals the end of the tape. The major subdivision between these records is by material. The data for a material is divided into files, and each file (MF number) contains the data for a certain class of information. A file is subdivided into sections, each containing data for a particular reaction type (MT number). Finally a section is divided into records. The content of each record is different and depends on whether a binary tape format or a BCD card-image format is used. Every record on a tape contains three identification numbers: MAT, MF, and MT. For a binary record, these numbers are given at the beginning of each record. For BCD card-image records, they are given in the last three fields of each record. These numbers are always in increasing numerical order, and the hierarchy is MAT, MF, MT. The end of a section, file, or material is signaled by special records.

The single record at the beginning of any ENDF tape, (TPID), consists of a 66 character free text field and a tape number. For a binary tape this record is 20 words. The first word is the integer value of the tape number. The second and third word are integer zeros for consistency with the other ENDF records which all have three integer values (MAT,MF,MT) to label the record

eral description of these nine numbers is given below, but the actual definition of each number will depend on its usage.

MAT is the material number (integer).

MF is the file number (integer).

MT is the reaction type number (integer).

C1 is a constant (floating point).

C2 is a constant (floating point).

L1 is an integer generally used as a test.

L2 is an integer generally used as a test.

N1 is a count of items in a list to follow.

N2 is generally a count of items in a second list to follow.

0.5.2.1. CØNT Records

The smallest possible record is a control (CØNT) record consisting of the nine numbers given above and no associated array. For convenience, a CØNT record is denoted by

(MAT, MF, MT/C1, C2; L1, L2; N1, N2)CØNT

The numbers within the brackets are symbolic of the numbers in a CØNT record. The semicolon is used to mark the separation between floating point numbers, test numbers, and counts. The slash is a reminder that the numbers MAT, MF, and MT appear in a different position on BCD card-image records then they do on the binary records. The BCD card-image format is described in Section 0.5.3 in more detail.

There are five special cases of a CØNT record, denoted by HEAD, SEND, FEND, MEND, and TEND. The HEAD record is the first in a section and has the same form as a CØNT record.

The structure of a typical HEAD record is

(MAT, MF, MT/ ZA, AWR, L1, L2, N1, N2)HEAD

where ZA is the (Z,A) designation for a material (see Appendix C),

AWR is the ratio of the mass of the atom (or molecule) to that of the neutron (carbon-12 system),

L1 is an integer to be used as a flag or a test,

L2 is an integer to be used as a flag or a test,

N1 is an integer to be used as a count of items in a list to follow except for MT=451, and

N2 is an integer to be used as a count of items in a second list to follow except for MT=451.

The symbolism used above to represent the HEAD record and to be used in the following format descriptions can be interpreted in either the binary format or the BCD-card image format. In the BCD-card image format, the six items after the slash are the contents of the first six fields on the card. Each field is eleven characters wide. After the first 66 characters, there are four characters for the MAT, two for the MF, and three for the MT. In the binary format, the symbolism just indicates the list of items to be read.

The SEND, FEND, MEND, and TEND records use only the first three numbers in the CØNT record, and they are used to signal the end of a section, file, material, and tape, respectively:

(MAT, MF, 0/0.0, 0.0; 0, 0; 0, 0)SEND

(MAT, 0 , 0/0.0, 0.0; 0, 0; 0, 0)FEND

(0 , 0 , 0/0.0, 0.0; 0, 0; 0, 0)MEND

(-1 , 0 , 0/0.0, 0.0; 0, 0; 0, 0)TEND

The values of $\bar{\nu}_p(E)$ given in this section are for the average number of prompt neutrons produced per fission event. Even though another section (MT = 455) that specifies the delayed neutron from fission may be given; $\bar{\nu}_d$, the number of delayed neutrons per fission, and $\bar{\nu}_p$, the number of prompt neutrons per fission, must be included in the values of $\bar{\nu}(E)$ given in the section (MT = 452); i.e., $\bar{\nu}(MT = 452) = \bar{\nu}_d(MT = 455) + \bar{\nu}_p(MT = 456)$.

1.5 Number of Neutrons from the Spontaneous Fissioning of the Target Nucleus (MT = 465, 466)

MT = 465 for $\bar{\nu}_{SD}$ (delayed component of spontaneous fission $\bar{\nu}$).

MT = 466 for $\bar{\nu}_{SP}$ (prompt component of spontaneous $\bar{\nu}$).

1.5.1. Formats

(MAT, 1, 465/	ZA	AWR	0	2	0	0)	HEAD*
(MAT, 1, 465/	0.0	0.0	0	0	1	2)	TAB 1
(MAT, 1, 465/	2	1	0	0	0	0)	
(MAT, 1, 465/	1.0E-5	$\bar{\nu}_{SD}$	2.0E+7	$\bar{\nu}_{SD}$	0	0)	
(MAT, 1, 0/	0.0	0.0	0	0	0	0)	SEND

and for MT = 466, the same format would be followed.

1.5.2. Procedures

Files 3 and 4 are not required for MT = 465 and 466.

*LNU = 1 (polynomial expansion) is not allowed as input.

1.6. Components of the Energy Release Due to Fission (MT = 458)

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

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

EFR is the kinetic energy of the fragments

ENP is the kinetic energy of the "prompt" fission neutrons

END is the kinetic energy of the delayed fission neutrons

EGP is the total energy released by the emission of "prompt" γ rays

EGD is the total energy released by the emission of delayed γ rays

EB is the total energy released by delayed β's

ENU is the energy carried away by the neutrinos

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

$E_i(0) = E_i(EINC) + \delta E_i$

where E_i is any of the energy release components

$E_i(0)$ is the value at EINC = 0

$E_i(EINC)$ is the value at incident energy EINC

EINC = 0 is ficticious and represents an artifice by which it is possible to recover the values at any EINC.

The δE_i's are given by the following:

$\delta QG = EINC - (1.057\ EINC - 8.07(\nu(EINC) - \nu(0)))$

$= - 0.057\ EINC + 8.07(\nu(EINC) - \nu(0))$.

$\delta EB = 0.075\ EINC$.

$\delta EGD = 0.075\ EINC$.

$\delta ENU = 0.100\ EINC$.

$\delta EFR = 0$.

$\delta ENP = - (1.307\ EINC - 8.07\ (\nu(EINC) - \nu(0))$.

$\delta EGP = 0$

1.6.1. Formats

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

The structure of a section is:

(MAT, 1, 458/ ZA, AWR, 0, 0, 0, 0) HEAD

(MAT, 1, 458/ 0.0, 0.0, 0, 0, 18, 9/

EFR, ΔEFR, ENP, ΔENP, END, ΔEND

EGP, ΔEGP, EGD, ΔEGD, EB, ΔEB

ENU, ΔENU, ER, ΔER, ET, ΔET) LIST

(MAT, 1, 0/ 0.0, 0.0, 0, 0, 0, 0) SEND,

where the Δ's allow the error estimates on the quantities listed above.

1.6.2. Procedures

This section should be used for fertile and fissile isotopes only. ($Z \geq 88$) for ENDF/B-V.

Consistency should be maintained between the Q values in File 3, the energies calculated from Files 5 and 15 and the energies listed in File 1. Note that ER = the pseudo-Q for fission (MT = 18) in File 3.

Other components are not so readily determined or checked. The procedure should be that File 5 and File 15 data take precedent, whenever available. That is, the "prompt" fission neutron energy calculated from File 5 spectra from MT = 18 should be used in File 1; the same holds true for the delayed neutron spectra given in File 5, MT = 455. The "prompt" gamma energy calculated from File 15 (MT = 18 for fission) should be input into File 1, that is the prompt gammas due to the fission process.

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

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

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

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

2. FILE 2, RESONANCE PARAMETERS

2.1. General Description

Every material must contain a File 2. It has only one section, which has been assigned the reaction type number MT = 151. If no resonance parameters are given for the material, the purpose of the File 2 section is to specify the scattering radius, AP. If resonance parameters are given for some isotopes of an elemental evaluation, an isotope without resonance parameters may be included. If it is included, the subsection for the first and only energy range of that isotope will consist of a single CONT record giving the spin, SPI, and scattering radius, AP. In these two cases, the inclusion of a scattering radius is solely for the convenience of users who wish an estimate of the potential scattering. It is not used to calculate a contribution to the scattering cross section, which in these two cases, is represented entirely in File 3.

The primary function of File 2 is to contain data for both resolved and unresolved resonance parameters. When resonance parameters are given the total (MT = 1), elastic scattering (MT = 2), fission (MT = 18), and radiative capture (MT = 102) cross sections given in File 3 must be added to corresponding contributions calculated from the resolved and/or unresolved parameters given in File 2 in order to obtain the correct reaction cross sections.

All other reactions, if any, are grouped together into a single "competitive width," Γ_x. This width is given explicitly in the unresolved resonance region, and implicitly in the resolved region. In the latter region, it is permissible for the total width to exceed the sum of the neutron, radiative capture, and fission widths. The difference is interpreted as the competitive width:

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

By convention, the individual competitive reactions (if any) given in File 3 represent the entire cross section and the contribution from File 2 is not to be added to them. (See Appendix D. Section D.3.3.)

For those isotopes with resonance parameters, the potential scattering term is given by

$$\sigma_{nn}^{\ell} = \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \phi_\ell, \quad \ell = 0, 1, 2,$$

where

$$k = 2.196771 \frac{AWRI}{AWRI + 1.0} \times 10^{-3} \sqrt{E}, \quad E \text{ in eV},$$

$$\phi_0 = \hat{\rho}, \ \phi_1 = \hat{\rho} - \tan^{-1} \hat{\rho}, \ \phi_2 = \hat{\rho} - \tan^{-1} \frac{3\hat{\rho}}{3 - \hat{\rho}^2},$$

and

$$\hat{\rho} = k(AP).$$

In order to calculate the penetrability and shift factors when resonances are present, the current ENDF convention is to employ the channel radius, a, also known as the "hard-sphere radius" or the "nuclear radius,"

$$a = .123 \ AWRI^{1/3} + .08 \quad \text{in units of } 10^{-12} \text{ cm.}$$

The resonance parameter data for a material are obtained by specifying the parameters for each isotope in the material. The data for the various isotopes

into no more than two energy ranges, one for resolved and the other for unresolved resonance parameters.

In the single-level Breit-Wigner formalism it is common for negative cross sections to occur, and this formalism ought not to be used for actual line-shape calculations. The problem can be avoided by the following procedures:

1. Use of the MLBW formalism, together with the addition of negative-energy levels to compensate the end-effect bias. High-energy resonances can likewise be added.
2. Insertion of File 3 "background" to produce a File 2 + File 3 cross section which is positive.

Further discussion of "Procedures" will be found in Section 2.4.

2.3. Unresolved Resonance Parameters (LRU = 2)

2.3.1. Formats

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

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

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

SPI is the spin of the target nucleus, I.

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

NE is the number of energy points at which energy-dependent widths are tabulated. (NE $\leq$ 250.)

NLS is the number of ℓ-values (NLS $\leq$ 3.)

ES_i is the energy of the i^{th} point used to tabulate energy-dependent widths.

L is the value of ℓ.

AWRI is the ratio of the mass of a particular isotope to that of the neutron.

NJS is the number of J-states for a particular ℓ-state. (NJS $\leq$ 6.)

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

D is the average level spacing for resonances with spin J. (It may be energy dependent if LRF = 2.)

AMUX is the number of degrees of freedom used in the competitive width distribution. (Assuming it is inelastic, 1.0 $\leq$ AMUX $\leq$ 2.0, determined by whether the spin of the first excited state is zero or not.)*

AMUN is the number of degrees of freedom in the neutron width distribution. (1.0 $\leq$ AMUN $\leq$ 2.0.)

*See Appendix D. Section D.2.2.6.

these cases either tabulated spectra or "mocked-up" levels can be constructed to supplement or replace simple evaporation spectra.

5. Note that prompt fission spectra are given under MT=18 with LF=11 preferred. The delayed fission spectra are given under MT=455 and 465.

5.4.2. LF = 1 (Tabulated Distributions)

Use only tabulated distributions to represent complicated energy distributions. Use the minimum number of incident energy points and secondary neutron energy points to accurately represent the data. The integral over secondary neutron energies for each incident energy point must be unity to within four significant figures. All interpolation schemes must be with linear-linear or log-linear (INT = 1, 2, or 3) to preserve probabilities upon interpolation. All secondary energy distributions must start and end with zero values for the distribution function $g(E \rightarrow E')$.

5.4.3. LF = 5 (General Evaporation Spectrum)

This law may be used for MT = 455 and 456, otherwise, LF = 1 should be used.

5.4.4. LF = 7 (Maxwellian Spectrum)

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

5.4.5. LF = 9 (Evaporation Spectrum)

An evaporation spectrum is preferred for most reactions. Care must be taken in describing the nuclear temperature near the threshold of a reaction. Nuclear temperatures that are too large can violate conservation of energy.

5.4.6. LF = 11 (Watt Spectrum)

This is the preferred law to use for the prompt fission spectrum. A linear-linear interpolation scheme is preferred for specifying the parameter as a function of energy.

5.4.7. Selection of the Integration Constant, U

1. When LF = 5, 7, 9, or 11 is used, an integration constant, U is required. This constant is used in defining the upper energy limit of secondary neutrons; i.e., $E'_{max} = E_n - U$, where E_n is the incident neutron energy. U is a constant for the complete energy range covered by a subsection in File 5 and is given in the LAB system.

2. U is negative for fission reactions. The preferred value is -20 MeV.

3. In practice, U can be taken to be the absolute value of Q for the lowest level (known or estimated) that can be excited by the particular reaction within the incident energy range covered by the subsection. U is actually a function of the incident neutron energy, but it can be shown that it is always greater than the absolute value of Q and less than the threshold energy of the reaction. At large AWR, since E_{th} and $|Q|$ are approximately equal, either could be used but the absolute value of Q is preferred. At small AWR, using $|Q|$ for U is the best approximation and must be used.

4. The following three cases commonly occur in data files; procedures are given for obtaining U values.

Case A: The complete reaction is treated as a continuum.

$U = -Q$

where Q is the reaction Q-values.

B(4) = E_{max}, the upper energy limit for the constant σ_{f0} (upper energy limit in which $S_0(\alpha,\beta,T)$ may be used).

B(5), not used.

B(6), not used.

The next six constants specify the analytic functions to be used in describing the scattering properties of the first non-principal scattering atom, (n = 1); i.e., for H_2O, this atom would be oxygen if the principal atom was hydrogen.

B(7) = a_1, a test indicating the type of analytic function used for this atom type.

a_1 = 1.0, use a free gas scattering law.

a_1 = 2.0, use a diffusive motion scattering law.

B(8) = $M_1\sigma_{f1}$, the total free atom cross section for this atom type.

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

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

B(11)= 0.0, B(11) is not used.

B(12)= 0.0, B(12) is not used.

The next six constants, B(13) through B(18), are used to describe the second nonprincipal scattering atom (n = 2), if required. The constants are defined in the same way as for n = 1; e.g., B(13) is the same type of constant as B(7).

The scattering law is given by tabulating S(α , β) at a specific temperature (°K) or at a series of temperatures. Since scattering law data are generally given at more than one temperature, it is extremely important to understand the data formats for specifying temperature-dependent data (see Appendix F for details). The data are presented at given values of β. The β's are ordered by increasing values. For each value of β, pairs of α vs $S(\alpha,\beta)$ are given. (The data are given in this form only for the first temperature; see Appendix F for

the formats for temperature dependent data.) Two interpolation schemes are given to interpolate between values of β and α.

In certain cases a more accurate temperature representation may be obtained by replacing the value of the actual temperature, T, that is used in the definition of α and β with a constant, T_o (T_o = 0.0253 eV or the equivalent depending on the units of Boltzmann's constant). A flag (LAT) is given for each material to indicate which temperature has been used in generating the $S(\alpha,\beta)$ data.

7.2. Formats

There is only one section in File 7, but the format varies slightly, depending on whether temperature-dependent data are given. The following quantities are defined:

LAT is a flag indicating which temperature has been used to compute α and β.

LAT = 0, the actual temperature was used.

LAT = 1, the constant T_o = 0.0253 eV has been used.

NS is the number of non-principal scattering atom types. For most moderating materials there will be (NS + 1) types of atoms in the molecule ($NS \leq 3$).

NI is the total number of items in the B(N) list. NI = 6*(NS + 1).

B(N) is the list of constants. Definitions are given above (Section 7.1).

NR is the number of interpolation ranges for a particular parameter, either β or α.

NB is the total number of β values given.

NP is the number of α values given for each value of β for the first temperature described, NP is the number of pairs, α and $S(\alpha,\beta)$, given.

8.3. Radioactive Decay Data (MT=457)

The spontaneous radioactive decay data are given in Section 457. This section is given for materials that are single nuclides in their ground state or an isomeric state. (An isomeric state is a "long lived" excited state of the nucleus.) The main purpose of MT=457 is to describe absolutely the energy spectra resulting from radioactive decay and give average parameters useful for applications such as decay heat, waste disposal, depletion and buildup studies, shielding, and fuel integrity. The information in this section can be divided into three parts:

a. General information about the material

ZA is the designation of the original (radioactive) nuclide (=1000* Z+A).

AWR is the ratio of the LIS state nuclide mass to that of neutron.

LIS is the state of the original nuclide (LIS=0, ground state, LIS=1, first excited state, etc.).

LISØ is the isomeric state number for original nuclide (LISØ=0, ground state; LISØ=1, first isomeric state; etc.).

$T_{\frac{1}{2}}$ is the half-life of the original nuclide (seconds).

$E_{"x"}$ is the average decay energy (eV) of "x" radiation for decay heat applications. The "β," "γ," and "α" energies are given in that order with space reserved for zero "β" or "γ" entries. See procedures for precise definitions of "β", "γ" and "α."

SPI is the spin of the nuclide in its LIS state. (SPI = - 77.777 = SPIN UNKNOWN)

PAR is the parity of the nuclide in its LIS state (±1.0).

b. Decay mode information - for each mode of decay:

NDK is the total number of decay modes given (cannot be zero).

RTYP is the mode of decay of the nuclide in its LIS state.

Decay modes defined:

RTYP	Mode of decay	
0.	γ	γ-ray (not used in 457)
1.	β^-	Beta decay
2.	e.c., (β^+)	Electron capture and/or positron emission
3.	IT	Isomeric transition (will in general be present only when the state being considered is an isomeric state)
4.	α	Alpha decay
5.	n	Neutron emission (not "delayed neutron decay" considered below)
6.	SF	Spontaneous fission
7.	p	Proton emission.
10.	-	Unknown origin.

Multiple particle decay is also allowed using any combination of the above RTYP variables as illustrated in the following examples:

RTYP	Mode of decay	
1.5	β^-,n	Beta decay followed by neutron emission ("delayed neutron decay")
1.4	β^-,α	Beta decay followed by alpha emission (N-16 decay)
2.4	β^+,α	Positron decay followed by alpha emission.

RFS is the isomeric state flag for daughter nuclide. (RFS=0.0, ground state; RFS=1.0, first isomeric state; etc.)

Q is the total decay energy (eV) available in the corresponding decay process. (This is not necessarily the same as the maximum energy of the emitted radiation. In the case of an isomeric transition Q will be the energy of the isomeric state. For both β^+ and β^-, Q equals the energy corresponding to the mass difference between the initial and final atoms.)

BR is the fraction of the decay of the nuclide in its LIS state which proceeds by the corresponding decay mode. (e.g. If only β^- occurs and no isomeric states in the daughter nucleus are excited then BR = 1.0 for β^-decay).

c. Resulting radiation spectra

NSP is the total number of radiation types (STYP) for which spectral information is given (NSP may be zero).

STYP is the decay radiation type

Decay radiations defined:

STYP	Radiation type	
0.	γ	Gamma rays
1.	β^-	Beta rays
2.	e.c., (β^+)	Electron capture and/or positron emission
4.	α	Alpha particles
5.	n	Neutrons
6.	SF	Spontaneous fission fragments
7.	p	Protons
8.	e^-	"Discrete electrons"

Decay Radiations Defined (Cont'd)

STYP	Radiation type	
9.	x	X-rays and annihilation radiation (photons not arising as transitions between nuclear states)

ER is the energy (eV) of radiation produced (E_{γ}, $E_{\beta-}$, $E_{e.c.}$, etc.)

RI is the intensity of radiation produced (relative units)

RP is the spectrum of the continuum component of the radiation in units of probability/eV such that $\int RP(ER)dER = 1$

TYPE is the type of transition for beta and electron capture

Types Defined:

TYPE	Spectrum Definition
0.0	not required for STYP
1.0	allowed, nonunique
2.0	First-forbidden unique
3.0	Second-forbidden unique

RICC is the total internal conversion coefficient (STYP=0.0 only)

RICK is the K-shell internal conversion coefficient (STYP=0.0 only)

RICL is the L-shell internal conversion coefficient (STYP=0.0 only)

RIS is the internal pair formation coefficient (STYP=0.0)

positron intensity (STYP=2.0)

0.0 (Otherwise)

LCON* is the continuum spectrum flag

LCON = 0, no continuous spectrum given

LCON = 1, only continuous spectrum given

*Spontaneous $\bar{\nu}$: For RTYP = 6. and STYP = 5. LCON = 1 and FC = $\bar{\nu}$ and FD = 0.0

LCON = 2, both discrete and continuous spectra

LCON = 5, spectral information in file 5 format

NT is the number of entries given for each discrete energy (ER)

FC* is the continuum spectrum normalization factor (absolute intensity/relative intensity)

FD is the discrete spectrum normalization factor (absolute intensity/relative intensity)

NER is the total number of tabulated discrete energies for a given spectral type (STYP)

$\overline{ER}$** is the average decay energy of radiation produced

NR is the number of interpolation ranges for the continuum spectrum

NP is the number of points at which the distribution will be given

X_{int} is the interpolation scheme for the continuum spectrum

NK is the number of partial energy distributions when LCON = 5 is used.

Δ is the uncertainty in any quantity.

8.3.1. Formats

The structure of this section always starts with a HEAD record and ends with a SEND record. This section is divided into subsections as follows:

(MAT, 8,457/ ZA AWR LIS LISØ b NSP) HEAD

(MAT, 8,457/ $T_{½}$ $\Delta T_{½}$ b b 6 b /

$\overline{E}_{"\beta"}$ $\Delta\overline{E}_{"\beta"}$ $\overline{E}_{"\gamma"}$ $\Delta\overline{E}_{"\gamma"}$ $\overline{E}_{"\alpha"}$ $\overline{\Delta E}_{"\alpha"}$) LIST

*Spontaneous $\bar{\nu}$: For RTYP = 6. and STYP = 5. LCON = 5 or LCON = 1 and FC = $\bar{\nu}$ and FD = 0.0

**For STYP = 2, this is the average positron energy; for STYP = 4, this includes energy of recoil nucleus.

(MAT,8,457/ SPI PAR b b 6*NDK NDK /

$RTYP_1$ RFS_1 Q_1 ΔQ_1 BR_1 ΔBR_1

.
.
.

$RTYP_{NDK}$ RFS_{NDK} Q_{NDK} ΔQ_{NDK} BR_{NDK} ΔBR_{NDK}) LIST

Repeat NSP times

(MAT,8,457/ b STYP LCON b 6 NER / (omit if NSP=0)

FD ΔFD $\overline{ER}$ $\overline{\Delta ER}$ FC ΔFC) LIST

(MAT,8,457/ ER_1 ΔER_1 b b NT b / (omit if LCON=1or5)

$RTYP_1$ $TYPE_1$ RI_1 ΔRI_1 RIS_1 ΔRIS_1

$RICC_1$ $\Delta RICC_1$ $RICK_1$ $\Delta RICK_1$ $RICL_1$ $\Delta RICL_1$) LIST

ER_{NER} ΔER_{NER} b b NT b / (omit if LCON=5)

$RTYP_{NER}$ $TYPE_{NER}$ RI_{NER} ΔRI_{NER} ----) LIST

(MAT,8,457/ RTYP 0.0 b b NR NP / (omit if LCON=0or5)

X_{int} / ER_K RP_K) TAB1

(MAT,8,457/ ZA AWR ER ΔER NK 0) HEAD (omit if LCON ≠5)

<SUBSECTION for K = 1>

<SUBSECTION for K = NK>

where subsections are described in Chapter 5, "File 5, Energy Distributions of Secondary Neutrons" page 5.1.

(MAT,8,0/ b b b b b b) SEND.

8.3.2. Procedures

I. The initial state of the parent nucleus is designated by LISØ which equals 0 for the ground state and equals n for the nth isomeric state. Only isomeric states are included in the count of LISØ. (In other files isomeric and non-isomeric states may be included in the count of levels.)

II. The average decay energy $\bar{E}_{\text{"x"}}$ for decay heat application is given for three general radiation types, $\bar{E}_{\text{"}\beta\text{"}}$, $\bar{E}_{\text{"}\gamma\text{"}}$, and $\bar{E}_{\text{"}\alpha\text{"}}$. The sum of these three quantities is the total average (neutrino energies excluded) energy available per decay to the decay heat problem. The three quantities are more precisely defined as

$$\bar{E}_{\text{"}\beta\text{"}} = \bar{E}_{\text{elect.}} = \bar{E}_{\beta-} + \bar{E}_{\beta+} + \bar{E}_{e-} + \ldots$$

$$\bar{E}_{\text{"}\gamma\text{"}} = \bar{E}_{\text{phot.}} = \bar{E}_{\gamma} + \bar{E}_{\text{x-ray}} + \bar{E}_{\text{ann. rad.}} + \ldots$$

$$\bar{E}_{\text{"}\alpha\text{"}} = \bar{E}_{\text{h.p.}} = \bar{E}_{\alpha} + \bar{E}_{SF} + \bar{E}_{p} + \bar{E}_{n},$$

where $\bar{E}_{\text{"}\beta\text{"}}$ ($\bar{E}_{\text{elect.}}$) means the average energy of all "electron-related" radiation such as β^-, β^+, conversion-electrons, Auger, etc. The quantity $\bar{E}_{\text{"}\gamma\text{"}}$ ($\bar{E}_{\text{phot.}}$) means the average energy of all "electromagnetic" radiations such as gamma rays, x-rays, and annihilation radiation. The quantity $\bar{E}_{\text{"}\alpha\text{"}}$ is the average energy of all heavy charged particles and delayed neutrons.

$\bar{E}_{\text{"}\beta\text{"}}$, $\bar{E}_{\text{"}\gamma\text{"}}$, and $\bar{E}_{\text{"}\alpha\text{"}}$ must be specified in that order with space reserved for zero or unknown information. The average alpha energy, $\bar{E}_{\alpha}$, also includes the recoil energy but the alpha energy alone can be separated out by the usual $\frac{M_R}{M_R+M_\alpha}$ factor where M_R and M_α are the recoil nucleus and alpha masses respectively.

III. The symbol RTYP indicates the mode of decay as determined by the initial event. A nucleus undergoing beta decay to an excited state of the daughter

nucleus which subsequently decays by gamma emission is in the beta decay mode. RTYP = 0.0 is not allowed in MT = 457 (although used under 8.1).

An isomeric state of the daughter nuclide resulting from the decay of parent nuclides is designated by RFS following the procedures used for LISØ. Q represents the total energy available in the decay process and is equal to the energy difference available between the initial and final states (both of which may be isomeric). The branching ratio BR for each decay mode is given as a fraction and the sum over all decay modes must equal unity. Multiple particle emission is also allowed by using any combination of the RTYP variables. This will account for particle emission from nuclear states excited in the decay of the parent ("delayed-particle" emission) whose half-lives are too short to warrant separate entry in the file. It will also allow users and processing codes to identify the various intermediate states, without having to examine all the spectrum listings to determine radiation types. The multiple-particle RTYP should be constructed in the order in which the particles are emitted. (e.g. RTYP = 1.5 indicates β decay followed by neutron emission).

IV. The source-of-radiation should be specified for each spectral line or continuous spectra. The source of radiation is a floating point integer corresponding to the RTYP definitions. If the source-of-radiation is not known RTYP = 10. should be used.

V. The energy spectra should be specified if they are known and identified by STYP. Gamma spectra are described using STYP = 0.0. Relative intensities and errors in the relative intensity should be specified. Absolute normalization is made through multiplication by FC and FD. If absolute discrete spectra are given FD must equal unity. The radiation intensity should total the contributions from all decays leading to radiation within a particular decay type, STYP, having an energy $E_r \pm \Delta E_r$.

a. For gamma ray emission (STYP = 0.0), no other information is required if X, Auger electron, conversion electron, and pair formation intensities have not been calculated for these transitions. In this case NT = 6.

The amount of additional information depends upon the detail in which quantities were obtained for inclusion in STYP = 8. or 9. spectra, and the number of decay modes. (This detail will also be reflected in the uncertainties assigned in STYP = 8. or 9. spectra.) If only the total conversion electron emission is calculated, RICC and ΔRICC should be included and NT is specified as 8. If contributors from the individual K, L, and M shells are calculated the K and L shell conversion coefficients should be included and NT = 12. In the rare case (i.e. $^{16}_{7}N$), where internal pair formation is included the internal pair formation coefficient should be included along with the conversion coefficients as the quantity RIS and ΔRIS.

b. For electron capture (STYP = 2.) the quantity RIS is 0.0 provided $E_{e.c.} \leq 1.022$ MeV. If positron emission is energetically possible, RIS and ΔRIS must be specified (as $I_{\beta+}$ and $\Delta I_{\beta+}$).

c. The spectra should be ordered in increasing values of STYP, and discrete spectral data should be specified before continuous spectra.

d. For STYP = 6. (spontaneous fission neutrons) LCON and NER must be zero and $\bar{E}_{SF}$ and $\Delta\bar{E}_{SF}$ should be given.

VI. The specification of data uncertainties is an important quantity which is difficult to represent in a simple way. Although a one sigma variance is desired, a number should be entered that at least indicates qualitatively how well the parameter is known.

For STYP = 8. and 9., ΔE will reflect the detail in which these values were derived. For example, if only the total conversion electron emission has been calculated, ΔE would be the spread between K-conversion and M-conversion electron energies. If a very detailed calculation has been made, ΔE would reflect the uncertainties in the electron binding energy and the transition energy.

VII. LCON = 5 should be used whenever data is given in MF = 5 as well as MF = 8, MT = 457 so that consistency between the two files is ensured.

VIII. Every effort should be made to determine the spin and parity of the original nucleus, either by experimental evidence or by strong theoretical arguments. If the spin cannot be determined, it should be reported as -777.77; if the parity cannot be determined it should be reported as zero.

GF. Because the covariance of ER and the other resonance parameters is very small in practice in File 32 we only concern ourselves with the variance of ER. The uncertainties on ER in practical applications are expected to be significant only for some calculations involving the thermal region for a few resonances. The value of the total angular momentum AJ of the resonance may only take on some discrete values. When the value of AJ can be determined from the experimental data, then its variance is zero as well as the covariance of AJ and of the other resonance parameters. However, frequently the exact value of AJ cannot be obtained from the experiments; it is then permissible (see 2.2.2 Procedures for File 2) to assign to it a value in File 2 such that the statistical weight factor g_L is given properly, on the average, for each value of L, the neutron angular momentum. In such cases it may not be possible within the resonance formalism used, to represent all of the available data and their uncertainties without assigning a variance to AJ and a covariance of AJ and of the other resonance parameters. In the above situation AJ is considered as a constrained parameter of the formalism and the covariances of AJ and of the other parameters a device for representing accurately the uncertainties in various quantities related to the resonance.

32.2. Formats

The format for File 32, MT=151, parallels the format for File 2, MT=151, with the restrictions that only resolved resonance parameters of the single-level and multi-level Breit-Wigner formalisms are allowed. The major difference is that in File 32 we require more information per resonance, the covariances of the resonance parameters, than in File 2. In the description of the format for File 32, MT=151, which follows, we use the same symbolism for naming the quantities as given in File 2, section 2, of the manual:

NIS is the number of isotopes in this material (NIS < 10).

ZAI is the (Z,A) designation for an isotope.

ABN is the abundance (weight fraction) of an isotope in this material.

EL is the lower energy limit of the energy range.

EH is the upper energy limit of the energy range.

LRF is a flag indicating which representation is used:

LRF=1, single-level B-W parameters.

LRF=2, multi-level B-W parameters.

The general structure of File 32 is as follows:

(MAT, 32, 151/ ZA, AWR; 0, 0; NIS, 0) HEAD

(MAT, 32, 151/ ZAI, ABN; 0, 0; 1, 0) CONT (isotope)

(MAT, 32, 151/ EL, EH; 1, LRF; 0, 0) CONT (range)

<subsection for the first isotope>

.

.

.

(MAT, 32, 151/ ZAI, ABN; 0, 0; 1, 0) CONT (isotope)

(MAT, 32, 151/ EL, EH; 1, LRF; 0, 0) CONT (range)

<subsection for the last isotope>

.

.

.

(MAT, 32, 0/ 0.0, 0.0; 0, 0; 0, 0) SEND

(MAT, 0, 0/ 0.0, 0.0; 0, 0; 0, 0) FEND

The structure of a subsection is the same for LRF=1 (single-level B-W parameters) as it is for LRF=2 (multi-level B-W parameters). The following quantities are defined:

33. FILE 33, COVARIANCES OF NEUTRON CROSS SECTIONS

33.1 General Description

The covariances of neutron cross section information appearing in File 3 are given in File 33. File 33 is intended to provide a measure of the "accuracies and their correlations" of the data in File 33 and does not indicate the precision with which the data are entered in the File 33. Since ENDF/B represents our knowledge of the microscopic data, the File 33 is used to give the covariances of these microscopic data. However, it should be stressed that for most practical applications to which the files are intended the data will be processed into group cross sections. While generating File 33 it should be remembered that one of their major aims is to represent adequately:

i. The variances of the group cross sections,

ii. The correlations of the uncertainties between the several adjacent groups, and

iii. The long-range correlations of the uncertainties over many groups.

Table 33.1 illustrates the relation of these three covariances with experimental uncertainties.

These primary considerations and the inherent difficulties associated with quantifying uncertainties should dictate the details given in Files 33.

In the resolved resonance region, some of the covariances of the cross sections, within each resonance, may be given through the covariances of the resonance parameters in File 32. In this case, the long-range components of the covariance matrix of the cross sections which span several resonances are given in File 33. It is permissible, in the resolved resonance region, to represent the covariance matrix in File 33, since often the major components of the matrix are

Table 33.1

Analogies Between File 33 Covariances Within One Section and Experimental Uncertainties*

File 33	Experimental	Energy Dependence
short-range	statistical	Rapid variation
medium-range	Detector Efficiency Multiple Scattering In/Out Scattering	Slowly varying
long-range	Geometry Flux Background Normalization	More or less constant

Example: If we had a 2% uncertainty due to statistics (short-range), 2% due to multiple scattering (medium-range) and, 1% due to background (long-range), we would cite a 3% uncertainty for a discrete measurement (one group covering a small ($\lesssim$ 200 keV) energy range); $\lesssim$ 2.5% over an energy range encompassing several measurements (several groups which together cover a 1- to 2-MeV range); and $\lesssim$ 1% over the entire energy range.

*As with all analogies, this should be used with care. It is designed to show in a familiar way of thinking how the covariance within a section are related.

long-range. In the unresolved resonance region the covariances of the cross sections must be given entirely in File 33.

33.2 Formats

File 33 is divided into sections identified by the value of MT. Within a section, (MAT,33,MT), several subsections may appear. Each section of File 33 starts with a HEAD record, ends with a SEND record, and has the following structure:

(MAT, 33, MT/ZA, AWR; b, MTL; b, NL) HEAD

<subsection for L = 1>

<subsection for L = 2>

.

.

.

<subsection for L = NL>

(MAT, 33, 0/ b, b; b, b; b, b) SEND

NL in the HEAD record denotes the number of subsections within a section. A non zero value of MTL is used as a flag to indicate that reaction MT is one component of the evaluator defined lumped reaction MTL, as discussed below; in this case, no covariance information is given for reaction MT (other than the HEAD record) and NL = 0.

Subsections

Each subsection of the section (MAT,33,MT) is used to describe a single covariance matrix. It is the covariance matrix of the energy-dependent cross sections given in section (MAT,3,MT) and energy-dependent cross sections given in section (MAT1,3,MT1) of the ENDF/B tape. The values of MAT1 and MT1 are given in the CONT record which begins every subsection. Each subsection is

therefore identified with a unique combination of values (MAT,MT) and (MAT1,MT1), and we may use the notation (MAT,MT;MAT1,MT1) to specify a subsection.

Each subsection may contain several sub-subsections. Two different types of sub-subsections may be used; they are referred to as "NC-type" and "NI-type" sub-subsections. Each sub-subsection describes an independent contribution, called component, to the covariance matrix given in the subsection. The total covariance matrix in the subsection is made up of the sum of the contributions of the individual sub-subsection.

The structure of a subsection describing the covariance matrix of the cross sections given in the ENDF/B type (MAT,3,MT) and (MAT1,3,MT1) is:

(MAT, 33, MT/ b, b; MAT1, MT1; NC, NI) CONT

<sub-subsection for n_c = 1>

<sub-subsection for n_c = 2>

.

.

.

<sub-subsection for n_c = NC>

<sub-subsection for n_i = 1>

<sub-subsection for n_i = 2>

.

.

.

<sub-subsection for n_i = NI>

NC is the number for "NC-type" sub-subsections which follow the CONT record.

NI is the number of "NI-type" sub-subsections which follow the "NC-type" sub-subsections.

Sub-subsections

There are two different types of sub-subsections which have a different structure, the "NC-type" and "NI-type" sub-subsections.

The "NC-type" sub-sections may be used to indicate that some or all of the contributions to the covariance matrix described in the subsection are to be found in a different subsection of the ENDF/B tape. The major purpose of the "NC-type" subsections is to eliminate from the ENDF/B tape a large fraction of the mostly redundant information which would otherwise be needed if only "NI-type" sub-subsections were used.

The "NI-type" sub-subsections are used to describe explicitly the various components of the covariance matrix of the subsection.

I. "NC-type" Sub-subsections

The "NC-type" sub-subsections may be used to describe the covariance matrices in energy ranges where the cross sections in (MAT,3,MT) can be "derived" in terms of other "evaluated" cross sections in the same energy range. In the context of File 33, and for purposes of discussing "NC-type" sub-subsections, we define an "evaluated" cross section, in a given energy range, as one for which the covariance matrix in that energy range is given entirely in terms of "NI-type" sub-subsections. The covariance matrices involving the "derived" cross sections may be obtained in terms of the covariance matrices of the "evaluated" cross sections already given in File 33 and therefore need not be given explicitly again.

a. LTY=0, "Derived Redundant Cross Sections"

In File 33 the evaluator may indicate by means of an LTY=0 sub-subsection that in a given energy range the cross sections in (MAT,3,MT) were strictly obtained, in the general sense of evaluated, as a linear combination of other "evaluated" cross sections having the same MAT number but different MT values. We recall that we use the definition of "evaluated" cross sections in the sense that the covariances of these cross sections are given in File 33 only in terms of "NI-type" sub-subsections. In general the linear relationship given in an LTY=0 sub-subsection applies not only to the range of energy specified, but also over the whole range of the file; however, it may not be the method whereby the cross sections were obtained, in the sense of evaluated, over the whole energy range of the file.

The structure of an "NC-type" sub-subsection with LTY=0 is:

(MAT, 33, MT/ b, b; b, LTY=0; b, b) CONT

(MAT, 33, MT/ E1, E2: b, b; 2*NCI, NCI/ {CI, XMTI}) LIST

In the LIST record, E1 and E2 define an energy range where the cross sections given in the section (MAT,3,MT) were "derived" in terms of other "evaluated" cross sections given in the sections (MAT,3,MTI)s.

NCI is the number of pairs of values in the array {CI, XMTI}.*

{CI, XMTI} are pairs of numbers. The coefficient CI is associated in the pair with a value of MTI, given as a floating point number and indicated as XMTI. The pairs of numbers indicate, in the energy range E1 to E2, that the cross sections in file (MAT,3,MT), written as $^{MAT}\sigma_{MT}$ (E), were obtained in terms of the cross sections in files (MAT,3,MTI), written as $^{MAT}\sigma_{MTI}$ (E), as follows:

*The notation {AI,BI} stands for A_1, B_1; A_2, B_2; ...; A_i, B_i in a LIST record.

$$ {}^{MAT}\sigma_{MT}(E) = \sum_{i=1}^{NCI} C_i * {}^{MAT}\sigma_{MT_i}(E). $$

In this expression we have written the CI's as C_i, and XMTI's as MT_i. The numbers CI are constant numbers over the whole range of energy El to E2, usually $\pm$ 1.

Note: In general each subsection describes a single covariance matrix. However, when an "NC-type" sub-subsection with LTY=0 is used in a subsection, several covariance matrices may be implied and these are not explicitly given as subsections in the File 33 (see procedure II-a-3). Therefore, in such cases the subsection may be thought of as describing several covariance matrices.

b. LTY=1, 2 and 3, "Covariances of Cross Sections Derived via Ratio Measurements"

Many important cross sections of ENDF/B are determined through "ratio" measurements. Evaluation of cross sections by means of "ratio" measurements is one of the main sources of information on covariances of cross sections having different MAT values. These covariances play an important role in many applications where the results depend on the relative magnitude of different cross sections. In order to represent efficiently these important covariance matrices in the Files 33, evaluators may use "NC-type" sub-subsections with LTY=1, 2 and 3 in appropriate subsections of the Files 33.

Let the cross sections in (MAT,33,MT) be strictly "derived", in the general sense of evaluated, in the energy range El to E2, through the evaluation of ratio measurements to other "evaluated" cross sections given in (MATS,3,MTS), referred to also as the "standard" cross sections for this "ratio evaluation".

Then in the subsection (MAT,MT;MAT,MT) of the File 33 for the material MAT, an LTY=1 sub-subsection must be used to describe in part the covariance matrix in the energy range E1 to E2. This part, or component, of the covariance matrix, given by the LTY=1 sub-subsection, is derived from the covariance matrix of the "standard" cross sections in the subsection (MATS,MTS;MATS,MTS) of the File 33 of the "standard" material MATS. The other part, or component, of the covariance matrix comes from the evaluation of the "ratios" and is given explicitly, over the range E1 to E2, by means of "NI-type" sub-subsections in the subsection (MAT,MT;MAT,MT) of the File 33. In addition, since this method of evaluation introduces a covariance of the "derived" cross sections in (MAT,3,MT) over the energy range E1 to E2 and the "standard" cross sections in (MATS,3,MTS) over their complete energy range, in the File 33 of the material MAT, in subsection (MAT,MT;MATS,MTS), there must be an LTY=2 sub-subsection to describe this covariance matrix. This LTY=2 sub-subsection (which contains the same information as the previously given LTY=1 sub-subsection in the subsection (MAT,MT;MAT,MT)) refers to a different covariance matrix than the LTY=1 sub-subsection previously mentioned, but it can also be derived from the covariance matrix of the "standard" cross sections in the subsection (MATS,MTS;MATS,MTS)of the File 33 of the "standard" material MATS. Finally, as a consequence of the evaluation of the cross sections in (MAT,3,MT) in the energy range E1 to E2, as a "ratio" to the "standard" cross sections in (MATS,3,MTS), there must be in the subsection (MATS,MTS;MAT,MT) of the File 33 of the "standard" material MATS an LTY=3 sub-subsection (which also contains the same information as the previously given LTY=1 sub-subsection in the subsection (MAT,MT;MAT,MT)) serves in the material MATS the same role as the LTY=2 sub-subsection in the material MAT since they describe the same covariance matrix. But, in addition, the LTY value of 3

serves as a "flag" to the user, and the processing codes, to indicate that there are additional covariances of cross sections using the same "standard" cross sections (MATS,3,MTS) not explicitly given in the Files 33. These additional covariance matrices can be derived from the appropriate LTY=3 sub-subsections and the covariance matrix of the "standard" cross sections in the subsection (MATS,MTS;MATS,MTS) of the File 33 of the "standard" material MATS.

The structure of an "NC-type" sub-subsection with LTY=1,2 and 3 is:

(MAT, 33, MT/ b, b; b, LTY; b, b) CONT

(MAT, 33, MT/ E1, E2; MATS, MTS; 2*NEI, NEI/ {EI, WEI}) LIST

In the LIST record, E1 and E2 define an energy range where the cross sections given in the section (MAT,3,MT) were "derived" in terms of ratio measurements to "evaluated" cross sections given in section (MATS,3,MTS).

For ENDF/B-V the only value of NEI allowed is 2 and the list EI, WEI must be: {E1, 1.; E2, 0.}.

Note A: The above structure for LTY=1, 2 and 3 is dictated by two considerations:

1. Compatibility with the LTY=0 sub-subsection structure,

2. The possible extension of the use of the format LTY=1, 2 and 3 when the cross sections given in (MAT,3,MT) are only partially determined from ratio measurements to the cross sections given in (MATS,3,MTS). In such cases the list {EI, WEI} will indicate the relative weights of the ratio measurements in the evaluation of the cross sections in (MAT,3, MT).

Note B: LTY=1, 2 and 3 sub-subsections are all used as flags in subsections to describe relative covariance matrix components obtained from the relative covariance matrix of the "standard" cross sections already given in a File 33. There is, however, a major difference between covariance matrices ob-

tained with LTY=1 sub-subsections and those obtained from LTY=2 and 3 sub-subsections. This difference results from the definition of their use given above. LTY=2 and 3 sub-subsections are always used in subsections where one of the cross sections involved is the "standard" cross section used. The LTY=2 subsection appears in the File 33 of the material whose cross sections are "derived," whereas the LTY=3 sub-subsection appears in the File 33 of the material whose cross sections are the "standard"; LTY=1 sub-subsections always appear in subsections describing covariance matrices of cross sections "derived" from a "standard" and no LTY=2 or 3 sub-subsections may appear in such subsections. An LTY=1 sub-subsection describes a covariance matrix which in principle is a "square matrix" of dimension E1 to E2. An LTY=2 or 3 sub-subsection describes in principle a "rectangular matrix": the covariance matrix of the "derived" cross sections over the energy range E1 to E2 and of the "standard" cross sections over their complete energy range.

In general, if cross sections in (MAT,3,MT) are "derived," over an energy range E1 to E2, by "ratios" to "standard" cross sections in (MATS,3,MTS), there will be three "NC-type" sub-subsections with LTY=1, 2 and 3 generated in File 33. The LTY=1 sub-subsection is given in the subsection (MAT,MT;MAT,MT); the LTY=2 sub-subsection is given in the subsection (MAT,MT;MATS,MTS). Both of these subsections are given in the File 33 of the material MAT of the "derived" cross sections (MAT,3,MT). The LTY=3 sub-subsection is given in the subsection (MATS,MTS;MAT,MT) which is in the File 33 of the material MATS of the "standard" cross sections (MATS,3,MTS). There are, however, some instances, such as the one taken in example 33.4A, where "still another cross section" such as those in (MAT,3,MT1) are "indirectly derived" from the cross sections in (MATS,3,MTS) through evaluation of ratios of the cross sections in (MAT,3,MT1) to those in

(MAT,3,MT). In such cases an LTY=1 sub-subsection will also be used in the subsections (MAT,MT1;MAT,MT1) and (MAT,MT;MAT,MT1) and LTY=2 sub-subsection will also be used in the subsection (MAT,MT1;MATS,MTS). All three of these subsections are in the File 33 of the material MAT. Corresponding to the LTY=2 sub-subsection in the subsection (MAT,MT1;MATS,MTS) of the File 33 of the material MAT, there will also be an LTY=3 sub-subsection in the subsection (MATS,MTS;MAT,MT1) of the File 33 of the material MATS.

Note C: For purposes of discussing the covariance matrices of cross sections "derived" through evaluation of ratio measurements, the label "standard" cross sections was used for the cross sections relative to which the ratio measurements were made and the symbol (MATS,3,MTS) was used for these cross sections. The cross sections for which the label "standard" was used may be any "evaluated" cross sections of ENDF/B and are not restricted to the special set of "standard cross sections" maintained in the ENDF/B library. The "standard cross sections of ENDF/B" are the preferred ones to use for ratio measurements in order to minimize the magnitude of the covariance matrix elements obtained from LTY=1, 2 and 3 sub-subsections. However, they may not always be the ones which were used in the data available to evaluators to perform evaluations.

II. "NI-type" Sub-subsections

The "NI-type" sub-subsections are used to describe explicitly the various components of the covariance matrix given in the subsection. In each "NI-type" sub-subsection there is a flag, the LB flag, whose numerical value indicates whether the components are "relative" or "absolute" and the kinds of correlations as a function of energy represented by the components in the sub-subsection.

For values of the LB flag from 0 to 4, the "NI-type" sub-subsection has the following structure:

$\lceil$MAT,33,MT/b,b; LT, LB; 2*NP, NP/$\{E_k , F_k\}\{E_\ell , F_\ell\}$) LIST

LB is a flag whose numerical value determines the meaning of the numbers given in the arrays $\{E_k , F_k\}\{E_\ell , F_\ell\}$.

NP is the total number of pairs of numbers in the arrays $\{E_k , F_k\}\{E_\ell , F_\ell\}$.

LT is the number of pairs of numbers in the second array, $\{E_\ell , F_\ell\}$.

LT may be zero, in which case we have a single array $\lceil E_k , F_k \rceil$. When LT$\neq$0, we have two arrays and the first one, $\lceil E_k , F_k \rceil$, has (NP-LT) pairs of numbers in it.

$\{E_k , F_k\}\{E_\ell , F_\ell\}$ are two arrays of pairs of numbers. Each array is referred to as an E table, the E_k table and the E_ℓ table. In each E table the first member of a pair is an energy, E_n; the second member of the pair, F_n, is a number associated with the energy interval between the two entries E_n and E_{n+1}.

The E_k table, and the E_ℓ table when present, must cover the complete energy range of the file. The first energy entry in an E table must therefore be 10^{-5} eV and the last one $2 \times 10^{+7}$ eV. Some of the F_k's, or F_ℓ's, may be zero, as must be the case below threshold for a threshold reaction, and the last value of F in an E table must be zero since it is not defined.

We now define the meaning of the F values entered in the E tables for different values of LB. Let X_i refer to the cross section in (MAT,3,MT) at energy E_i and Y_j refer to the cross section in (MAT1,3,MT1) at energy E_j. The contribution of the sub-subsection to the covariance matrix $COV(X_i,Y_j)$, having the units

of "barns squared," described in the subsection, is defined as follows for the different values of LB:

LB=0 Absolute components only correlated within each E_k interval

$$COV(X_i,Y_j) = \sum_k P^{i;k}_{j;k} F_{xy,k}$$

LB=1 Fractional components only correlated within each E_k interval

$$COV(X_i,Y_j) = \sum_k P^{i;k}_{j;k} F_{xy,k} X_i Y_j$$

LB=2 Fractional components correlated over all E_k intervals

$$COV(X_i,Y_j) = \sum_{k,k'} P^{i;k}_{j;k'} F_{xy,k} F_{xy,k'} X_i Y_j$$

LB=3 Fractional components correlated over E_k and E_ℓ intervals

$$COV(X_i,Y_j) = \sum_{k,\ell} P^{i;k}_{j;\ell} F_{x,k} F_{yk\ell} X_i Y_j$$

LB=4 Fractional components correlated over all E_ℓ intervals within each E_k interval

$$COV(X_i,Y_j) = \sum_{K,\ell,\ell'} P^{i;k,\ell}_{j;k,\ell'} F_k F_{xy,\ell} F_{xy,\ell'} X_i Y_j.$$

For LB=0, 1 and 2 we have LT=0, i.e., only one E_k table. For LB=3 and LB=4 we have LT≠0, i.e., two E tables, the E_k and the E_ℓ tables.

The dimensionless operators P in the above definitions are defined in terms of the operator S as follows:

$$P^{i;k,\ell,\ldots}_{j;m,n,\ldots} \equiv S^k_i S^\ell_i \cdots S^m_j S^n_j \cdots ,$$

where

$S^k_i \equiv 1$ when the energy E_i is in the interval E_k to E_{k+1} of an E_k table,

$S^k_i \equiv 0$ when the energy E_i is outside the range of E_k to E_{k+1} of an E_k table.

It is often possible during the evaluation process to generate the relative covariance matrix of some cross sections averaged over some energy intervals. Such relative covariance matrices may be suitable for use in File 33. Although the use of LB=3 sub-subsections allows the representation of such matrices, one row (or one column) at a time this method of representation is very inefficient since one sub-subsection must be used for every row (or column) and the same energy mesh is repeated in the E_k table (or E_ℓ table) of every sub-subsection. Often, in addition, such relative covariance matrices are symmetric about their diagonal and there is no way to avoid repeating almost half of the entries with LB=3 sub-subsections. In order to allow such relative covariance matrices to be entered efficiently in the files directly LB=5 sub-subsections may be used. The following definition applies for LB=5 sub-subsections:

LB=5 Relative covariance matrix components

$$COV(X_i,Y_j) = \sum_{k,k'} P^{i;k}_{j;k'} F_{xy;k,k'} X_i Y_j$$

A single list of energies $\{E_k\}$ is required to specify the energy intervals labeled by the indices k and k'. The numbers $F_{xy;k,k'}$ represent fractional components correlated over the energy intervals E_k and $E_{k'}$.

Since we no longer have the need for the E_k tables with pairs of numbers (E_k,F_k) found in sub-subsections with LB<5 we need a new structure for LB=5 sub-subsections. The structure of an LB=5 sub-subsection is:

(MAT, 33, MT/ b, b; LS, LB=5; NT, NE/ $\{E_k\}\{F_{k,k'}\}$) LIST.

NT is the total number of entries in the two arrays $\{E_k\}$ and $\{F_{k,k'}\}$.

NE is the number of entries in the array $\{E_k\}$ defining (NE-1) energy intervals.

LS is a flag indicating whether the $F_{k,k'}$ matrix is symmetric or not:

LS=0 Asymmetric matrix

The matrix elements $F_{k,k'}$ are ordered by rows in the array $\{F_{k,k'}\}$:

$$\{F_{k,k'}\} \equiv F_{1,1} ; F_{1,2} ;\cdots; F_{1,NE-1} ; F_{2,2} ;\cdots; F_{NE-1,N}$$

There are $(NE-1)^2$ numbers in the array $\{F_{k,k'}\}$ and $NT=NE + (NE-1)^2$

LS=1 Symmetric matrix

The matrix elements $F_{k,k'}$ are ordered by rows starting from the diagonal term in the array $\{F_{k,k'}\}$:

$$\{F_{k,k'}\} \equiv F_{1,1} ; F_{1,2} ;\cdots; F_{1,NE-1} ; F_{2,2} ; F_{2,3} ;\cdots; F_{NE-1,NE-1}$$

There are NE*(NE-1)/2 numbers in the array $\{F_{k,k'}\}$ and

$$NT = NE + NE*(NE-1)/2$$

A lumped reaction is an evaluator-defined "redundant' cross section, defined in File 33 for the purpose of specifying the uncertainty in the sum of a set of cross sections, such as those for a set of neighboring discrete inelastic levels. The uncertainty in a lumped-reaction cross section, as well as its correlations with other reactions, are given in the usual way using the formats described above. On the other hand, the uncertainties and correlations of the individual parts or components of a lumped reaction are not given.

The File-33 section for one component of a lumped reaction consists of a single HEAD record that contains, in the second integer field, the section number MTL of the lumped reaction to which the component contributes. The value of MTL must lie in the range 851-870, which has been reserved specifically for lumped reactions. These MT-numbers may not be used in Files 3, 4 or 5, so the

net cross section and net scattering matrix for a lumped reaction must be constructed at the processing stage by summing over the reaction components.

A list of the components of a given lumped reaction is given only indirectly, namely, on the above-mentioned HEAD records. These special HEAD records, with MTL $\neq$ 0 and NL = 0, form a kind of index that can be scanned easily by the processing program in order to control the summing operation.

Except for the need to sum the cross-section components during uncertainty processing, lumped reactions are "normal" reactions, in that all covariance formats can be used to describe their uncertainties. For example, one expects in general that the covariances of a lumped reaction with other reactions, including other lumped reactions, will be given by the evaluator. Also, a lumped reaction may be represented, using an "NC-type" sub-subsection with LTY = 0, as being "derived" from other reactions, including other lumped reactions. (However, since uncertainties are not provided for the separate component reactions, a lumped reaction may not be represented as being "derived" from its components.)

33.3 Procedures

Although it is not necessary to have a section in File 33 for every section in File 3, the most important values of MT for the applications to which the evaluation was intended should have a section in File 33.

I. Ordering of Sections, Subsections and Sub-subsections

a. Sections

The sections in File 33 are ordered by increasing value of MT.

b. Subsections

Within a section, (MAT,33,MT), the subsections are ordered in a rigid manner. A subsection of File 33 is uniquely identified by the quartet of num-

bers: (MAT,MT;MAT1,MT1); the first pair of numbers indicate the section and the second pair of numbers appear in the appropriate field, MAT1 and MT1, of the CONT record which begins every subsection.

1. The subsections within a section are ordered by increasing values of MAT1.

2. In order to have the covariance matrices of the cross sections for which MAT1=MAT appear first in a section, and follow procedure I-b-1, the value MAT1=0 shall be used to mean MAT1=MAT in the CONT record which begins the subsection.

3. When there are several subsections with the same value of MAT1 in a section, these subsections shall be ordered by increasing values of MT1 given in the CONT record which begins the subsections.

4. When MAT1=0, which according to procedure I-b-2 means that MAT1=MAT, only subsections for MT1 $\geq$ MT shall be given.

c. Sub-subsections

When both "NC-type" and "NI-type" sub-subsections are present in a subsection, the format requires that the "NC-type" sub-subsections be given first.

1. "NC-type" sub-sections. Several "NC-type" sub-subsections may be given in a subsection. When more than one is given, these must be ordered according to the value of the energy range E1 to E2 given in the LIST record. We note that by definition, if several "NC-type" sub-subsections are given in a subsection, the energy ranges E1 to E2 of these different sub-subsections cannot overlap. The value of the LTY flag of "NC-type" sub-subsections does not affect the ordering of the sub-subsections within a subsection.

2. "NI-type" sub-subsections. There is no special ordering requirement of a "NI-type" sub-subsection within a subsection. However, it often happens that the full energy range of the file is covered by different sub-subsections, the F-values being set to zero in the E-tables outside the different ranges. It would improve the readability of the files if these different sub-subsections were grouped together by the energy range effectively covered in the sub-subsections.

II. Completeness

As previously stated, there is presently no minimum requirement on the number of sections and subsections in File 33. However, the presence of some subsections in a File 33, as well as the presence of some sub-subsections in a subsection, implies the presence of other subsections either in the same File 33 or the File 33 of another material. In what follows we shall identify the subsections by their value of the quartet:

(MAT,MT;MAT1,MT1)

a. Subsections for which MAT1=0

By subsections for which MAT1=0, we mean the subsection having the quartet: (MAT,MT;0,MT1), which according to procedure I-b-2 means MAT1=MAT.

1. If there is a subsection (MAT,MT;0,MT1) with MT1≠MT, there must be within the same File 33 the two subsections: (MAT,MT;0,MT) and (MAT,MT1;0,MT1). Note that the converse is not necessarily true since the two cross sections (MAT,3,MT) and (MAT,3,MT1) may have zero covariances, which are not required to be explicitly stated in the files. This procedure and procedure I-b-4 guarantee that every section of File 33, (MAT,33,MT), starts with the subsection (MAT,MT;0,MT).

2. In a subsection (MAT,MT;0,MT), if there is an "NC-type" sub-subsection with LTY=0, it contains a list of MTI values. There must be a subsection (MAT,MT;0,MTI) for every value of MTI given in the "NC-type" sub-subsection.

3. "NC-type" sub-subsections with LTY=0 must be given only in sub-sections of the type (MAT,MT;0,MT), i.e. with MT1=MT. "NC-type" sub-subsections with LTY=0, for "derived redundant cross sections," imply many covariance matrices of the "derived" cross sections and of the "evaluated" cross sections. It is the task of the processing code to generate these covariance matrices from the information given in the File 33.

4. In a subsection (MAT,MT;0,MT) if there is an "NC-type" sub-subsection with LTY=1, this sub-subsection contains values of MATS, MTS. There must be another material MATS with a File 33 containing the subsection (MATS,MTS;0,MTS). However, in the same File 33, there must be a sub-subsection (MAT,MT;MATS,MTS). Note that according to procedure III-a, given below, MATS must be different from MAT in an "NC-type" sub-subsection with LTY=1.

5. In a subsection (MAT,MT;0,MT), if there is an "NC-type" sub-subsection with LTY=1 which covers the energy range E1 to E2, in the same subsection there must be some "NI-type" sub-subsections with F-values different from zero in this energy range E1 to E2. These "NI-type" sub-subsections represent the relative covariance matrix of the evaluated ratio measurements.

b. Subsection for MAT1≠0

If there is a subsection (MAT,MT;MAT1,MT1) with MAT1≠0, similar to procedure II-a-1, there must also be a subsection (MAT,MT;0,MT) in the same File 33, but there must also be the two sub-subsections: (MAT1,MT1;0,MT1) and (MAT1,MT1;MAT,MT) in the File 33 for material MAT1.

III. Other Procedures

a. "NC-type" sub-subsections with LTY=1 shall only be used with MATS≠MAT. The use of LTY=1 sub-subsections is reserved for covariance matrix components arising out of ratio measurements of cross sections of different nuclides, i.e. different values of MAT.

b. If a single "NC-type" sub-subsection with LTY=0 is used in a subsection and there are no "NI-type" sub-subsections, the value of E1 must be 10^{-5} eV and the value of E2 must be $2 \times 10^{+7}$ eV.

c. As a consequence of the definition of "NC-type" sub-subsections with LTY=0, if there are any "NI-type" sub subsections in the same sub-section, the F-values in their E-tables must be zero within the range E1 to E2 of these "NC-type" sub-subsections.

d. "NI-type" sub-subsections with LB=0 shall in general be avoided and forbidden in the case of cross sections involved in ratio measurements. Therefore the "standard cross sections of ENDF/B" shall not have LB=0, "NI-type" sub-subsections. The use of LB=0 "NI-type" sub-subsections should be reserved for the description of covariance matrices of cross sections which fluctuate rapidly and for which details of the uncertainties in the "deep valleys" of the cross sections are important.

e. The formats of File 33 allow for the possibility of great details to be entered in the files if needed. The number of "NI-type" sub-subsections and the number of energy entries in their E_k and E_ℓ tables will be a function of the details of the covariance matrices available and the need to represent them within their estimated accuracies. However, good judgement should be used to minimize as much as possible the number of different entries in the E_k and E_ℓ tables. The important quantity to remember is the union of all of the E values

of the E_k and E_ℓ tables of a File 33. A reasonable upper limit of the order of 100 different E values for the union of all energy entries in all of the E_k and E_ℓ tables in a File 33 should be considered.

f. The lumping of reactions for uncertainty purposes will be useful mainly in connection with discrete-level inelastic scattering cross sections. However, other reactions, such as (n,n'p), (n,n'α), and (n,n' continuum), may also be treated in this way.

g. In order not to lose useful uncertainty information, reactions lumped together should have similar characteristics. Ordinarily, the level energies of discrete inelastic levels lumped together should not span a range greater than 30-40%, and the angular distributions should be similar.

h. The components of a lumped reaction need not have adjacent MT-numbers.

i. Lumped-reaction MT-numbers must be assigned sequentially, beginning at 851. The sequence is determined by ordering the lumped reactions according to the lowest MT-number of their respective components. Thus, the first value of MTL encountered on any component-reaction HEAD record will be 851. The next new value of MTL encountered will be 852, and so on.

j. Lumped reactions with only a single component are permitted. This is recommended practice when, for example, an important discrete inelastic level is treated individually, while all of its neighbors are lumped. Covariances for both the individual level and the nearby lumped levels can then be placed together in sections 851-870.

33.4 Example

We illustrate here the use of File 33 by means of two concrete examples.

A. Use of LTY=1 and LTY=2 "NC-type" subsections

Let us consider the hypothetical evaluation of Pu-239, MAT=1264. The decision is made that in File 33 only the fission cross sections and the capture cross sections shall have covariances represented. The following methods were used in performing the evaluation:

1. Fission cross sections, MT=18

Let X_i stand for the fission cross section of Pu-239 at the energy E_i.

a. From 10^{-5} eV to an energy ES, X_i was evaluated in terms of "direct" or "absolute" measurements, A_i. By this we mean that in this energy range, X_i and its uncertainties are independent of any other cross sections. In this energy range $X_i \equiv A_i$.

b. From ES to 20 MeV, X_i was evaluated by means of ratio measurements to Y_i the fission cross section of U-235, to which we assign the MAT number 1261. In this energy range $X_i = R_i Y_i$, where R_i is the evaluated ratio at energy E_i.

2. Capture cross sections, MT=102

Let Z_i stand for the capture cross section of Pu-239 at the energy E_i. In this evaluation, Z_i was obtained by the evaluation of a_i over the complete range of the file. Therefore we have $Z_i = a_i X_i$.

In this evaluation then, only 3 quantities were evaluated: A_i from 10^{-5} eV to ES, R_i from ES to 20 MeV, and a_i from 10^{-5} eV to 20 MeV. The evaluation of these quantities resulted in the evaluation of three covariance matrices: $COV(A_i,A_j)$, $COV(R_i,R_j)$ and $COV(a_i,a_j)$. Let us now assume that in addition it has been determined that the uncertainties in these three different

quantities are uncorrelated, i.e. covariances such as $COV(A_i,a_j)$ are essentially zero.

Let us denote relative covariance matrices such as $\frac{COV(A_i,A_j)}{A_i\ A_j}$ as $\langle dA_i \cdot dA_j \rangle$, and similarly for the other quantities.

From 10^{-5} eV to ES, since $X_i = A_i$ and $Z_i = a_i X_i$, we have:

$$\langle dX_i \cdot dX_j \rangle = \langle dA_i \cdot dA_j \rangle$$

$$\langle dX_i \cdot dZ_j \rangle = \langle dA_j \cdot dA_j \rangle$$

$$\langle dZ_i \cdot dZ_j \rangle = \langle da_i \cdot da_j \rangle + \langle dA_i \cdot dA_j \rangle$$

From ES to 20 MeV, since $X_i = R_i Y_i$ and $Z_i = a_i X_i$, we have:

$$\langle dX_i \cdot dX_j \rangle = \langle dR_i \cdot dR_j \rangle + \langle dY_i \cdot dY_j \rangle$$

$$\langle dX_i \cdot dZ_j \rangle = \langle dR_i \cdot dR_j \rangle + \langle dY_i \cdot dY_j \rangle$$

$$\langle dX_i \cdot dY_j \rangle = \langle dY_i \cdot dY_j \rangle$$

$$\langle dZ_i \cdot dZ_j \rangle = \langle da_i \cdot da_j \rangle + \langle dR_i \cdot dR_j \rangle + \langle dY_i \cdot dY_j \rangle$$

$$\langle dZ_i \cdot dY_j \rangle = \langle dY_i \cdot dY_j \rangle$$

We note that in the above we have expressed all of the covariance matrices of the cross sections only in terms of the covariance matrices of the evaluated quantities and the covariance matrix of the U-235 fission.

For purposes of illustrating the use of the formats we need not know the details of how the covariance matrices $\langle dA_i \cdot dA_j \rangle$, $\langle dR_i \cdot dR_j \rangle$ and $\langle da_i \cdot da_j \rangle$ are represented. They must be represented by one or more "NI-type" sub-subsections having an E_k table, or could be so represented. For our purposes, we symbolically represent each one of them in terms of a single "NI-type" sub-subsection with a single E_k table:

$$\langle dA_i \cdot dA_j \rangle \rightarrow \{E_k^A, F_k^A\}$$

$$\langle dR_i \cdot dR_j \rangle \rightarrow \{E_k^R, F_k^R\}$$

$$\langle da_i \cdot da_j \rangle \rightarrow \{E_k^a, F_k^a\}$$

Whether one or more "NI-type" sub-subsection is used, each one of the E tables used in the sub-subsections can be written as:

$$\{E_k^A, F_k^A\} = \{1.0E\text{-}5,\ F_1^A; \ldots;\ E_k^A, F_k^A; \ldots;\ ES,\ 0.0;\ 2.0E+7, 0.0\},$$

$$\{E_k^R, F_k^R\} = \{1.0E\text{-}5,\ 0.0;\ ES,\ F_1^R; \ldots;\ E_k^R,\ F_k^R; \ldots;\ 2.0E+7, 0.0\},$$

$$\{E_k^a, F_k^a\} = \{1.0E\text{-}5,\ F_1^a;\ \ldots;\ E_k^a, F_k^a;\ \ldots;\ 2.0E+7,\ 0.0\},$$

the E and F values explicitly shown must have the values indicated above for this example.

In the listing given in Table 33.2 for the File 33 of MAT=1264, corresponding to our example, we have shown with only one sub-subsection each of the matrices $\langle dA_i \cdot dA_j \rangle$, $\langle dR_i \cdot dR_j \rangle$ and $\langle da_i, da_j \rangle$ with the E tables indicated symbolically as:

(EAK, FAK) for $\{E_k^A, F_k^A\}$, etc.

Note: In the File 33 of MAT-1261 in the subsections (1261, 18;1264,18) and (1261,18;1264,102) and LTY=3 "NC-type" sub-subsection corresponding to the LTY=2 sub-subsections of Table I-33 must be inserted.

B. Use of LTY=0, "NC-type" sub-subsections

Let us consider a hypothetical evaluation of C-12, MAT=1274. The decision is made that in File 33 the MT values 1,2,4,102 and 107 shall have covariances represented. We shall use the notation developed in the previous example. The following method was used in this evaluation:

Table 33.2

```
                                  (1264,18;0,18)
9.42390+ 4 2.36999+ 2          0           0           0          3126433 18 HEAD
0.00000+ 0 0.00000+ 0          0          18           1          2126433 18 CONT
0.00000+ 0 0.00000+ 0          0           1           0          0126433 18 CONT
2.00000+ 5 2.00000+ 7       1261          18           4          2126433 18 LIST
2.00000+ 5 1.00000+ 0 2.00000+ 7 0.00000+ 0                        126433 18<dYi•dYj>
0.00000+ 0 0.00000+ 0          0           1          14          7126433 18 LIST
1.00000- 5 0.00000+ 0 1.00000+ 0 2.50000- 3 3.00000+ 2 3.60000- 3126433 18<dAi•dAj>
3.00000+ 4 4.90000- 3 1.00000+ 5 6.40000- 3 2.00000+ 5 0.00000+ 0126433 18
2.00000+ 7 0.00000+ 0                                              126433 18
0.00000+ 0 0.00000+ 0          0           1           6          3126433 18 LIST
1.00000- 5 0.00000+ 0 2.00000+ 5 4.00000- 4 2.00000+ 7 0.00000+ 0126433 18<dRi•dRj>
                                  (1264,18;0,102)
0.00000+ 0 0.00000+ 0          0         102           1          2126433 18 CONT
0.00000+ 0 0.00000+ 0          0           1           0          0126433 18 CONT
2.00000+ 5 2.00000+ 7       1261          18           4          2126433 18 LIST
2.00000+ 5 1.00000+ 0 2.00000+ 7 0.00000+ 0                        126433 18<dYi•dYj>
0.00000+ 0 0.00000+ 0          0           1          14          7126433 18 LIST
1.00000- 5 0.00000+ 0 1.00000+ 0 2.50000- 3 3.00000+ 2 3.60000- 3126433 18<dAi•dAj>
3.00000+ 4 4.90000- 3 1.00000+ 5 6.40000- 3 2.00000+ 5 0.00000+ 0126433 18
2.00000+ 7 0.00000+ 0                                              126433 18
0.00000+ 0 0.00000+ 0          0           1           6          3126433 18 LIST
1.00000- 5 0.00000+ 0 2.00000+ 5 4.00000- 4 2.00000+ 7 0.00000+ 0126433 18<dRi•dRj>
                               (1264,18;1261,18)
0.00000+ 0 0.00000+ 0       1261          18           1          0126433 18 CONT
0.00000+ 0 0.00000+ 0          0           2           0          0126433 18 CONT
2.00000+ 5 2.00000+ 7       1261          18           4          2126433 18 LIST
2.00000+ 5 1.00000+ 0 2.00000+ 7 0.00000+ 0                        126433 18<dYi•dYj>
0.00000+ 0 0.00000+ 0          0           0           0          0126433  0 SEND
                                  (1264,102;0,102)
9.42390+ 4 2.36999+ 2          0           0           0          2126433102 HEAD
0.00000+ 0 0.00000+ 0          0         102           1          3126433102 CONT
0.00000+ 0 0.00000+ 0          0           1           0          0126433102 CONT
2.00000+ 5 2.00000+ 7       1261          18           4          2126433102 LIST
2.00000+ 5 1.00000+ 0 2.00000+ 7 0.00000+ 0                        126433102<dYi•dYj>
0.00000+ 0 0.00000+ 0          0           1          14          7126433102 LIST
1.00000- 5 0.00000+ 0 1.00000+ 0 2.50000- 3 3.00000+ 2 3.60000- 3126433102<dAi•dAj>
3.00000+ 4 4.90000- 3 1.00000+ 5 6.40000- 3 2.00000+ 5 0.00000+ 0126433102
2.00000+ 7 0.00000+ 0                                              126433102
0.00000+ 0 0.00000+ 0          0           1           6          3126433102 LIST
1.00000- 5 0.00000+ 0 2.00000+ 5 4.00000- 4 2.00000+ 7 0.00000+ 0126433102<dRi•dRj>
0.00000+ 0 0.00000+ 0          1           5          21          6126433102 LIST
1.00000- 5 2.53000- 2 9.00000- 2 2.50000- 1 1.00000+ 0 2.00000+ 7126433102<dαi•dαj>
2.21000- 3 4.84000- 4 3.62000- 4 3.56000- 4 0.00000+ 0 4.84000- 4126433102
3.10000- 4 3.04000- 4 0.00000+ 0 6.25000- 4 2.30000- 4 0.00000+ 0126433102
2.21000- 3 0.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0126433102
                               (1264,102;1261,18)
0.00000+ 0 0.00000+ 0       1261          18           1          0126433102 CONT
0.00000+ 0 0.00000+ 0          0           2           0          0126433102 CONT
2.00000+ 5 2.00000+ 7       1261          18           4          2126433102 LIST
2.00000+ 5 1.00000+ 0 2.00000+ 7 0.00000+ 0                        126433102<dYi•dYj>
0.00000+ 0 0.00000+ 0          0           0           0          0126433  0 SEND
```

1. Total cross sections, MT=1

The total cross sections, σ_i^T, were evaluated over the complete energy range, with the covariance matrix obtained, and:

$$<d\sigma_i^T \cdot d\sigma_j^T> \rightarrow \{E_k^T, F_k^T\} ,$$

with

$$\{E_k^T, F_k^T\} = \{1.0E\text{-}5,\ F_1^T; \ldots;\ E_k^T, F_k^T; \ldots;\ 2.0E+7,\ 0.0\}$$

2. Elastic cross sections, MT=2

The elastic cross sections, σ_i^E, were "derived" up to 8.5 MeV from the "evaluated" cross sections:

$$\sigma_i^E = \sigma_i^T - \sigma_i^I - \sigma_i^C - \sigma_i^\alpha .$$

Above 8.5 MeV the elastic cross sections were evaluated and:

$$<d\sigma_i^E \cdot d\sigma_j^E> \rightarrow \{E_k^E, F_k^E\} ,$$

with

$$\{E_k^E, F_k^E\} = \{1.0E\text{-}5,\ 0.0;\ 8.5E+6,\ F_1^E;\ \ldots;\ E_k^E, F_k^E; \ldots; 2.0E+7,\ 0.0\}.$$

3. Inelastic cross sections, MT=4

The inelastic cross sections, σ_i^I, were evaluated from threshold, 4.8 MeV, to 8.5 MeV and:

$$<d\sigma_i^I, d\sigma_i^I> \rightarrow \{E_k^I, F_k^I\} ,$$

with

$$\{E_k^I, F_k^I\} = \{1.0E\text{-}5,\ 0.0;\ 4.8E+6,\ F_1^I; \ldots;\ E_k^I, F_k^I; \ldots;\ 8.5E+6,\ 0.0;\ 2.0E+7,\ 0.0\}\ .$$

Above 8.5 MeV the inelastic cross sections were "derived" and:

$$\sigma_i^I = \sigma_i^T - \sigma_i^E - \sigma_i^C - \sigma_i^\alpha\ .$$

4. Capture cross sections, MT=102

The capture cross sections, σ_i^C, were evaluated over the complete energy range and:

$$\langle d\sigma_i^C \cdot d\sigma_j^C \rangle \rightarrow \{E_k^C, F_k^C\}\ ,$$

with

$$\{E_k^C, F_k^C\} = \{1.0E\text{-}5,\ F_1^C; \ldots;\ E_k^C,\ F_k^C; \ldots;\ 2.0E+7,\ 0.0\}\ .$$

5. The (n,α) cross sections, MT=107

The (n,α) cross sections, σ_i^α, were evaluated from threshold, 6.18 MeV to 20 MeV and:

$$\langle d\sigma_i^\alpha \cdot d\sigma_j^\alpha \rangle \rightarrow \{E_k^\alpha, F_k^\alpha\}$$

with

$$\{E_k^\alpha, F_k^\alpha\} = \{1.0E\text{-}5,\ 0.0;\ 6.18E+6,\ F_1^\alpha; \ldots;\ E_k^\alpha,\ F_k^\alpha; \ldots;\ 2.0E+7,\ 0.0\}\ .$$

In the listing given in Table 33.3 for File 33 of MAT=1274, corresponding to our example, we have shown only one "NI-type" sub-subsection for each evaluated covariance matrix with the E tables indicated symbolically as:

$$\text{(ETK, FTK) for } \{E_k^T,\ F_k^T\} \text{ etc...}$$

The above example has great similarity to the way the evaluation of C-12 was made, the major difference being that instead of MT=4 being evaluated, the evaluation was made for MT=51 and MT=91. Since it will illustrate some of the procedures of File 33, let us now consider adding to the above File 33 for MAT=1274 the covariance matrices for MT=51 and MT=91.

a. MT=51

The inelastic scattering to the first excited state, σ_i^{51}, up to 8.5 MeV is identical to σ_i^I. Therefore we may consider up to 8.5 MeV that σ_i^{51} is a "derived" cross section with: $\sigma_i^{51} = \sigma_i^I$. This is permissible because MT=4 has only "NI-type" sub-subsections in this energy range.

From 8.5 MeV to 20 MeV, MT=51 was evaluated and:

$$\langle d\sigma_i^{51} \cdot d\sigma_j^{51} \rangle \rightarrow \{E_k^{51},\ F_k^{51}\}\ .$$

with

$$\{E_k^{51},\ F_k^{51}\} = \{1.0E\text{-}5,\ 0.0;\ 8.5E+6,\ F_1^{51};\ldots;\ E_k^{51},\ F_k^{51};\ldots;\ 2.0E+7,0.0\}.$$

b. MT=91

From 8.5 to 20 MeV, the continuum inelastic, σ_i^{91}, was "derived" as: $\sigma_i^{91} = \sigma_i^I - \sigma_i^{51}$. However, we cannot use this relationship for

purposes of File 33 because σ_i^I in this energy range is indicated in the file as being already "derived."

Therefore, for purposes of File 33, we must write:

$$\sigma_i^{91} = \sigma_i^T - \sigma_i^E - \sigma_i^{51} - \sigma_i^C - \sigma_i^\alpha$$

which now only refers to cross sections having exclusively "NI-type" sub-subsections. Therefore we may now add the sections to the File 33, MAT=1274, shown in Table 33.4, to have a more complete File 33.

Table 33.3

```
                                    (1274,1;0,1)
 6.01200+ 3 1.18969+ 1          0          0          0          1112733  1 HEAD
 0.00000+ 0 0.00000+ 0          0          1          0          1112733  1 CONT
 0.00000+ 0 0.00000+ 0          0          1          6          3112733  1 LIST
 1.00000- 5 0.00000+ 0 2.00000+ 6 2.50000- 5 2.00000+ 7 0.00000+ 0112733  1
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  0 SEND
                                    (1274,2;0,2)
 6.01200+ 3 1.18969+ 1          0          0          0          1112733  2 HEAD
 0.00000+ 0 0.00000+ 0          0          2          1          1112733  2 CONT
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  2 CONT
 1.00000- 5 8.50000+ 6          0          0          8          4112733  2 LIST
 1.00000+ 0 1.00000+ 0-1.00000+ 0 4.00000+ 0-1.00000+ 0 1.02000+ 2112733  2
-1.00000+ 0 1.07000+ 0                                                 112733  2
 0.00000+ 0 0.00000+ 0          0          1          8          4112733  2 LIST
 1.00000- 5 4.00000- 6 1.00000+ 3 8.00000- 6 2.00000+ 6 2.50000- 5112733  2
 2.00000+ 7 0.00000+ 0                                                 112733  2
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  0 SEND
                                    (1274,4;0,4)
 6.01200+ 3 1.18970+ 1          0          0          0          1112733  4 HEAD
 0.00000+ 0 0.00000+ 0          0          4          1          1112733  4 CONT
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  4 CONT
 8.50000+ 6 2.00000+ 7          0          0          8          4112733  4 LIST
 1.00000+ 0 1.00000+ 0-1.00000+ 0 2.00000+ 0-1.00000+ 0 1.02000+ 2112733  4
-1.00000+ 0 1.07000+ 2                                                 112733  4
 0.00000+ 0 0.00000+ 0          0          1         20         10112733  4 LIST
 1.00000- 5 0.00000+ 0 8.29600+ 6 1.00000- 2 8.45000+ 6 2.50000- 3112733  4
 8.95000+ 6 1.00000- 2 1.10000+ 7 4.00000- 2 1.20000+ 7 4.00000- 2112733  4
 1.30000+ 7 2.25000- 2 1.40000+ 7 1.00000- 2 1.50000+ 7 4.00000- 2112733  4
 2.00000+ 7 0.00000+ 0                                                 112733  4
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  0 SEND
                                  (1274,102;0,102)
 6.01200+ 3 1.18969+ 1          0          0          0          1112733102 HEAD
 0.00000+ 0 0.00000+ 0          0        102          0          1112733102 CONT
 0.00000+ 0 0.00000+ 0          0          1          6          3112733102 LIST
 1.00000- 5 3.60000- 3 1.00000+ 3 4.00000- 2 2.00000+ 7 0.00000+ 0112733102
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  0 SEND
                                  (1274,107;0,107)
 6.01200+ 3 1.18969+ 1          0          0          0          1112733107 HEAD
 0.00000+ 0 0.00000+ 0          0        107          0          1112733107 CONT
 0.00000+ 0 0.00000+ 0          0          0          8          4112733107 LIST
 1.00000- 5 0.00000+ 0 6.32000+ 6 1.00000- 4 7.36000+ 6 0.00000+ 0112733107
 2.00000+ 7 0.00000+ 0                                                 112733107
 0.00000+ 0 0.00000+ 0          0          0          0          0112733  0 SEND
```

Table 33.4

```
                                    (1274,51;0,51)
 6.01200+ 3 1.18969+ 1           0           0           0           1127433 51 HEAD
 0.00000+ 0 0.00000+ 0           0          51           1           1127433 51 CONT
 0.00000+ 0 0.00000+ 0           0           0           0           0127433 51 CONT
 1.00000- 5 8.50000+ 6           0           0           2           1127433 51 LIST
 1.00000+ 0 4.00000+ 0                                                127433 51
 0.00000+ 0 0.00000+ 0           0           1           6           3127433 51 LIST
 1.00000- 5 0.00000+ 0 8.29600+ 6 2.50000- 3 2.00000+ 7 0.00000+ 0127433 51
 0.00000+ 0 0.00000+ 0           0           0           0           0127433  0 SEND
                                    (1274,91;0,91)
 6.01200+ 3 1.18969+ 1           0           0           0           1127433 91 HEAD
 0.00000+ 0 0.00000+ 0           0          91           1           0127433 91 CONT
 0.00000+ 0 0.00000+ 0           0           0           0           0127433 51 CONT
 8.50000+ 6 2.00000+ 7           0           0          10           5127433 51 LIST
 1.00000+ 0 1.00000+ 0-1.00000+ 0 2.00000+ 0-1.00000+ 0 5.10000+ 1127433 51
-1.00000+ 0 1.02000+ 2-1.00000+ 0 1.07000+ 2                          127433 51
 0.00000+ 0 0.00000+ 0           0           0           0           0127433  0 SEND
```

MT	Description
114	(n,d2α) cross section
115-119	(to be assigned)
120	Target destruction = nonelastic less total (n,n'γ)
121-150	(to be assigned)
151	General designation for resonance information
152-200	(to be assigned for specific resonance information)
201-202	(to be assigned)
203	Total hydrogen production
204	Total deuterium production
205	Total tritium production
206	Total ^{3}He production
207	Total ^{4}He production
208-250	(to be assigned)
251	$\bar{\mu}_L$, the average cosine of the scattering angle (laboratory system) for elastic scattering
252	ξ, the average logarithmic energy decrement for elastic scattering
253	γ, the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic decrement for elastic scattering
254-300	(to be assigned)
301-450	Energy release rate parameters, $\overline{E^*\sigma}$, for total and partial cross sections. Subtract 300 from this number to obtain the specific reaction type identification. For example, MT = 302 = (300 + 2) denotes elastic scattering
451	Heading or title information (given only in File 1)
452	$\bar{\nu}$, average total (prompt plus delayed) number of neutrons released per fission event
454	Independent fission product yield data
455	Delayed neutrons from fission

MT	Description
456	Prompt neutrons from fission
457	Radioactive decay data
458	Energy Release in fission
459	Cumulative fission product yield data
465	Delayed neutrons from spontaneous fission
466	Prompt neutrons from spontaneous fission
467-500	(to be assigned)
501	Total photon interaction cross section
502	Photon coherent scattering
503	(to be assigned)
504	Photon incoherent scattering
505-514	(to be assigned)
515	Pair production, electron field
516	Pair production, nuclear and electron field (i.e., pair plus triplet production)
517	Pair production, nuclear field
518	Photofission (γ,f)
519-531	(to be assigned)
532	Photoneutron (γ,n)
533	Total photonuclear
534-601	(to be assigned)
602	Photoelectric
603-699	(to be assigned)
700	(n,p_0) cross section (cross section for leaving the residual nucleus in the ground state)
701	(n,p_1) cross section for 1st excited state
702	(n,p_2) " " " 2nd "

MT	Description
703	(n,p_3) " " " 3rd "
704	(n,p_4) cross section for 4th excited state
.	
.	
.	
718	(n,p_c) " " " continuum excited state
719	(n,p_c') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing proton)
720	(n,d_0) cross section for ground state
721	(n,d_1) cross section for 1st excited state
722	(n,d_2) cross section for 2nd excited state
.	
.	
.	
738	(n,d_c) cross section for continuum excited state
739	(n,d_c') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing deuteron)
740	(n,t_0) cross section for ground state
741	(n,t_1) " " " 1st excited state
742	(n,t_2) " " " 2nd " "
.	
.	
.	
750	(n,t_c) " " " continuum excited state
759	(n,t_c') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing triton)
760	$(n,{}^3He_0)$ cross section for ground state
761	$(n,{}^3He_1)$ cross section for 1st excited state
.	
.	
.	
778	$(n,{}^3He_c)$ cross section for continuum
779	$(n,{}^3He_c)$ cross section for continuum specifically not included in σ total (redundant, used for describing outgoing ^3He)
780	(n,α_0) cross section for ground state

MT	Description
781	(n,α_1) cross section for 1st excited state
.	
.	
.	
798	(n,α_c) cross section for continuum
799	(n,α_c') cross section for continuum specifically not included in σ_T (redundant, used to describe outgoing α)
800-999	(to be assigned)

$$\sigma^{\ell}_{n,f}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{fr}}{(E-E'_r)^2 - \frac{1}{4}\Gamma_r^2}$$

and Γ_{fr} is the fission width.

4. The Competitive Reaction Cross Section The competitive reaction cross section, $\sigma_{n,x}(E)$, is given in terms of analogous formulas involving Γ_{xr} the competitive width. By convention, the cross section for the competitive reaction is given entirely in File 3, and is not to be computed from the resonance parameters. The reason for this is that the latter calculation can be done correctly only in the case of a single competitive channel, since the file can define only a single competitive width.

The statistical factor $g_J = (2J+1)/2(2I+1)$ is obtained from the target spin I and the resonance spin J given in File 2 as SPI and AJ, respectively.

The sum on ℓ extends over all ℓ-states described. There will be NLS terms in the sum. NLS is given in File 2 for each isotope. It is important for the evaluator to provide, and processing codes to include, contributions from ℓ-values for which there are no resonances, in order that the potential scattering be correctly calculated.

The sum on J extends over all possible J-states for a particular ℓ-state. NR is the number of resonances for a given pair of ℓ and J values.

$$NRS = \sum_{J} NR_J$$

NRS is given in File 2 for each ℓ-value.

$\Gamma_{nr}(|E_r|) \equiv GN_r$ is the neutron width, for the r^{th} resonance for a particular value of ℓ, evaluated at the resonance energy E_r. For bound levels, the absolute value $|E_r|$ is used.

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

$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr} + \Gamma_{xr}$ is the total width, a function of energy through Γ_{nr} and (possibly) Γ_{xr} since $\Gamma_{\gamma r}$ and Γ_{fr} are assumed constant with respect to energy. The "competitive" width, Γ_{xr} is not entered explicitly in File 2. It is calculated implicitly from the equation:

$$\Gamma_{xr} = \Gamma_r - \Gamma_{nr} - \Gamma_{\gamma r} - \Gamma_{fr} \quad \text{at } E_r$$

The following quantities are given in File 2 for each resonance:

E_r = ER, the resonance energy

J = AJ, the spin of the resonance state

$\Gamma_{nr}(|E_r|)$ = GN, the neutron width

$\Gamma_{\gamma r}$ = GG, the radiation width

Γ_{fr} = GF, the fission width and

$\Gamma_r(|E_r|)$ = GT, the total width evaluated at the resonance energy.

Since the competitive width, Γ_{xr}, is not given, Γ_r should be obtained from File 2 directly, and <u>not</u> by summing partial widths. Γ_{xr}, if non-zero, should be obtained by subtraction.

For p-, d-, and higher ℓ-values, the primed resonance energy E_r' is energy-dependent:

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

although the fact that the shift is zero at <u>each</u> E_r is an artifact of the SLBW formalism, and implies a different R-matrix boundary condition for each resonance.

$$k = 2.196771 \frac{AWRI}{AWRI + 1.0} \times 10^{-3}\sqrt{E},$$

is the neutron wave number in the center-of-mass system, in terms of the laboratory energy, and AWRI is the ratio of the mass of a particular isotope to that of the neutron. E is the incident neutron energy (Laboratory system, eV); S_ℓ is the shift factor,

$$S_o = 0$$

$$S_1 = -\frac{1}{1 + \rho^2}$$

$$S_2 = -\frac{18 + 3\rho^2}{9 + 3\rho^2 + \rho^4}$$

P_ℓ is the penetration factor,

$$P_o = \rho$$

$$P_1 = \frac{\rho^3}{1 + p^2}$$

$$P_2 = \frac{\rho^5}{9 + 3\rho^2 + \rho^4}$$

where $\rho = ka$ and "a" is the channel radius (in units of 10^{-12} cm), defined as

$$a = .123\ AWRI^{1/3} + .08;\ AWRI = A/1.00865^*$$

ϕ_ℓ is the (negative of a) hard-sphere phase shift,

$$\phi_0 = \hat{\rho}$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho}$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\frac{3\hat{\rho}}{3-\hat{\rho}^2},$$

where $\hat{\rho} = k\,(AP)$ and AP is the scattering radius, given in File 2, which determines the low energy potential scattering cross section.

D.1.2. Multilevel Breit-Wigner Formula: LRU=1, LRF=2

The equations are exactly the same as above, except that a resonance-resonance interference term is included in the equation for elastic scattering of ℓ-wave neutrons, $\sigma^{\ell}_{n,n}(E)$:

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

This form, which as $\sim N^2/2$ energy-dependent terms and can involve a great deal of computer time, can be written in the following form with only N terms: (See Section 2.4.15)

*A is the target mass in amu. The channel radius, strictly speaking, involves $A^{1/3}$, and not $(AWRI)^{1/3}$, but as long as the mass of the incident particle is approximately unity, as it is for neutrons, the difference is not important.

$$\frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{G_r \Gamma_r + 2H_r (E-E'_r)}{(E-E'_r)^2 + (\Gamma_r/2)^2} \tag{2}$$

where

$$G_r = \frac{1}{2} \sum_{\substack{s=1 \\ (s \neq r)}}^{NR_J} \frac{\Gamma_{nr} \Gamma_{ns} (\Gamma_r + \Gamma_s)}{(E'_r - E'_s)^2 + \frac{1}{4}(\Gamma_r + \Gamma_s)^2} , \tag{3}$$

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

For the user who does not require ψ- and χ-broadening, the following equations, which are mathematically identical to the MLBW equations, require very little computing time: (See Section 2.4.20)

$$\sigma_{n,n}(E) = \sum_{\ell=0}^{NLS} \sigma^{\ell}_{n,n}(E) \tag{5}$$

$$\sigma^{\ell}_{nn}(E) = \frac{\pi}{k^2} \sum_{J} g_J \left| 1 - U^J_{nn}(E) \right|^2 \tag{6}$$

$$U^J_{nn}(E) = \exp(2i\phi_\ell) - \sum_{r=1}^{NR_J} \frac{i\Gamma_{nr}}{E'_r \quad \Gamma_r/2} \tag{7}$$

D.1.3. Reich-Moore Formulae

A detailed derivation of these formulae is to be found in Reich and Moore.[2] Neutron cross sections with an exit channel c are given by*

$$\sigma_{nc} = \frac{\pi}{k^2} \sum_J g_J \left| \delta_{nc} - U^J_{nc} \right|^2 \quad , \tag{1}$$

where k and g_J are the same as in the previous section.

In the Reich-Moore formalism one has for the scattering matrix, labelled by channel subscripts (n in, c out)

$$U^J_{nc} = e^{-i(\phi_n + \phi_c)} \left\{ 2\left((I-K)^{-1} \right)_{nc} - \delta_{nc} \right\} \quad , \tag{2}$$

where

$$(I-K)_{cc'} = \delta_{cc'} - \frac{i}{2} \sum_r \frac{\Gamma^{1/2}_{cr} \Gamma^{1/2}_{c'r}}{E_r - E - \frac{i}{2}\Gamma_{\gamma r}} \tag{3}$$

*These formulae are to be used for the 0°K case (no Doppler broadening terms given).

(2) C.W. Reich and M. S. Moore, Phys. Rev. 111, 929 (1958).

b. Radiative Captive Cross Section

$$\sigma_{n,\gamma}(E) = \sum_{\ell=0}^{NLS} \sigma^{\ell}_{n,\gamma}(E) \quad ,$$

$$\sigma^{\ell}_{n,\gamma}(E) = \frac{2\pi^2}{k^2} \sum_{J}^{NJS_{\ell}} \frac{g_J}{\bar{D}_{\ell,J}} \left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{\ell,J} .$$

c. Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{\ell=0}^{NLS} \sigma^{\ell}_{n,f}(E) \quad ,$$

$$\sigma^{\ell}_{n,f}(E) = \frac{2\pi^2}{k^2} \sum_{J}^{NJS_{\ell}} \frac{g_J}{\bar{D}_{\ell,J}} \left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle_{\ell,J} .$$

The sum over ℓ in the above equations extends up to $\ell = 2$ or to NLS (the number of ℓ-states for which data are given). For each value of ℓ, the sum over J has NJS_{ℓ} terms (the number of J-states for a particular ℓ-state). NLS and NJS are given in File 2.

The averages are re-written as

$$\left\langle \frac{\Gamma_n \Gamma_n}{\Gamma} \right\rangle_{\ell,J} = \left(\frac{\bar{\Gamma}_{n_{\ell,J}} \bar{\Gamma}_{n_{\ell,J}}}{\bar{\Gamma}_{\ell,J}} \right) R_{n_{\ell,J}}$$

$$\left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{\ell,J} = \left(\frac{\bar{\Gamma}_{n_{\ell,J}} \bar{\Gamma}_{\gamma_{\ell,J}}}{\bar{\Gamma}_{\ell,J}} \right) R_{\gamma_{\ell,J}}$$

$$\left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle_{\ell,J} = \left(\frac{\bar{\Gamma}_{n_{\ell,J}} \bar{\Gamma}_{f_{\ell,J}}}{\bar{\Gamma}_{\ell,J}} \right) R_{f_{\ell,J}}$$

where $R_{\gamma_{\ell,}}$, $R_{f_{\ell,}}$, and $R_{n_{\ell,J}}$ are width-fluctuation factors for capture, fission, and elastic scattering, respectively. Associated with each factor is the number of degrees of freedom for each of the average widths, and the integrals are to be evaluated using the MC^2-II method.

Data given in File 2 for each (ℓ, J) state

$\mu_{n_{\ell,J}}$ = AMUN, the number of degrees of freedom for neutron widths

$\mu_{f_{\ell,J}}$ = AMUF, " " " " " " " fission widths

$\mu_{x_{\ell,J}}$ = AMUX, " " " " " " " competitive

$\mu_{\gamma_{\ell,}}$ = AMUG, " " " " " " " radiation widths

$\bar{\Gamma}_{x_{\ell,J}}$ = GX, the average competitive reaction width

$\bar{\Gamma}^{o}_{n_{\ell,J}}$ = GNO. the average reduced neutron width

$\bar{\Gamma}_{\gamma_{\ell,J}}$ = GG, the average radiation width

$\bar{\Gamma}_{f_{\ell,J}}$ = GF, the average fission width

$\bar{D}_{\ell,J}$ = D, the average level spacing

The average neutron widths are defined in Section D.2.2.2, Equation 10, where $\bar{\Gamma}_{n_{\ell,J}} = \langle \Gamma_n(\ell,J) \rangle$.

File 5 Energy Distributions of Secondary Neutrons

(Energy Dependent Watt Spectrum)

LF = 11, Energy dependent Watt spectrum:

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

I is the normalization constant,

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

a and b are energy dependent;

U is a constant introduced to define the proper upper limit for the final neutron energy such that $0 \leq E' \leq E - U$.

File 7 Scattering Law Data

There is only one section in File 7, but the format varies slightly, depending on whether temperature-dependent data are given. The following quantities are defined:

LAT is a flag indicating which temperature has been used to compute α and β.

LAT = 0, the actual temperature was used.

LAT = 1, the constant T_o = 0.0253 eV has been used.

NS is the number of non-principal scattering atom types. For most moderating materials there will be (NS + 1) types of atoms in the molecule (NS $\leq$ 3).

NI is the total number of items in the B(N) list. NL = 6*(NS + 1).

B(N) is the list of constants. Definitions are given above (Section 7.1).

NR is the number of interpolation ranges for a particular parameter, either β or α.

NB is the total number of β values given.

NP is the number of a values given for each value of β for the first temperature described, NP is the number of pairs, α and $S(\alpha,\beta)$, given.

β_{int} and α_{int} are the interpolation schemes used (see Appendix E for interpolation formats).

In the energy range E1 to E2, the cross sections in file (MAT,3,MT), written as ${}^{MAT}\sigma_{MT}(E)$, are obtained in terms of the cross sections in files (MAT,3,MTI), written as ${}^{MAT}\sigma_{MT_i}(E)$, as follows:

$$ {}^{MAT}\sigma_{MT}(E) = \sum_{i=1}^{NCI} C_i * {}^{MAT}\sigma_{MT_i}(E). $$

Let X_i refer to the cross section in (MAT,3,MT) at energy E_i and Y_j refer to the cross section in (MAT1,3,MT1) at energy E_j. The contribution of the sub-subsection to the covariance matrix $COV(X_i,Y_j)$, having the units of "barns squared," described in the subsection, is defined as follows for the different values of LB:

LB=0 Absolute components only correlated within each E_k interval

$$ COV(X_i,Y_j) = \sum_k P^{i;k}_{j;k} F_{xy,k} $$

LB=1 Fractional components only correlated within each E_k interval

$$ COV(X_i,Y_j) = \sum_k P^{i;k}_{j;k} F_{xy,k} X_i Y_j $$

LB=2 Fractional components correlated over all E_k intervals

$$ COV(X_i,Y_j) = \sum_{k,k'} P^{i;k}_{j;k'} F_{xy,k} F_{xy,k'} X_i Y_j $$

LB=3 Fractional components correlated over E_k and E_ℓ intervals

$$ COV(X_i,Y_j) = \sum_{k,\ell} P^{i;k}_{j;\ell} F_{x,k} F_{yk\ell} X_i Y_j $$

LB=4 Fractional components correlated over all E_ℓ intervals within each E_k interval

$$ COV(X_i,Y_j) = \sum_{K,\ell,\ell'} P^{i;k,\ell}_{j;k,\ell'} F_k F_{xy,\ell} F_{xy,\ell'} X_i Y_j. $$

For LB=0, 1 and 2 we have LT=0, i.e., only one E_k table. For LB=3 and LB=4 we have LT≠0, i.e., two E tables, the E_k and the E_ℓ tables.

The dimensionless operators P in the above definitions are defined in terms of the operator S as follows:

$$ P^{i;k,\ell,\ldots}_{j;m,n,\ldots} \equiv S^k_i S^\ell_i \cdots S^m_j S^n_j \cdots , $$

where

$S^k_i \equiv 1$ when the energy E_i is in the interval E_k to E_{k+1} of an E_k table,

$S^k_i \equiv 0$ when the energy E_i is outside the range of E_k to E_{k+1} of an E_k table.

LB=5 Relative covariance matrix components

$$ COV(X_i,Y_j) = \sum_{k,k'} P^{i;k}_{j;k'} F_{xy;k,k'} X_i Y_j $$

A single list of energies $\{E_k\}$ is required to specify the energy intervals labeled by the indices k and k'. The numbers $F_{xy;k,k'}$ represent fractional components correlated over the energy intervals E_k and $E_{k'}$.

MT52-MT59 are lumped into MT851 and MT60-MT64 are lumped into MT852. The important level MT51 is treated individually. MT51, MT851, and MT852 are "evaluated," while MT4 is "derived" as the sum of these 3 reactions.

```
 6.00000+ 3 1.18969+ 1          0          0          0          1130633  4  101
 0.00000+ 0 0.00000+ 0          0          4          1          0130633  4  102
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  4  103
 4.81200+ 6 2.00000+ 7          0          0          6          3130633  4  104
 1.00000+ 0 5.10000+ 1 1.00000+ 0 8.51000+ 2 1.00000+ 0 8.52000+ 2130633  4  105
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  106
 6.00000+ 3 1.18969+ 1          0          0          0          1130633 51  107
 0.00000+ 0 0.00000+ 0          0         51          0          2130633 51  108
 0.00000+ 0 0.00000+ 0          0          1         20         10130633 51  109
 1.00000- 5 0.00000+ 0 4.81200+ 6 1.00000- 2 8.45000+ 6 2.50000- 3130633 51  110
 8.95000+ 6 1.00000- 2 1.10000+ 7 4.00000- 2 1.20000+ 7 4.00000- 2130633 51  111
 1.30000+ 7 2.25000- 2 1.40000+ 7 1.00000- 2 1.50000+ 7 4.00000- 2130633 51  112
 2.00000+ 7 0.00000+ 0                                             130633 51  113
 0.00000+ 0 0.00000+ 0          0          1          6          3130633 51  114
 1.00000- 5 0.00000+ 0 4.81200+ 6 2.50000- 3 2.00000+ 7 0.00000+ 0130633 51  115
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  116
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 52  117
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  118
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 53  119
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  120
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 54  121
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  122
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 55  123
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  124
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 56  125
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  126
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 57  127
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  128
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 58  129
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  130
 6.00000+ 3 1.18969+ 1          0        851          0          0130633 59  131
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  132
 6.00000+ 3 1.18969+ 1          0        852          0          0130633 60  133
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  134
 6.00000+ 3 1.18969+ 1          0        852          0          0130633 61  135
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  136
 6.00000+ 3 1.18969+ 1          0        852          0          0130633 62  137
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  138
 6.00000+ 3 1.18969+ 1          0        852          0          0130633 63  139
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  140
 6.00000+ 3 1.18969+ 1          0        852          0          0130633 64  141
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  142
 6.00000+ 3 1.18969+ 1          0          0          0          1130633851  143
 0.00000+ 0 0.00000+ 0          0        851          0          1130633851  144
 0.00000+ 0 0.00000+ 0          0          1          6          3130633851  145
 1.00000- 5 0.00000+ 0 8.29600+ 6 4.00000- 2 2.00000+ 7 0.00000+ 0130633851  146
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  147
 6.00000+ 3 1.18969+ 1          0          0          0          1130633852  148
 0.00000+ 0 0.00000+ 0          0        852          0          1130633852  149
 0.00000+ 0 0.00000+ 0          0          1          6          3130633852  150
 1.00000- 5 0.00000+ 0 1.43640+ 7 4.00000- 2 2.00000+ 7 0.00000+ 0130633852  151
 0.00000+ 0 0.00000+ 0          0          0          0          0130633  0  152
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