

The Data Covariance Files for ENDF/B-V

F. G. Perey

MASTER

OAK RIDGE NATIONAL LABORATORY

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ABSTRACT

In this report we present the formats and procedures for the data covariances of ENDF/B-V.

INTRODUCTION

The Cross Section Evaluation Working Group (CSEWG) for over ten years has periodically issued a library of reference cross sections called the Evaluated Neutron Data Files (ENDF/B). Currently the fifth version of this library is being prepared and will be called ENDF/B-V. With each version of ENDF/B the coverage of the library has grown as more elements and new types of data have been included. ENDF/B represents today the most complete library of evaluated data for neutronics calculations and is widely used for many transport applications. Although primarily intended to be used in various neutronics calculations, the library aims at providing our best current knowledge of the microscopic data.

Until ENDF/B-IV the only means available to evaluators for communicating the estimated uncertainties in the data was through publication of the documentation of the evaluations. During the preparation of ENDF/B-IV a Data Covariance Subcommittee of CSEWG was formed to coordinate the efforts at standardizing statements made about the data uncertainties and their correlations. One of the important aspects of nuclear data and of cross sections in particular is that the uncertainties in the various data tend to be highly correlated through the measurement processes and the different corrections made to the observable quantities to obtain the microscopic cross sections. In many applications when one is interested in estimating the uncertainties in calculated results based on the cross sections, the correlations in the uncertainties of the different data play a crucial role. In principle the uncertainties in the results of a calculation due to the data uncertainties can be calculated provided one is given all of the covariances of the data. In practice, in addition to the uncertainties due to the basic data, the results of calculations have uncertainties due to the calculational models used which may not represent perfectly the actual situation for which the calculations are intended. In some situations "modeling uncertainties" may dominate the uncertainties in computed results; in others they are negligible compared to the microscopic data uncertainties. In principle "modeling uncertainties" may be reduced by improving the models, although

sometimes at large cost. The data uncertainties may also be reduced, often at large cost, by performing better measurements, new kinds of measurements or more refined analysis of existing data.

The Data Covariance Subcommittee of CSEWG was charged with trying to improve substantially the treatment of uncertainties in ENDF/B. Very rapidly the idea of improving the method of reporting uncertainties in the documentation was abandoned as not providing the desired answer. This is due to the fact that in calculations the microscopic data and their uncertainties are rarely used directly, but are usually processed to yield quantities, such as group cross sections, which are then used as "basic data" in the calculations. One of the requirements of the uncertainty information is that it be easily processed to yield the covariances in the "data" used in the calculations themselves. For ENDF/B-IV the principle of having the uncertainty information on the data tape was adopted and a trial formalism was developed. This formalism has the virtue that the information is in such a form that it can be easily processed with minor modification to existing processing codes. Only a few evaluations of ENDF/B-IV were issued with data covariance information in this format as a trial measure. Since then, considerably more work has been done in trying to quantify data covariances within the ENDF/B-IV formalism and using the information for purposes of sensitivity studies. These sensitivity studies have been made in three different areas where the data covariances play a crucial role: propagation of uncertainties to final calculated results, adjustment of data sets incorporating information from some integral measurements and, determination of data accuracies needed to meet targeted uncertainties in results taking into account the correlations in uncertainties in the present data sets. Although most of the work done to date within the ENDF/B structure can only be termed exploratory in nature, some significant results have already been obtained. It is therefore with much greater confidence in the ultimate usefulness of this effort that the formalism and formats for representing data covariances in ENDF/B-V have been extended to cover most of the neutron cross section data in the files.

In this report we present, in the usual style of the Formats and Procedures Manual of ENDF/B, the formats and procedures for representing the data covariances in ENDF/B-V for the neutron cross sections. It should be noted here that two important classes of data, energy distributions (File 5) and angular distributions (File 4), have not yet received formats for representing the data uncertainties and their correlations. It is realized that in some applications this will limit the usefulness of the present data covariance file for neutron transport applications. Hopefully, these deficiencies will be removed in the near future; however, it should be realized that very possibly an enormous processing task lies ahead for these types of data since one must now generate covariance matrices for group-to-group transfer cross sections as well as their Legendre moments! For many applications the lack of treatment of covariances in continuous energy distributions is most serious. However, within the current formats of ENDF/B, it is possible to bypass the problem, at least for inelastic scattering, by using the subterfuge of pseudodiscrete levels to treat a continuum. In this case the current formats may be used since we have then effectively eliminated the continuum from the files. Unfortunately, this expedient is of little use for some important continuum data such as $(n,2n)$ spectra.

The formats and procedures given below have been approved by the Codes and Formats Subcommittee of CSEWG for ENDF/B-V. This document is therefore the official Formats and Procedures Manual of CSEWG for ENDF/B-V. A more detailed report covering the justifications for these formats, remarks concerning quantification of the data uncertainties, and a complete description of processing algorithms to obtain group cross section covariance matrices will soon be issued.

31. FILE 31, COVARIANCES OF THE AVERAGE NUMBER OF NEUTRONS PER FISSION

31.1 General Description

For fissionable materials, in File 1, MT=452 must be used to specify $\bar{\nu}$, the average total number of neutrons per fission. MT=455 may be used to specify the average total number of delayed neutrons per fission, $\bar{\nu}_d$, and MT=456 may also be used to specify the average number of prompt neutrons per fission, $\bar{\nu}_p$. The average number of neutrons per fission is given as a function of incident neutron energy. This energy dependence may be given by tabulating the values as a function of incident neutron energy or by providing the coefficients for a polynomial expansion as a function of incident neutron energy. Whichever method is used, the result is that the quantities are specified as a function of incident neutron energy and in this sense are similar to the data given in File 3. Therefore, the problems associated with representing the covariances of the average number of neutrons per fission are identical to those in File 33.

31.2 Formats

The formats for File 31, MT=452, 455 and 456 are the same as those for File 33 given in section 33.2.

31.3 Procedures

All procedures given in 33.3 concerning the ordering and completeness of sections of File 33 apply to sections of File 31: (MAT,31,452), (MAT,31,455) and (MAT,31,456).

We note that in File 1 $\bar{\nu}$ (MT=452), $\bar{\nu}_d$ (MT=455) and $\bar{\nu}_p$ (MT=456) satisfy the relation:

$$\bar{\nu}(E) = \bar{\nu}_d(E) + \bar{\nu}_p(E)$$

Therefore if one of these quantities is "derived" in terms of the other two, it is permissible to use "NC-type" sub-subsections with LTY=0 to indicate that it is a "derived redundant cross section."

When a section of File 31 for either MT=452, 455 or 456 is used, there must be a section in File 33 for the fission cross sections, i.e., section (MAT,33,18).

Note: 1. Since \bar{v}_d is much smaller than \bar{v}_p , it should never be evaluated by subtracting \bar{v}_p from \bar{v} .

2. When a polynomial representation is used to describe the data in File 1 MT=452, 455 and 456, the covariance file applies to the tabular reconstruction of the data as a function of energy and not to the polynomial coefficients.

32. FILE 32, COVARIANCES OF RESONANCE PARAMETERS

32.1 General Description

In File 32, MT=151, the covariances of the resonance parameters of the resolved resonances in File 2, MT=151, may be given. The resonance parameters in File 2, MT=151, used with the appropriate resonance formalism, provide an efficient way to represent the important correlations in the magnitude of the different partial cross sections over the resonances, compared to the use of File 3 only. Similarly with File 32, the use of the covariances of the resonance parameters of individual resonances provides an efficient way of representing the rapid variation of the covariances of the partial cross sections over the individual resonances. In the resonance region the covariances of the partial cross sections are often characterized by a) "long-range" components which affect the covariances over many resonances, which should be given in File 33, and b) "short-range" components affecting the covariances of the different partial cross sections over the individual resonances, which should be given in File 32. When the cross sections are averaged over many resonances, as is often the case for some applications in the higher energy range of the resolved resonance energy region and for the unresolved resonance energy region, the effects of the "short-range" components tend to "average out" and the covariances of the averaged cross sections are dominated by the long-range components given in File 33. Therefore the covariances of the cross sections in the unresolved resonance energy region should be given by means of File 33 only. In the resolved resonance energy region the covariances of the partial cross sections may be given using only File 33, in which case the "short range" variations which occur over individual resonances are ignored. For some applications such as: a) the calculation of the uncertainties in Doppler effects and selfshielding and b) the calculation of group cross section covariances where the groups are narrow compared to the resonance width (or when only very few resonances are within a group), a knowledge of the "short-range" correlations of uncertainties within the resonances is needed. It is for these purposes that File 32 should be used, with File 33, to describe the covariances of the cross sections. Because this

situation may only be important in the lower energy range of the resolved resonance region, File 32 may only contain data for the lowest energy resonances and need not cover the whole range of resonances given in File 2. It should be noted that it is the sum of the covariances in Files 32 and 33 which gives the total covariances of the partial cross sections and that in the resolved and unresolved resonance energy region one should not identify the components of the covariance matrix given in File 33 with the covariances of the "residual cross sections" which may or may not be present in File 3.

For ENDF/B-V the use of File 32 is limited to the Breit-Wigner representations (LRF=1 or 2). For the Adler-Adler representation one is limited to the description of the "long-range" components given in File 33.

For the Breit-Wigner representations (LRF=1, single level; or LRF=2, multilevel formalism) for each resonance given in File 2 we have:

- ER the resonance energy (in the laboratory system);
- AJ the floating-point value of J (the spin, or total angular momentum of the resonance);
- GT the resonance total width Γ evaluated at the resonance energy ER;
- GN the neutron width Γ_n evaluated at the resonance energy ER;
- GG the radiation width Γ_γ evaluated at the resonance energy ER;
- GF the fission width Γ_f evaluated at the resonance energy ER.

We note that in ENDF/B-V GT is no longer redundant since a "competitive width" GX is allowed in File 2. However, for purposes of File 32 we ignore GX and therefore only concern ourselves with the covariance matrix of the parameters ER, AJ, GN, GG and 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 of the resonance AJ may only take on 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 ENDF/B-V 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:

SPI is the nuclear spin of the target nucleus, I (positive number).

AP is the spin-dependent effective scattering radius, A_+ (for spin-up) in units of 10^{-12} cm.

QX is an effective Q-value.

NLS is the number of sets of resonance parameters given. A set of parameters is given for each ℓ -state (neutron angular momentum quantum number) $NLS \leq 3$.

L is the value of the ℓ -state (neutron angular momentum quantum number).

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

NRS is the number of resonances for a given ℓ -state, $NRS \leq 500$.

The symbols for the resonance parameters and the covariances of the resonance parameters are:

ER the resonance energy (in the laboratory system);

AJ the floating-point value of J (the spin, or total angular momentum of the resonance);

GT the resonance total width Γ evaluated at the resonance energy ER;

GN the neutron width Γ_n evaluated at the resonance energy ER;

GG the radiation width Γ_γ evaluated at the resonance energy ER;

GF the fission width Γ_f evaluated at the resonance energy ER;

\underline{DE}^2 the variance of ER in units of eV squared;
 \underline{DJ}^2 the variance of AJ;
 \underline{DJDN} the covariance of AJ and of GN in units of eV;
 \underline{DN}^2 the variance of GN in units of eV squared;
 \underline{DJDG} the covariance of AJ and of GG in units of eV;
 \underline{DNDG} the covariance of GN and of GG in units of eV squared;
 \underline{DG}^2 the variance of GG in units of eV squared;
 \underline{DJDF} the covariance of AJ and of GF in units of eV;
 \underline{DNDF} the covariance of GN and of GF in units of eV squared;
 \underline{DGDF} the covariance of GG and of GF in units of eV squared;
 \underline{DF}^2 the variance of GF in units of eV squared.

The structure of a subsection is as follows:

[MAT, 32, 151/ SPI, AP; 0, 0; NLS, 0] CONT

[MAT, 32, 151/ AWRI, QX; L, 0; 18*NRS, NRS/

ER₁, AJ₁, GT₁, GN₁, GG₁, GF₁,

DE₁², DN₁², DNDG₁, DG₁², DNDF₁, DGDF₁,

DF₁², DJDN₁, DJDG₁, DJDF₁, DJ₁², 0.0,

ER₂, AJ₂, GT₂, GN₂, GG₂, GF₂,

DE₂², DN₂², DNDG₂, DG₂², DNDF₂, DGDF₂,

DF₂², DJDN₂, DJDG₂, DJDF₂, DJ₂², 0.0,

.

.

.

ER_{NRS}, AJ_{NRS}, GT_{NRS}, GN_{NRS}, GG_{NRS}, GF_{NRS},

DE_{NRS}², DN_{NRS}², DNDG_{NRS}, DG_{NRS}², DNDF_{NRS}, DGDF_{NRS},

DF_{NRS}², DJDN_{NRS}, DJDG_{NRS}, DJDF_{NRS}, DJ_{NRS}², 0.0/ LIST.

32.3 Procedures

The data in File 32 for each resonance are only intended to provide information concerning the rapid variations of the covariance matrices of the different partial cross sections over the resonance, the long-range components of the covariance matrices being given in File 33. Since the long-range components of the covariance matrices may be the dominant ones, in particular in the higher energy range of the resolved resonance region for some material, it is not necessary to provide in File 32 the covariances of the resonance parameters for all the resonances given in File 2, although it might be desirable to do so.

I. Correspondence between File 32 and File 2

The following procedures indicate the relationships which may or must exist between corresponding quantities in File 2 and File 32. We shall indicate quantities in File 2 with the index 2 and the corresponding quantities in File 32 with the index 32.

1. In File 2 for each subsection EL_2 and EH_2 indicate the range of energies where the resonance formalism must be used to generate the partial cross sections even though some of the resonances may have a resonance energy outside the range of EL_2 to EH_2 . In File 32, since the resonances with resonance energies outside EL_{32} and EH_{32} may only contribute long-range components to the covariance matrices of the partial cross sections in the range EL_{32} to EH_{32} , it is not necessary to include them in File 32 if their contributions to the covariance matrices have been given in File 33.

2. In the corresponding subsections of File 2 and File 32 the value of EL must be the same, i.e. $EL_{32} = EL_2$. However, since the long-range components of the covariance matrices given in File 33 may dominate completely the covariance matrices in the higher energy region of the resolved resonance range EH_{32} may be lower than EH_2 , i.e. $EH_{32} \leq EH_2$.

3. Within the energy range EL_{32} to EH_{32} all of the resonances given in the subsections of File 2 must also be given in File 32.

II. Completeness of File 32

Procedure I-3 above requires that all the resonances of File 2 within the energy range EL_{32} to EH_{32} be given in File 32. All of the

covariances of the parameters of each resonance need not be non-zero in File 32. In particular, the variance of AJ , DJ^2 , and the covariances of AJ and of the other parameters will be zero when the value of AJ is known or when it is not used as a constrained free parameter of the formalism. However, when the covariance of two different resonance parameters is non-zero, the variances of each of these parameters must be non-zero. We note that because of selfshielding effects the analysis of most experimental data results in a large covariance of GN and of GG as well as a large covariance of GN and of GF .

32.4 Example

In order to illustrate the use of the formats and procedures for File 32, we give below Files 2 and 32 for an hypothetical evaluation of Fe-56, MAT=1180. Although hypothetical, this example is based upon work performed for ENDF/B-V. The resonance parameters were evaluated using: transmission data which yielded values of $g\Gamma_n$ and their variances, angular distribution data which yielded J , and capture resonance areas ($g\Gamma_n\Gamma_\gamma/\Gamma_t$) with their variances after correction for selfshielding effects in the samples. Without going into the details of the evaluation of the various resonances most of the covariances of Γ_n and Γ_γ came from the variance in the resonance areas. When $\Gamma_n \gg \Gamma_\gamma$ the capture area is essentially a measure of Γ_γ and since Γ_n was known the covariance of Γ_n and Γ_γ was small and neglected in the File 32. When $\Gamma_\gamma \gg \Gamma_n$ the capture area is essentially a measure of Γ_n . Since the selfshielding is small, the covariance of Γ_n and Γ_γ was small and it was neglected in the File 32.

In the example which follows we do not give the File 33 which would accompany this File 32. This File 33 would contain a section for MT=1, the total cross sections, with long-range components; it would also contain a section for MT=102, the capture cross sections with a long-range component of about 10% to account for the normalization of all of the capture data.

To illustrate the procedures, in File 2 we indicate the range of the resolved resonance energy region as 10^{-5} eV to 100 keV and give a few resonances outside the range. In File 32 we indicate the range from 10^{-5} eV to 85 keV with variances and some covariances for all the resonances in File 2 within this range. Presumably the File 33, not shown for this material, would represent entirely the covariances of the cross sections above 85 keV.

Table I-32. Example of File 2.

2.6056E+4	5.5454E+1	0	0	1	01180	2151	HEAD
2.6056E+4	1.0	0	0	1	01180	2151	C0NT
1.0E-5	1.0E+5	1	2	0	01180	2151	C0NT
0.0	0.46	0	0	3	01180	2151	C0NT
5.5454E+1	0.0	0	0	36	61180	2151	LIST
-2.000E+3	0.5	1.8064E+2	1.80E+2	0.64	1180	2151	
2.767E+4	0.5	1.5214E+3	1.52E+3	1.40	1180	2151	
7.398E+4	0.5	5.3573E+2	5.35E+2	0.73	1180	2151	
8.365E+4	0.5	1.2513E+3	1.25E+3	1.3	1180	2151	
1.298E+5	0.5	5.0110E+2	5.00E+2	1.10	1180	2151	
1.404E+5	0.5	2.7022E+3	2.70E+3	2.20	1180	2151	
5.5454E+1	0.0	1	0	114	191180	2151	LIST
1.149E+3	0.5	0.6600	0.0600	0.60	1180	2151	
1.245E+4	0.5	0.5423	0.0023	0.54	1180	2151	
1.775E+4	0.5	0.5590	0.0190	0.54	1180	2151	
2.279E+4	0.5	0.8100	0.2700	0.54	1180	2151	
3.420E+4	1.5	1.3300	0.7900	0.54	1180	2151	
3.840E+4	1.5	0.8600	0.3200	0.54	1180	2151	
4.804E+4	0.5	10.530	10.000	0.53	1180	2151	
5.212E+4	1.5	12.420	12.000	0.42	1180	2151	
5.354E+4	0.5	1.6700	1.0000	0.67	1180	2151	
5.537E+4	0.5	2.0200	1.9000	0.12	1180	2151	
5.920E+4	1.5	4.4900	4.0000	0.49	1180	2151	
6.344E+4	1.5	1.3500	0.8000	0.55	1180	2151	
7.298E+4	0.5	20.720	20.000	0.72	1180	2151	
7.704E+4	0.5	3.9300	3.6000	0.33	1180	2151	
9.029E+4	1.5	14.460	14.900	0.46	1180	2151	
9.278E+4	1.5	1.0600	0.5200	0.54	1180	2151	
9.629E+4	0.5	1.7000	1.3000	0.40	1180	2151	
9.657E+4	1.5	2.9000	2.5000	0.40	1180	2151	
1.025E+5	1.5	21.36	21.000	0.36	1180	2151	
5.5454E+1	0.0	2	0	36	61180	2151	LIST
2.350E+3	1.5	0.8402	0.0002	0.84	1180	2151	
2.017E+4	1.5	0.8447	0.0047	0.84	1180	2151	
3.670E+4	2.5	0.9500	0.1100	0.84	1180	2151	
8.080E+4	2.5	7.7400	7.0000	0.74	1180	2151	
9.265E+4	1.5	2.2500	1.6000	0.65	1180	2151	
9.614E+4	2.5	1.7700	0.6700	1.10	1180	2151	
0.0	0.0	0	0	0	01180	2	0 SEND
0.0	0.0	0	0	0	01180	0	0 FEND

Table II-32. Example of File 32 for File 2 shown in Table I-32.

2.6056E+4	2.5454E+1	0	0	1	0118032151	HEAD
2.6056E+4	1.0	0	0	1	0118032151	CONT
1.0E-5	8.5E+4	1	2	0	0118032151	CONT
0.0	J.46	0	0	3	0118032151	CONT
5.5454E+1	0.0	0	0	54	3118032151	LIST
2.767E+4	0.5	1.5214E+3	1.52E+3	1.40	0.0	118032151
9.0E+2	9.0E+2	0.0	1.0E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
7.398E+4	0.5	5.3573E+2	5.35E+2	0.73	0.0	118032151
2.5E+3	1.0E+2	0.0	4.9E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
8.365E+4	0.5	1.2513E+3	1.25E+3	1.3	0.0	118032151
6.4E+3	2.5E+3	0.0	1.7E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
5.5454E+1	0.0	1	0	252	14118032151	LIST
1.149E+3	0.5	0.6600	0.6600	0.60	0.0	118032151
4.0E+0	1.6E-5	1.4E-4	3.6E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
1.245E+4	0.5	0.5423	0.0023	0.54	0.0	118032151
1.6E+3	9.0E-8	0.0	2.5E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
1.775E+4	0.5	0.5590	0.0190	0.54	0.0	118032151
2.5E+3	4.0E-6	0.0	2.5E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
2.279E+4	0.5	0.6100	0.2700	0.54	0.0	118032151
2.5E+3	3.0E-3	-5.9E-3	2.5E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
3.420E+4	1.5	1.3300	0.7900	0.54	0.0	118032151
2.5E+3	9.0E-2	-4.3E-2	2.5E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
3.840E+4	1.5	0.8600	0.3200	0.54	0.0	118032151
2.5E+3	6.4E-3	-9.3E-3	2.5E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
4.604E+4	0.5	10.530	10.000	0.53	0.0	118032151
2.5E+3	9.0E+0	0.0	2.5E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
5.212E+4	1.5	12.420	12.000	0.42	0.0	118032151
4.0E+2	1.0E+0	0.0	1.6E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
5.354E+4	0.5	1.6700	1.0000	0.67	0.0	118032151
4.0E+2	1.6E-1	-5.5E-2	2.9E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
5.537E+4	0.5	2.0200	1.9000	0.12	0.0	118032151
4.0E+2	9.0E-2	0.0	2.5E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
5.920E+4	1.5	4.4900	4.0000	0.49	0.0	118032151
4.0E+2	2.5E-1	0.0	2.5E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
6.344E+4	1.5	1.3500	0.8000	0.55	0.0	118032151
4.0E+2	2.6E-2	-1.5E-2	1.7E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
7.298E+4	0.5	20.720	20.000	0.72	0.0	118032151
2.5E+3	1.6E+1	0.0	4.9E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
7.704E+4	0.5	3.9300	3.6000	0.33	0.0	118032151
4.0E+2	2.5E-1	0.0	9.0E-4	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
5.3454E+1	0.0	2	0	72	4118032151	LIST
2.350E+3	1.5	0.8402	0.0002	0.84	0.0	118032151
2.5E+3	3.0E-0	0.0	6.2E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
2.017E+4	1.5	0.8447	0.0047	0.64	0.0	118032151
2.5E+3	2.5E-7	0.0	6.2E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
3.670E+4	2.5	0.9500	0.1100	0.84	0.0	118032151
2.5E+3	1.0E-4	0.0	6.2E-2	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
8.000E+4	2.5	7.7400	7.0000	0.74	0.0	118032151
4.0E+2	4.9E-1	0.0	6.4E-3	0.0	0.0	118032151
0.0	0.0	0.0	0.0	0.0	0.0	118032151
0.0	0.0	0	0	0	0118032	0 SEND
0.0	0.0	0	0	0	01180	0 0 FEND

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. The Files 33 are intended to provide a measure of the "accuracies and their correlations" of the data in Files 3 and do not indicate the precision with which they are entered in the Files 3. Since ENDF/B represents our knowledge of the microscopic data, the Files 33 are 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 and the Files 33 will yield the covariances of these group cross sections. While generating the Files 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.

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 covariances of the cross sections entirely by means of File 33, since often the major components of the covariance matrix are 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, b; 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.

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-subsections.

The structure of a subsection describing the covariance matrix of the cross sections given in the ENDF/B tape (MAT,3,MT) and (MAT1,3,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 of "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-subsections may be used to indicate that some or all of the contributions to the covariance matrix described in the subsection are to be found in a different subsection of the ENDF/B tape. The major purpose of the "NC-type" sub-subsections is to eliminate from the ENDF/B tape a large fraction of the mostly redundant information which would otherwise be needed if only "NI-type" sub-subsections were used.

The "NI-type" sub-subsections are used to describe explicitly 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 the Files 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. It should be emphasized here that the Files 33 are intended to provide a measure of the "accuracy" of the cross sections in Files 3 and not the precision to which they are entered in the files. 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

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

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 $\text{MAT}_{\sigma_{\text{MT}}}(E)$, were obtained in terms of the cross sections in files (MAT,3,MTI), written as $\text{MAT}_{\sigma_{\text{MTI}}}(E)$, as follows:

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

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 E1 to E2, usually ± 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 E1 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. This 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 obtained with LTY=1 sub-subsections and those obtained from LTY=2 and 3 sub-subsections. This difference results from the definition of their use given above. LTY=2 and 3 sub-subsections are always used in subsections where one of the cross sections involved is the "standard" cross section used. The LTY=2 sub-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;" no LTY=1 sub-subsections may appear in such subsections. 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 the Files 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 an 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:

[MAT, 33, MT/ b, b; LT, LB; 2*NP, NP/ {E_k, F_k} {E_l, F_l}] LIST .

LB is a flag whose numerical value may be from 0 to 4 and determines the meaning of the numbers given in the arrays {E_k, F_k} {E_l, F_l}.

NP is the total number of pairs of numbers in the arrays {E_k, F_k} {E_l, F_l}.

LT is the number of pairs of numbers in the second array, {E_l, F_l}.

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

{E_k, F_k} {E_l, F_l} 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 x 10¹⁷ 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 $\text{COV}(X_i, Y_j)$, 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

$$\text{COV}(X_i, Y_j) = \sum_k P_{j;k}^{i;k} F_{xy,k}$$
- LB=1 Fractional components only correlated within each E_k interval

$$\text{COV}(X_i, Y_j) = \sum_k P_{j;k}^{i;k} F_{xy,k} X_i Y_j$$
- LB=2 Fractional components correlated over all E_k intervals

$$\text{COV}(X_i, Y_j) = \sum_{k,k'} P_{j;k'}^{i;k} F_{xy,k} F_{xy,k'} X_i Y_j$$
- LB=3 Fractional components correlated over E_k and E_ℓ intervals

$$\text{COV}(X_i, Y_j) = \sum_{k,\ell} P_{j;\ell}^{i;k} F_{x,k} F_{y,\ell} X_i Y_j$$
- LB=4 Fractional components correlated over all E_ℓ intervals within each E_k interval

$$\text{COV}(X_i, Y_j) = \sum_{k,\ell,\ell'} P_{j;k,\ell'}^{i;k,\ell} F_k F_{xy,\ell} F_{xy,\ell'} X_i Y_j$$

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 $LT \neq 0$, i.e., two E tables, the E_k and the E_ℓ tables.

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

$$P_{j;m,n,\dots}^{i;k,\ell,\dots} \equiv S_i^k S_i^\ell \dots S_j^m S_j^n \dots$$

where

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

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

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 Files 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

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

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 $\{F_{k, k'}\}$:

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

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 $\{F_{k,k'}\}$:

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

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

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

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 numbers: (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 another File 33 of the ENDF/B tape. 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 $MT1 \neq MT$, 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 subsections 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 also be on the ENDF/B tape in a different File 33 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 a different File 33.

III. Other Procedures

a. "NC-type" sub-subsections with LTY=1 shall only be used in ENDF/B-V with MATS≠MAT. The use of LTY=1 sub-subsections in ENDF/B-V 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 subsection, 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.

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 of ENDF/B. 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 α_i over the complete range of the file. Therefore we have $Z_i = \alpha_i X_i$.

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 α_i from 10^{-5} eV to 20 MeV. The evaluation of these quantities resulted in the evaluation of three covariance matrices: $\text{COV}(A_i, A_j)$, $\text{COV}(R_i, R_j)$ and $\text{COV}(\alpha_i, \alpha_j)$. 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 $\text{COV}(A_i, \alpha_j)$ are essentially zero.

Let us denote relative covariance matrices such as $\frac{\text{COV}(A_i, A_j)}{A_i A_j}$ 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 $Z_i = \alpha_i X_i$, we have:

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

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

$$\langle dZ_i \cdot dZ_j \rangle = \langle d\alpha_i \cdot d\alpha_j \rangle + \langle dA_i \cdot dA_j \rangle$$

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

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

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

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

$$\langle dZ_i \cdot dZ_j \rangle = \langle d\alpha_i \cdot d\alpha_j \rangle + \langle dR_i \cdot dR_j \rangle + \langle dY_i \cdot dY_j \rangle$$

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

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 $\langle d\alpha_i \cdot d\alpha_j \rangle$ 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:

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

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

$$\langle d\alpha_i \cdot d\alpha_j \rangle \rightarrow \{E_k^\alpha, F_k^\alpha\}$$

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:

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

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

$$\{E_k^\alpha, F_k^\alpha\} = \{1.0E-5, F_1^\alpha; \dots; E_k^\alpha, F_k^\alpha; \dots; 2.0E+7, 0.0\} ,$$

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

In the listing given below 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 $\langle d\alpha_i, d\alpha_j \rangle$ with the E tables indicated symbolically as:

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

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

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:

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

with

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

Table I-33. Example of File 33 with "NC-type" LTY=1 sub-subsection.

9.4239E+4	2.36999E+2	0	C	0	3126433	18	HEAD					
0.0	0.0	0	1E	1	2126433	18	C0NT					
0.0	0.0	0	1	0	0126433	18	C0NT					
ES	2.0E+7	1261	1E	4	2126433	18	LIST	} <dY _i ·dY _j >	}			
ES	1.0	2.0E+7	0.0	0.0	126433	18	"					
0.0	0.0	LT	LB	2*NP	NP126433	18	LIST					
***** (EAK,FAK) *****												
					126433	18	"	} <dA _i ·dA _j >	}	(1264, 18; 0, 18)		
0.0	0.0	LT	LB	2*NP	NP126433	18	LIST					
***** (ERK,FRK) *****												
					126433	18	"	} <CR _i ·dR _j >	}			
0.0	0.0	0	102	1	2126433	18	C0NT					
0.0	0.0	0	1	0	0126433	18	C0NT					
ES	2.0E+7	1261	1E	4	2126433	18	LIST	} <dY _i ·dY _j >	}			
ES	1.0	2.0E+7	0.0	0.0	126433	18	"					
0.0	0.0	LT	LB	2*NP	NP126433	18	LIST					
***** (EAK,FAK) *****												
					126433	18	"	} <dA _i ·dA _j >	}	(1264, 18; 0, 102)		
0.0	0.0	LT	LB	2*NP	NP126433	18	LIST					
***** (ERK,FRK) *****												
					126433	18	"	} <dR _i ·dR _j >	}			
0.0	0.0	1261	1E	1	0126433	18	C0NT					
0.0	0.0	0	2	0	0126433	18	C0NT					
ES	2.0E+7	1261	1E	4	2126433	18	LIST	} <dY _i ·dY _j >	}	(1264, 18; 1261, 18)		
ES	1.0	2.0E+7	0.0	0.0	126433	18	"					
0.0	0.0	0	0	0	0126433	0	SEND					
9.4239E+4	2.36999E+2	0	0	0	2126433102	HEAD						
0.0	0.0	0	102	1	3126433102	C0NT						
0.0	0.0	0	1	0	0126433102	C0NT						
ES	2.0E+7	1261	1E	4	2126433102	LIST	} <dY _i ·dY _j >	}				
ES	1.0	2.0E+7	0.0	0.0	126433102	"						
0.0	0.0	LT	LB	2*NP	NP126433102	LIST						
***** (EAK,FAK) *****												
					126433102	"	} <dA _i ·dA _j >	}		(1264, 102; 0; 102)		
0.0	0.0	LT	LB	2*NP	NP126433102	LIST						
***** (ERK,FRK) *****												
					126433102	"	} <dR _i ·dR _j >	}				
0.0	0.0	LT	LB	2*NP	NP126433102	LIST						
***** (EAK,FAK) *****												
					126433102	"	} <dA _i ·dA _j >	}		(1264, 102; 1261, 18)		
0.0	0.0	1261	1E	1	0126433102	C0NT						
0.0	0.0	0	2	0	0126433102	C0NT						
ES	2.0E+7	1261	1E	4	2126433102	LIST	} <dY _i ·dY _j >	}				
ES	1.0	2.0E+7	0.0	0.0	126433102	"						
0.0	0.0	0	E	0	0126433	0	SEND					
0.0	0.0	0	G	0	01264	0	FEND					

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:

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

with

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

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:

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

with

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

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

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

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

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

In the listing given below 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:

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

The above example has great similarity to the way the ENDF/B-IV 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:

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

with

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

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 following sections to the File 33, MAT=1274, shown above, to have a more complete File 33.

Table II-33. Example of File 33 with "NC-type" LTY=0 sub-subsection.

6.012E+3	1.1897E+1	0	0	0	1127433	1	HEAD	
0.0	0.0	0	1	0	1127433	1	C0NT	
0.0	0.0	LT	LB	2*NP	NP127433	1	LIST	
***** (ETK,FTK) *****					127433	1	"	(1274, 1; 0, 1)
0.0	0.0	0	0	0	0127433		SEND	
6.012E+3	1.1897E+1	0	0	0	1127433	2	HEAD	
0.0	0.0	0	2	1	1127433	2	C0NT	
0.0	0.0	0	0	0	0127433	2	C0NT	
1.0E-5	8.5E+6	0	0	8	4127433	2	LIST	
1.0	1.0	-1.0	4.0	-1.0	102.	127433	2	"
-1.0	107.	0.0	0.0	0.0	102.	127433	2	"
0.0	0.0	LT	LB	2*NP	NP127433	2	LIST	"derived" (1274, 2; 0, 2)
***** (EEK,FEK) *****					127433	2	"	
0.0	0.0	0	0	0	0127433		SEND	
6.012E+3	1.1897E+1	0	0	0	1127433	4	HEAD	
0.0	0.0	0	4	1	1127433	4	C0NT	
0.0	0.0	0	0	0	0127433	4	C0NT	
8.5E+6	2.0E+7	0	0	8	4127433	4	LIST	
1.0	1.0	-1.0	2.0	-1.0	102.	127433	4	"
-1.0	107.	0.0	0.0	0.0	102.	127433	4	"
0.0	0.0	LT	LB	2*NP	NP127433	4	LIST	"derived" (1274, 4; 0, 4)
***** (EIK,FIK) *****					127433	4	"	
0.0	0.0	0	0	0	0127433		SEND	
6.012E+3	1.1897E+1	0	0	0	1127433102		HEAD	
0.0	0.0	0	102	0	1127433102		C0NT	
0.0	0.0	LT	LB	2*NP	NP127433102		LIST	(1274, 102; 0, 102)
***** (ECK,FCK) *****					127433102		"	
0.0	0.0	0	0	0	0127433		SEND	
6.012E+3	1.1897E+1	0	0	0	1127433107		HEAD	
0.0	0.0	0	107	0	1127433107		C0NT	
0.0	0.0	LT	LB	2*NP	NP127433107		LIST	(1274, 107; 0, 107)
***** (EOK,FOK) *****					127433107		"	
0.0	0.0	0	0	0	0127433		SEND	
0.0	0.0	0	0	0	01274		FEND	

Table III-33. Additional sections of File 33 which could be added to File 33 given in Table II-33.

6.012E+3	1.1097E+1	0	0	0	1127433	51	HEAD	} (1274, 51; 0, 51)
0.0	0.0	0	51	1	1127433	51	COMT	
0.0	0.0	0	0	0	0127433	51	COMT	
1.0E-5	8.5E+6	0	0	2	1127433	51	LIST	
1.0	4.0	0.0	0.0	0.0	127433	51	"	
0.0	0.0	0	0	2*NP	NP127433	51	LIST	
***** (E51K,F51K) *****								
0.0	0.0	0	0	0	127433	51	"	
0.012E+3	1.1897E+1	0	0	0	0127433	91	SEND	} (1274, 91; 0, 91)
0.0	0.0	0	91	1	1127433	91	HEAD	
0.0	0.0	0	0	0	0127433	91	COMT	
8.5E+0	2.0E+7	0	0	10	0127433	91	COMT	
1.0	1.0	-1.0	2.0	-1.0	5127433	91	LIST	
-1.0	102.	-1.0	107.	0.0	127433	91	"	
0.0	0.0	0	0	0	127433	91	"	
0.0	0.0	0	0	0	0127433	91	SEND	

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