33. FILE 33, COVARIANCES OF NEUTRON CROSS SECTIONS

33.1. General Description

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

i. the variances of the group cross sections,
ii. the correlations between the cross sections of the several adjacent groups, and
iii. the long-range correlations among the cross sections for many groups.

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

These primary considerations and the inherent difficulties associated with quantifying uncertainties should dictate the level of detail given in File 33.

In the resolved resonance region, some of the covariances of the cross sections may be given through the covariances of the resonance parameters in File 32. In this case, the long-range components of the covariance matrix of the cross sections, which span many resonances, may be given in File 33, since often the most important components of the matrix are long-range.

Table 33.1
Analogies Between File 33 Covariances Within One Section and Uncertainties in a Hypothetical Experiment [1]

File 33	Experimental	Energy Dependence
Short range	Statistical	Rapid variation
Medium range	Detector Efficiency Multiple Scattering In/Out Scattering	Slowly varying
Long range	Geometry Background Normalization	More or less constant

Example: If there is 2% uncertainty due to statistics (short-range), 2% due to multiple scattering (medium-range) and, 1% due to geometry (long-range), cite a 3% uncertainty for a discrete measurement (one group covering a small energy range); ≈2.5% over an energy range encompassing several measurements (several groups which together cover a 1- to 2-MeV range); and closer to 1% average over the entire energy range.

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

3.2. Formats

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

The following quantities are defined:

ZA,AWR	Standard material charge and mass parameters.
MTL	Nonzero value of MTL is used as a flag to indicate that reaction MT is one component of the evaluator-defined lumped reaction MTL, as discussed in paragraphs at the end of 33.2. and 33.3. below; in this case, no covariance information subsections are given for reaction MT and NL=0.
NL	Number of subsections within a section.

The structure of a section is:

```
[MAT, 33, MT/  ZA, AWR, 0, MTL, 0, NL] HEAD
               <subsection for n = 1>
               <subsection for n = 2>
               <subsection for n = NL>
[MAT, 33,  0/ 0.0, 0.0, 0,   0, 0,  0] SEND
```

3.2.1. Subsections

Each subsection of the section (MAT,33,MT) is used to describe a single covariance matrix. It is the covariance matrix of the energy-dependent cross sections given in section (MAT,3,MT) and energy-dependent cross sections given in section (MAT1,MF1,MT1) of the ENDF tape. [If MF1=0, then in the subsection (MAT1,10,MT1.LFS1)]. The values of MAT1, XMF1 = Float(MF1), MT1, and XLFS1 =Float(LFS1) if MF1=10, are given in the CONT record which begins each subsection. Each File 33 subsection is therefore identified with a unique combination of values (MAT,MT) and (MAT1,MF1,MT1,[LFS1]), and we may use the notation (MAT,MT;MAT1,MF1,MT1,[LFS1]) to specify a subsection.

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

The following quantities are defined:

XMF1	Floating point equivalent of MF for 2nd energy-dependent cross section of pair for which correlation matrix is given. If MF1=MF, XMF1 = 0.0 or blank.
XLFS1	Floating point equivalent for final excited state of 2nd energy-dependent cross section, For MF1=10, XLFS1 = 10; if MF1≠10, XLFS1 = 0.0 or blank.
MAT1	MAT for 2nd energy-dependent cross section
MT1	MT for 2nd energy-dependent cross section
NC	Number of "NC-type" sub-subsections which follow the CONT record.
NI	Number of "NI-type" sub-subsections which follow the "NC-type" sub-subsections.

The structure of a subsection describing the covariance matrix of the cross sections given in the ENDF/B tape (MAT,3,MT) and (MAT1,MF1,MT1,[LFS1]) is:

```
[MAT,33,MT/ MF1, XLFS1, MAT1, MT1, NC, NI]CONT
              <sub-subsection for n  =1>
              <sub-subsection for n  =2>
            ----------------------------
            ----------------------------
              <sub-subsection for n = NC>
              <sub-subsection for n =1>
              <sub-subsection for n =2>
            ----------------------------
            ----------------------------
              <sub-subsection for n = NI>
```

3.2.2. Sub-subsections

The "NC-type" and "NI-type" sub-subsections have different structures.

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

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

I. <u>"NC-type" sub-subsections</u>

The "NC-type subsections may be used to describe the covariance matrices in energy ranges where the cross sections in (MAT,3,MT) can be "derive" in terms of other "evaluated" cross sections in the same energy range. In the context of File 33, and for purposes of discussing "NC-type" sub-subsections, we define an "evaluated" cross section, in a given energy range, as one for which the covariance matrix in that energy range is given entirely in terms of "NI-type" sub-subsections. The covariance matrices involving the "derived" cross sections may be obtained in part in terms of the covariance matrices of the "evaluated" cross sections given elsewhere in File 33.

The following quantity is defined:

LTY Flag used to indicate the procedure used to obtain the covariance matrix

a.) <u>LTY=0, "Derived Redundant Cross Sections"</u>. In File 33, the evaluator may indicate by means of an LTY=0 sub-subsection that in a given energy range the cross sections in (MAT,3,MT) were obtained as a linear combination of other "evaluated" cross sections having the same MAT number but different MT values. By the definition of "evaluated" the covariances of these cross sections are given in File 33 wholly in terms of "NI-type" sub-subsections. [In general the linear relationship given in an LTY=0 sub-subsection applies not only to the range of energy specified, but also over the whole range of the file.]

The following additional quantities are defined:

E1, E2 Energy range (eV) where the cross sections given in the section (MAT,3,MT) were "derived" in terms of other "evaluated" cross sections given in the sections (MAT,3,MTI)s.

NCI Number of pairs of values in the array {CI, XMTI}[2].

{CI, XMTI} Array of pairs consisting of coefficient CI and a value of XMTI, (MTI given as a floating point number). The pair of numbers indicate that, in the energy range E1 to E2, the cross sections in file (MAT,3,MT), were obtained in terms of the cross sections in files (MAT,3,MTI), as follows:

$$\sigma_{MT}^{MAT}(E) = \sum_{i=1}^{NC1} C_i \times \sigma_{MT}^{MAT}(E) \quad .$$

[At the minimum, the use of an LTY=0 sub-subsection implies that the evaluator wishes the corresponding covariance components to be derived as if this expression were valid.]

In this expression we have written the CI's as C_i, and XMTI's as MT_i. The numbers CI are constant numbers over the whole range of energy E1 and E2, usually ± 1.

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

```
[MAT,33,MT/ 0.0, 0.0,   0, LTY,     0,   0] CONT              (LTY=0)
[MAT,33,MT/  EL,  E2,   0,   0, 2*NCI, NCI/ {CI, XMTI}] LIST
```

Note: In general, each subsection describes a single covariance matrix. However, when an "NC-type" sub-subsection with LTY=0 is used in a subsection, portions of NCI+1 covariance matrices are implied and these are not explicitly given as subsections in the File 33 (see procedure 33.3.2-a-3). In such cases the subsection may be thought of as describing in part several covariance matrices.

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

Many important cross sections of ENDF/B are based on measurements of cross sections ratios. When an evaluated cross section is obtained from such measurements, covariances so generated between the cross sections for the two reactions may become important. This is a primary origin of ENDF-6 covariances linking cross sections for different materials. As seen below, these covariances depend on the covariances of the standard cross section and on the covariances of the evaluated cross section ratios to those standards. When the resulting multigroup covariance files are utilized, the covariances of the ratios themselves play an important role if the performance of some system depends on the relative magnitude of two cross sections.

[2] The Notation {AI,BI} stands for A_1, B_1; A_2, B_2; ...; A_i, B_i in a list record.

In order efficiently to represent in File 33 the covariances that depend on "absolute" ratio measurements to standards, evaluators may use "NC"-type sub-subsections with LTY=1, 2 and 3 in appropriate File 33 subsections. [In other cases of covariance components induced by ratio measurements, it is necessary for the evaluator to represent the covariance components that arise may be found in the literature.[3]]

First we identify the covariances induced if an evaluator obtains cross section $\sigma_a(E)$ for (MAT,MT) within the interval (E1,E2) entirely from ***absolute*** ratio measurements to a cross section standard $\sigma_S(E)$ for (MATS,MTS). That is,

$$\sigma_a(E) = \alpha(E)\ \sigma_S(E)\ , \quad \text{for } (E1 \le E < E2)$$

The evaluated ratio itself is assumed to be independent of the standard cross section evaluation because the relevant measurements are similarly independent. If so, then

$\mathrm{Rvar}[\sigma_a(E)] = \mathrm{Rvar}[\alpha(E)] + \mathrm{Rvar}[\sigma_S(E)]$, for $(E1 \le E < E2)$

$\mathrm{Rvar}[\sigma_a(E),\sigma_a(E')] = \mathrm{Rvar}[\alpha(E),\alpha(E')] + \mathrm{Rvar}[\sigma_S(E),\sigma_S(E')]$,
for $(E1 \le E < E2)$ and $(E1 \le E' < E2)$

$\mathrm{Rvar}[\sigma_a(E),\sigma_S(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_S(E')]$, for $(E1 \le E < E2)$ and $(E1 \le E' < E2)$

Rvar and Rcov are the relative variance and relative covariance defined in Chapter 30, and the values generated by the specified ratio evaluation are zero outside the specified ranges. The variance and covariance terms in (MAT,MT) depend on those for both the standard and the ratio, and only for energies in ranges where the cross section is specified to depend on this standard. However, the covariance matrix between the cross sections (MAT,MT) and (MATS,MTS) does not depend on the covariances of the ratio determination but spans all values o the energy E′.

A cross section $\sigma_a(E)$ may be obtained from measurements relative to (MATS,MTS) energy region $(E1 \le E < E2)$ and cross section $\sigma_b(E')$ from (MATS′,MT′) in energy region $(E1' \le E' < E2')$. If the cross sections for the two standards are correlated and the two sets of ratio measurements are uncorrelated, then one obtains the additional results:

$\mathrm{Rvar}[\sigma_a(E),\sigma_b(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_{S'}(E')]$, for $(E1 \le E < E2)$ and $(E1' \le E < E2')$, zero otherwise;
$\mathrm{Rvar}[\sigma_a(E),\sigma_{S'}(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_{S'}(E')]$, for $(E1 \le E < E2)$ and all E′ ,zero otherwise;
$\mathrm{Rvar}[\sigma_S(E),\sigma_b(E')] = \mathrm{Rvar}[\sigma_S(E),\sigma_{S'}(E')]$, for $(E1' \le E' < E2')$ and all E, zero otherwise;

Note that the above expressions apply when $\sigma_a(E)$ and $\sigma_b(E')$ refer to the same (MAT,MT) for which cross sections are obtain by ratios to different standards in the two energy regions.

The most far-reaching relationship correlates $\sigma_a(E)$ with all cross sections correlated to the standard relative to which it was measured. That is,

$\mathrm{Rcov}[\sigma_a(E), \sigma_x(E')] = \mathrm{Rcov}[\sigma_S(E), \sigma_x(E;)]$, for $(E1 \le E < E2)$ and all $\sigma_S(E')$, zero otherwise.

The right side may nonzero for many (MATX, MTX), and discretion may be required to avoid generation in cross section processing of negligible but nonzero multigroup covariances matrices.

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[3] W. P. Poenitz, "Data Interpretation, Objective Evaluation Procedures, and Mathematical Techniques for the Evaluation of Energy-Dependent Ratio, Shape, and Cross Section Data", **BNL-NCS-51363**, *Conf. on Nuclear Data Evaluation and Techniques*, p. 264, B. A. Magurno and S. Pearlstein, eds. (March, 1981)

R. W. Peele, "Uncertainties and Correlations in Evaluated Data Sets Induced by the Use of Standard Cross Sections", **NBS Special Publication 425**, *Conf. on Nuclear Cross Sections and Technology*, p.173, R. A. Schrack and C. D. Bowman, eds. (1975)

Let the cross sections in (MAT,3,MT) be strictly "derived" in the energy range E1 to E2 through the evaluation of ratio measurements to the "evaluated" cross sections given in (MATS,MFS,MTS,[LFSS]), referred to also as the **"standard" cross sections** for this "ratio evaluation". Then, in the subsection (MAT,MT;MAT,3,MT,0) of the File 33 for the material MAT, an LTY=1 sub-subsection must be used to describe, in part, the covariance matrix in the energy range E1 to E2. (LFS=0 when MF=3). The part, or component, of the covariance matrix represented by the LTY=1 sub-subsection is obtained by the user from the **covariance matrix of the "standard" cross sections** in the File (MFS+30) subsection (MATS,MTS,[LFSS]; MATS,MFS,MTS,[LFSS]) of the material MATS. The other part, or component, of the covariance matrix comes from the evaluation of the "ratios" and is given explicitly, over the range E1 to E2, by means of "NI-type" sub-subsections in the File 33 subsection (MAT,MT;MAT,3,MT,0).

This method of evaluation introduces a covariance of the "derived" cross sections in (MAT,3,MT) over the energy range E1 to E2 and the "standard" cross section in over its complete energy range. Therefore, in the File 33 of the material MAT, in subsection contsining the covariance of the "standard" cross section, there must be an LTY=2 sub-subsection to represent this covariance matrix. This LTY=2 sub-subsection [which contains the same information as the previously given LTY=1 sub-subsection in the subsection (MAT,MT; MAT,3,MT,0)] refers to a different covariance matrix than the LTY=1 sub-subsection previously mentioned, but it can also be derived from the covariance matrix of the "standard" cross sections in File MFS+30 subsection of the standard material MATS.

Finally, as a consequence of the evaluation of the cross sections in (MAT,3,MT) in the energy range E1 to E2, as a "ratio" to the "standard" cross sections, there must be in the subsection (MATS,MTS,[LFSS]; MAT,MT) of the File (MFS+30) of the "standard" material MATS and LTY=3 sub-subsection in the File 33 subsection (MAT,MFT; MAT,3,MT,0)] which serves in the material MATS the same role as the LTY=2 sub-subsection in the material MAT since they describe the same covariance matrix. In addition, the LTY value of 3 serves as a "flag" to the user, and the processing codes, to indicate existence of any additional covariances among cross sections using the same "standard" cross sections, covariances not explicitly given in the covariance files. These additional covariance matrices can be derived from the appropriate LTY=3 sub-subsections and the covariance matrix of the "standard" cross sections in the File (MFS+30) subsection.

The following quantities are defined:

E1, E2	Energy range where the cross sections given in the section (MAT,3,MT) were obtained to a significant extent in terms of ratio measurements to "standard" cross sections.
NEI	Number of energies that demarcate (NEI-1) regions where this standard was employed in measurements with WEI.
WEI	Fractional evaluated weight.

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

```
[MAT,33,MT/0.0, 0.0,     0, LTY,        0,    0] CONT
[MAT,33,MT/ E1,  E2, MATS, MTS, 2*NEI+2, NEI/
           (XMFS,XLFSS),  {EI,WEI}           ] LIST
```

The number of items in the list record is 2*NEI+2. The file number that contains the standard cross sections is the integer equivalent of XMFS, except that XMFS=0.0 is entered when MFS=3. The value of XLFSS is always zero unless MFS=10.

The use of the format LTY=1, 2 and 3 is allowed when the cross sections given in (MAT,3,MT) are only partially determined from ratio measurements to the "standard" cross section. In such cases the list {EI,WEI} indicates the fractional weight of the ratio measurements to this standard in the evaluation of the cross sections in (MAT,3,MT). That fractional weight is WE_i in the interval $E_i \leq E < E_{i+1}$. The first value of E_i in the sub-subsection shall equal the E1 given, and E_{NEI} =E2.

Note A: LTY=1, 2 and 3 sub-subsections are all used as flags in subsections to represent relative covariance matrix components obtained from the relative covariance matrix of the "standard" cross sections that is given in a File 33, 31, or 40. There is, however, as seen in the formulae above, a major difference between covariance matrices obtained with LTY=1 sub-subsections and those obtained from LTY=2 and 3 sub-subsections. This difference results from the definition of their use given above. LTY=2 and 3 sub-subsections are always used in subsections where one of the cross sections involved is the "standard" cross section used. The LTY=2 subsection appears in the File 33 [in the present case] of the material whose cross sections are "derived," whereas the LTY=3 sub-subsection appears in the File (MFS+30) of the material whose cross sections are the "standard",; LTY=1 sub-subsections always appear in subsections describing covariance matrices of cross sections "derived" from a "standard" and no LTY=2 or 3 sub-subsections may appear in such subsections. An LTY=1 sub-subsection represents a covariance matrix which in principle is a "square matrix" covering the ranges E1 to E2. An LTY=2 or 3 sub-section describes in principle a "rectangular matrix": the covariance matrix of the "derived" cross sections over the energy range E1 or E2 and of the "standard" cross sections over their complete energy range.

In general, if cross sections in (MAT,3,MT,0) are "derived," over an energy range E1 to E2, by "ratios" to "standard" cross sections, there will be three "NC-type" sub-subsections with LTY=1, 2 and 3 generated in the covariance files. The LTY=1 sub-subsection is given in the subsection (MAT,MT; MAT,3,MT,0); the LTY=2 sub-subsection is given in the subsection (MAT,MT; MATS,MFS,MTS,[LFSS]). Both of these subsections are given in the File 33 of the material MAT of the "derived" cross sections (MAT,3,MT). The LTY=3 sub-subsection is given in the subsection (MATS,MFS,MTS,[LFSS]; MAT,3,MT,0) which is in the File (MFS+30) of the material MATS of the "standard" cross sections.

There are, however, some instances, such as the one taken in the Example 33.1, where other cross sections, such as those in (MAT,3,MTI), are "indirectly derived" from the cross sections in (MATS,3,MT) through evaluation of ratios of the cross sections in (MAT,3,MTI) to those in (MAT,3,MT). In such cases, an LTY=1 sub-subsection will also be used in the subsections (MAT,MT1,MAT,MT1) and (MAT,MT; MAT,MT1) and LTY=2 sub-subsection will also be used in the subsection (MAT,MT1; MATS,MFS,MTS,[LFSS]). All three of these subsections are in File 33 of the material MAT. Corresponding to the LTY=2 sub-subsection in the subsection (MAT,MT1; MATS,MFS,MTS,[LFSS]) of the File 33 of the material MAT, there will also be an LTY=3 sub-subsection in the subsection (MATS,MTS,[LFSS]; MAT,MT1) of the File (MFS+30) of the material MATS.

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

II. "NI-type" Sub-subsections

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

The following quantity is defined:

LB Flag whose numerical value determines the meanings of the numbers given in the arrays $\{E_k, F_k\}\{E_l, F_l\}$.

a. Flag LB=0-4

The following additional quantities are defined:

NP Total number of pairs of numbers in the arrays $\{E_k, F_k\}\{E_l,F_l\}$.

NT Total number of numbers in the LIST record. NT=2∗NP

LT Number of pairs of numbers in the second array, $\{E_l,F_l\}$.LT=0, when the table contains is a single array $\{E_k,F_k\}$. LT≠0, when the table contains two arrays; the first array, $\{E_k,F_k\}$, has (NP-LT) pairs of numbers in it.

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

For a values of the LB flag from 0 through 4, "NI-type" sub-subsections have the following structure:

[MAT,33,MT/ 0.0, 0.0, LT, LB, NT, NP/ $\{E_k, F_k\}\{E_1, F_1\}$] LIST

The E_n table, and the E_l table, when present, must cover the complete energy range of the File 3 for the same (MAT,MT). The first energy entry in an E table must therefore be 10^{-5} eV, or the reaction threshold, and the last one 20×10^6 eV unless a large upper-energy limit has been defined. Some of the F_k's, or F_l's, may be zero, and the last value of F in an E table must be zero.

We now define the meaning of the F values entered in the E tables for different values of LB. [Note that the units of F vary]. Let X_i refer to the cross section in (MAT,3,MT) at energy E_i and Y_j refer to the cross section in (MAT1,3,MT1) at energy E_j. The contribution of the sub-subsection to the covariance matrix $COV(X_i,Y_j)$, having the units of "barns squared," is defined as follows for the different values of LB:

LB=0 Absolute components correlated only within each E_k interval

$$Cov\left(X_i,Y_i\right)=\sum_k P_{j;k}^{i;k}F_{xy;k}$$

LB=1 Fractional components correlated only within each E_k interval

$$Cov\left(X_i,Y_i\right)=\sum_k P_{j;k}^{i;k}F_{xy;k}X_iY_j$$

LB=2 Fractional components correlated over all E_k intervals

$$Cov\left(X_i,Y_i\right)=\sum_{k,k'} P_{j;k}^{i;k}F_{xy;k}F_{xy;k'}X_iY_j$$

LB=3 Fractional components correlated over E_k and E_l intervals

$$Cov\left(X_i,Y_i\right)=\sum_{k,l} P_{j;l}^{i;k}F_{x;k}F_{y;l}X_iY_j$$

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

$$Cov\left(X_i,Y_i\right)=\sum_{k,l,l'} P_{j;k,l'}^{i;k,l}F_kF_{xy,l}F_{xy,l'}X_iY_j$$

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

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

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

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

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

$$Cov\left(X_i,Y_i\right)=\sum_{k,k} P_{j;k}^{i;k}F_{xy;k,k}X_iY_j$$

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

Since there is no need for E_k tables with pairs of numbers (E_k,F_k) like those found in sub-subsections with LB<5, a new structure is required for LB=5 sub-subsections.

The following quantities are defined:

NT	Total number of entries in the two arrays $\{E_k\}$ and $\{F_{k,k'}\}$.
NE	Number of entries in the array $\{E_k\}$ defining (NE-1) energy intervals.
LS	Flag indicating whether the $F_{k,k'}$, matrix is symmetric or not.

The structure of an LB=5 sub-subsection is:

`[MAT,33,MT/ 0.0, 0.0, LS, LB=5, NT, NE/ {E_k}{F_k,k'}] LIST.`

LS=0 Asymmetric matrix

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

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

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

$$NT = NE + (NE-1)^2 = NE(NE-1) + 1$$

LS=1 Symmetric matrix

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

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

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

$$NT = NE + [NE\ (NE-1)]/2 = [NE\ (NE+1)]/2$$

c.) Flag LB=6. A covariance matrix interrelating the cross sections for two different reaction types or materials generally has different energy grids for its rows and columns. The LB=6 format described below allows efficient representation of a rectangular (not square) matrix in one LIST record with no repetition of energy grids.

The following definition applies for LB=6 sub-subsections:

$$Cov\left(X_i, Y_i\right) = \sum_{k,l} P^{i;k}_{j;l} F_{xy;k,l} X_i Y_j$$

where X_i as before refers to the cross sections at E_i in (MAT,3,MT) and
Y_j refers to the cross section at E_j in (MAT1,MF1,MT1,[LFS1]).

The dimensionless operator P is as defined for other LB's. A single "stacked" list of energies $\{E_{kl}\}$ is required to specify the energy intervals with lower boundaries labeled by the indices k and *l*. That is, a single array contains the energies for the rows (E_k) and then the columns (E_l) of the matrix with the energies corresponding to the rows given first: (ER_1, ER_2, ..., ER_{NER}, EC_1, EC_2, ..., EC_{NEC}). The numbers $F_{xy;k,l}$ represent fractional components correlated over the energy intervals with lower boundaries E_k and E_l.

The following quantities are defined:

NT	Total number of entries in the two arrays $\{E_{k,l}\}\{F_{k,l}\}$. See below.
NER	Number of energies corresponding to the rows of the matrix and defining (NER-1) energy intervals.
NEC	Number of energies corresponding to the columns of the matrix and defining (NEC-1) energy intervals. NEC may be inferred from NT and NER.

The structure of an LB=6 sub-subsection is:

`[MAT,33,MT/ 0.0, 0.0, 0, LB, NT, NER/ {`$E_{k,l}$`}{`$F_{k,l}$`}] LIST` (LB=6)

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

$$\{F_{k,l}\} = F_{1,1}, F_{1,2}, ..., F_{1,NEC-1}; F_{2,1}, ..., F_{2,NEC-1}; ...; F_{NER-1,1}, F_{NER-1,2}, ..., F_{NER-1,NER-1}$$

There are (NER-1)(NEC-1) numbers in the array $\{F_{k,l}\}$. Therefore, the total number of entries in the two arrays $\{E_{k,l}\}$ and $\{F_{k,l}\}$ is:

$$NT = NER + NEC + (NER-1)(NEC-1) = 1 + NER*NEC.$$

d.) Flag LB=8, Short Range Variance Representation. A short range self-scaling variance component should be specified in each File 33 subsection of the type (MAT,MT; 0,MT) by use of an LB=8 sub-subsection, unless the cross section is known to be free from unresolved underlying structure. [See section 33.3.3.].

The following quantities are defined:

NP	Total number of pairs of numbers in the arrays $\{E_k, F_k\}\{E_l,F_l\}$.
NT	Total number of numbers in the LIST record. NT=2*NP
$\{E_k,F_k\}$	Array of pairs of numbers; the first member of a pair is an energy, E_n; the second member of the pair, F_n, is a number associated with the energy interval between the two entries E_n and E_{n+1}.

The format of an LB=8 sub-section is (just as for LB=0):

`[MAT,33,MT/ 0.0, 0.0, LT, LB, NT, NP/ {`E_k`,`F_k`}] LIST` (LT=0,LB=8)

Only one E_k table is required. The F_k values for LB=8 have the dimension of squared cross sections. The magnitude of the resulting variance component for a processed average cross section depends strongly on the size of the energy group as well as on the values of F in the sub-subsection. For the simplest case of a multigroup covariance matrix processed on the energy grid of this sub-subsection with a constant weighting function, the variance elements VAR_{kk} for the LB=8 component are just F_k and the off diagonal elements are zero.

In general, each F_k characterizes an uncorrelated contribution to the absolute variance of the indicated cross section averaged over any energy interval (sub-group) ΔE_j that includes a portion of the energy interval ΔE_k. The variance contribution VAR_{jj} from an LB=8 sub-subsection to the processed group variance for the energy group (E_j,E_{j+1}) is inversely proportional to its width ΔE_j when (E_j,E_{j+1}) lies within (E_k,E_{k+1}) and is obtained from the relation

$$VAR_{jj} = F_k \Delta E_k/\Delta Ej \text{ , where } E_k \le E_j \le E_{j+1} \le E_{k+1}$$

Note that the VAR_{jj} are variances in average cross sections. This rule suffices for arbitrary group boundaries if subgroup boundaries are chosen to include all the E_k. No contributions to off-diagonal multigroup covariance matrix elements are generated by LB=8 sub-subsections.

3.2.3. Lumped Reaction Covariances

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

The File-33 section for one component of a lumped reaction consists of a single HEAD record that contains, in the second integer field, the section number MTL of the lumped reaction to which the component contributes. (See definition of the HEAD record at the beginning of this Section.)

```
[MAT, 33, MT/ ZA,  AWR,  0,  MTL,  0,  NL] HEAD                (NL=0)
```

The value of MTL must lie in the range 851-870, which has been reserved specifically for covariance data for lumped reactions. These MT-numbers may not be used in File 3, 4 or 5, so the net cross section and net scattering matrix for a lumped reaction must be constructed at the processing stage by summing over the reaction components.

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

Except for the need to sum the cross-section components during uncertainty processing, lumped reactions are "normal" reactions, in that all covariance formats can be used to describe their uncertainties in MF=33, MT=MTL. For example, one expects in general that the covariances of a lumped reaction with other reactions, including other lumped reactions, will be given by the evaluator. Also, a lumped reaction may be represented, using an "NC-type" sub-section with LTY=0, as being "derived" from other reactions, including other lumped reactions. However, since uncertainties are not provided for the separate component reactions, a lumped reaction may not be represented as being "derived" from its components.

33.3. Procedures

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

33.3.1. Ordering of Sections, Subsections and Sub-subsections

a.) 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 set of numbers: (MAT,MT;MAT1,MF1,MT1,[LFS1]); the first pair of numbers indicated the section and the second set of numbers appears in the appropriate fields, XMF1, XLFS1, MAT1 and MT1, of the CONT record which begins every subsection. [When MT≠10, XLFS1=0.0.]

1. The subsections within a section are ordered by increasing values of MAT1. In order to have the covariance matrices of the cross sections for which MAT1=MAT appear first in a section the value MAT1=0 shall be used to mean MAT1=MAT in the CONT record which begins the subsection.

2. When there are several subsections with the same value of MAT1 in a section, these subsections shall be ordered by increasing values of XMF1. When MF1=MF-30, the XMF1 field shall be entered as blank or zero. Therefore, within a given section and for a given MAT1, the subsections for MF1=MF-30 will always appear before those for other MF1 values.

3. When there are several subsections with the same value of MAT1 and MF1 in a section, these subsections shall be ordered by increasing values of MT1 given in CONT record which begins the subsections.

4. When MAT1=0, when according to procedure 33.3.1-b-2 means that MAT1=MAT, and XMF1=0.0 meaning MF1=MF-30, only subsections for which MT1>MT shall be given.

5. When there are several subsections with the same values of MAT1, MF1=10, and MT1 in a section, these subsections shall be ordered by increasing values of LFS1.

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

1. "NC-type" sub-sections. Several "NC-type" sub-subsections may be given in a subsection. When more than one is given, these must be ordered according to the value of the energy range lower endpoint E1 given in the LIST record. We note that by definition, if several LTY=0 "NC-type" sub-subsections are given in a subsection, the energy ranges E1 to E2 of the these different sub-subsections cannot overlap with each other or with any LTY=1 sub-subsection. However, in ENDF-6 formats it is permitted to have overlapping (E1,E2) ranges for LTY≥1, provided that the sum of the WEI values in one subsection is no greater than unity at any energy. The value of the LTY flag of "NC-type" sub-subsections does not affect the ordering of the sub-subsections within a subsection.

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

33.3.2. Completeness

As previously stated, there is presently no minimum requirement on the number of sections and subsections in File 33. Lack of a File 33 for a reaction does not imply zero uncertainty. However, the presence of some subsections in a File 33, as well as the presence of some sub-subsections in a subsection, implies the presence of other subsections either in the same File 33 or the File 33 (or 31 or 40) of another material. In what follows we shall identify the File 33 subsections by their value of the sextet:

```
[MAT,MT; MAT1,MF1,MT1,(LFS1)]
```

a.) Subsections for which MAT1=0. By subsections for which MAT1=0, we mean the subsections of the class (MAT,MT; 0,MF1,MT1,[LFS1]), which according to procedure 33.3.1-b-1 implies that MAT1=MAT.

1. If there is a File 33 subsection (MAT,MT; 0,MF1,MT1,[LFS1] with MT1≠MT, there must be within the same material the two subsections: (MAT,MT; 0,3,MT,0) in File 33 and (MAT,MT1; 0,MF1,MT1,[LMF1]) in file MF1+30. Note that the converse is not necessarily true since the two cross sections (MAT,3,MT) and (MAT,MF1,MT1,[LMF1]) may have zero covariances between them, which are not required to be explicitly stated in the files. (However, see the discussion in paragraph 33.3.2.b below concerning the desirability of explicitly representing some zero covariances.) This procedure and procedure 33.3.1-b-4 guarantee that every section of File 33, (MAT,33,MT), starts with the subsection (MAT,MT; 0,3,MT,0).

2. In a subsection (MAT,MT; 0,3,MT,0), if there is an "NC-type" sub-subsection with LTY=0, it contains a list of MTI given in the "NC-type" sub-subsection.

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

4. In a subsection (MAT,MT; 0,3,MT,0) if there is an "NC-type" sub-subsection with LTY=1, this sub-subsection contains values of (MATS,MFS,MTS,[LFSS]). In the same File 33, there must be a sub-subsection (MAT,MT; MATS,MFS,MTS,[LFSS]). There must be another material MATS with a File (MFS+30) containing the subsection (MATS, MTS,[LFSS]; 0,MFS,MTS,[LFSS]). Note that according to procedure 33.3.3.a, given below, MATS must be different from MAT in an "NC-type" sub-subsection with LTY=1.

5. In a subsection (MAT,MT; 0,3,MT,0), if there is an "NC-type" sub-subsection with LTY=1 which covers the energy range E1 to E2, in the same subsection there must be at least one "NI-type" subsections represent the relative covariance matrix of the evaluated ratio measurements. In the energy range where WEI is the relative weight given to the evaluated ratio to the indicated standard cross section, the processing code takes into account the value of WEI when it applies the standards covariances. The evaluator is responsible for multiplying the covariances of the evaluated ratios by WEI^2 before entry into the NI-type sub-subsections. Note that, where the weight is not unity in a given energy region, the NI-type sub-subsections that represent the covariance data for the ratios are mixed together without identification in File 33.

b.) Subsections for MAT1=0. If there is a File 33 subsection (MAT,MT; MAT1,MF1,MT1,[LFS1]) with MAT1≠0, similar to procedure 33.3.2-a-1, there must also be a subsection (MAT,MT; 0,3,MT,0) in the same File 33. There must also be two sub-subsections, (MAT1,MT1,[LFS1]; 0,MF1,MT1,[LFS1]) and (MAT1,MT1,[LFS1]; MAT,3,MT,0) in the File (MF1+30) for material MAT1.

33.3.3. Other Procedures

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

b.) If a single "NC-type" sub-subsection with LTY=0 is used in a subsection and there are no "NI-type" sub-subsections, the value of E1 must be 10^{-5} eV, or the reaction threshold, and the value of E2 must be the highest energy for which the corresponding cross section is given, at least 2×10^{7} eV.

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

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

e.) The formats of File 33 allow for the possibility of great details to be entered in the files if needed. The number of "NI-type" sub-subsections and the number of energy entries in their E_k and E_l tables will be a function of the details of the covariance matrices available and the need to represent them in such detail. However, good judgement should be used to minimize as much as possible the number of different entries in the E_k and E_l tables. An important quantity to note is the union of all of the E values of the E_k and E_l tables of a File 33. A reasonable upper limit of the order of a few hundred different E values for the union of all energy entries in all of the E_k and E_l tables in a File 33 should be considered.

Note that the evaluator's covariance values will be most readily recognized in a processed multigroup covariance matrix when the energies in the E_k and E_l tables can be chosen from the set of standard multigroup energy boundaries. If in the File 33 the uncertainties in a cross section are represented using LB=0 or 1 in regions of width ΔE_i, and if the file is processed to give a multigroup covariance library with group width in that energy region ΔE_a such that $\Delta E_i > \Delta E_a$, the correlation patterns in ENDF-6 are defined so that the processed group uncertainties are lowest and the intergroup correlations greatest when an energy group of the processed covariance matrix is evenly split by a covariance file E value. This behavior has alarmed some users. However, because of the correlation pattern set up, no big anomalies arise in the uncertainty projected for an integral quantity that is sensitive to a broad spectrum of incident particle energies. The magnitude of the effect can be reduced by using narrower intervals in LB=0, 1 files, or more favorably by using overlapping files with staggered energy edges.

f.) The ground rules above (see 33.2, under LT=1 sub-subsections) state that if cross sections are obtained by evaluating ratio measurements to a "standard cross section," the latter cross section should be "evaluated" in the sense that there are no NC-type sub-subsections with LTY=0 or 1 describing the covariance data for that cross section. This leads to procedural requirements.

1. Evaluators of established standard cross sections should endeavor to avoid the use of any LTY=0 or LTY=1 sub-subsections. If the physics of an evaluation problem should require that this rule be broken, the CSEWG should be informed and the text documentation should call attention to the situation.
2. If an evaluated cross section is best obtained as the ratio to a cross section in another material that is not an established standard, than an evaluator needs to contact the evaluator of that material to be reassured that NC-type sub-subsections will not appear in the files for the reference cross section for the energy region of concern.

Such communication is required in any case to encourage the evaluation of the covariance data for that reference cross section, without use of LB=0 sub-subsections, and to assure that the required LTY=3 sub-subsection will be entered. To aid the review process, a written form of this communication should be sent to the CSEWG.

g.) The ENDF-6 formats allow the evaluator to recognize the partial dependence of a cross section on a standard cross section. This means that it is possible to recognize in the covariance files an evaluation that utilizes some absolute data as well as ratio data to one or more standard cross sections. Use of this capability is expected to be necessary to properly represent some covariance information. Since processing complexity is thereby induced, evaluators are urged to use this capability with caution, and in no case to represent the dependence of a cross section in a given energy region on ratio measurements to more than two standard cross sections.

h.) The discussion of the covariance terms that arise from evaluated cross section ratio measurements was based entirely on so-called absolute ratio measurements. Evaluators should note that various types of cross section "shape" measurements induce additional covariance terms that can be derived for specific situations. Within ENDF-6 formats the evaluator must include them in NI-type sub-subsections in the covariance files of the derived cross section.

i.) When cross section A is correlated to B, and cross section C is also correlated to B even though A is uncorrelated to C, evaluators should include the file segments that express this zero correlation to signify to reviewers and users that an unusual case is recognized. This is the exception to the general rule that zero covariances need not be openly expressed in the covariance files.

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

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

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

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

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

o.) An LB=8 sub-subsection should be included in each (MAT, MT; 0, MT) subsection unless the cross section is known to be free from unresolved underlying structure[4]. The Doppler effect in reactor applications smooths cross sections on an energy scale too narrow to be of concern for LB=8 covariance evaluation. This sub-subsection must cover the entire energy range of the section (threshold to at least 20 MeV). Use of zero values for F_k in any part of this energy range should be avoided because such usage could induce the problem of nonphysical full correlation between neighboring fine-group cross sections, the problem that the LB=8 format was designed to solve. The LB=8 format may not be used for cross-reaction covariances.

Note that the law for processing LB=8 sub-subsections directly references the variance of an average cross section rather than the variance of a pointwise cross section. If a fine-grid covariance matrix is developed and then collapsed to the evaluator's E_k grid with constant weighting, the resulting variance components are just the F_k. (A complete multigroup covariance matrix cannot in general be correctly "reprocessed" to a finer energy mesh; one must process the ENDF/B-VI covariance files).

The values of F_k may be chosen by the evaluator to account for statistical fluctuations in fine-group average cross sections that are induced by the width and spacing distributions of the underlying resonances. Values may also be chosen to represent the uncertainty inherent in estimating the average cross sections for small energy intervals where little or no experimental data exist and smoothness is not certain.

The LB=8 sub-subsections help prevent mathematical difficulties when covariance matrices are generated on an energy grid finer than that used by the evaluator, but F_k values must be chosen carefully to avoid accidental significant dilution of the evaluated covariance patterns represented in the other Sub-sections. If no physical basis is apparent for choosing the F_k values, they may be given values about 1% as large on the evaluator's grid as the combined variance from the other sub-subsections. Such values would be small enough not to degrade the remainder of the covariance evaluation and large enough to assure that the multigroup covariance matrix will be positive definite for any energy grid if the matrix on the evaluator's energy grid is positive definite.

Since LB=8 specifies absolute covariances, it should not be employed near reaction thresholds. In particular, for threshold reactions having an effective threshold above 0.1 MeV, LB=8 should not be employed for incident energies less than 1 MeV above the effective threshold.

[4] For example, if covariance data for neutron scattering from hydrogen were to be represented in File 33, one would expect no component that could be properly represented by an LB=8 sub-section. Covariance data in such cases may best be represented in File 30.

33.4. Examples

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

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

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

1. Fission cross sections, MT=18

   Let X_i stand for the fission cross section of ^{239}Pu at the energy E_i.

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

   b. From ES to 20 MeV, X_i was evaluated by means of ratio measurements to Y_i , the fission cross section of ^{235}U, to which we assign the MAT number 1261. In this energy range $X_i = R_i Y_i$, 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 ^{239}Pu at the energy E_i. In this evaluation, Z_i was obtained by the evaluation of a_i, the ratio of capture to fission cross sections, over the complete range of the file. Therefore we have $Z_i = a_i X_i$.

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 these three different quantities are uncorrelated, *i.e.*, covariances such as $COV(A_i,a_j)$ can be neglected.

Let us denote relative covariance matrices such as $COV(A_iA_j)/(A_iA_j)$ as $\langle dA_i,dA_j\rangle$, and similarly for the other quantities.

From 10^{-5} to ES, since $X_i = A_i$ and $Z_i = a_i X_i$, 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 in terms of the covariance matrices of the evaluated quantities and the covariance matrix of the ^{235}U fission.

For purposes of illustrating the use of the formats we need not know the details of how the covariance matrices $\langle dA_i \cdot dA_j \rangle$, $\langle dR_i \cdot dR_j \rangle$ 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:

$\langle dA_j \cdot dA_j \rangle \rightarrow \{E_k^A, F_k^A\}$
$\langle dR_j \cdot dR_j \rangle \rightarrow \{ER_k^R, FR_k^R\}$
$\langle da_j \cdot da_j \rangle \rightarrow \{E_K^a, F_k^a\}$

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:

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

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

In the listing given in Example 33.1 for the File 33 of MAT=1264, corresponding to our example, we have shown with only one sub-subsection each of the matrices $\langle dA_i \cdot dA_j \rangle$, $\langle dR_i \cdot dR_j \rangle$ and $\langle da_i \cdot da_j \rangle$. E_S is taken as 2×10^5 eV.

Note: In the File 33 of MAT-1261 in the subsections (1261,18; 1264,18) and (1261, 18; 1264,102) an LTY=3 "NC-type" sub-subsection corresponding to the LTY=2 sub-subsections of Example 33.2 must be inserted.

Example 33.1. File 33 with "NC-type" LTY=1 sub-subsections

```
9.42390+4 2.36999+2          0          0         0       NL=3126433 18 HEAD
0.00000+0 0.00000+0     MAT1=0      T1=18       NC=1      NI=2126433 18 CONT
0.00000+0 0.00000+0          0      LTY=1          0         0126433 18 CONT
2.00000+5 2.00000+7 MATS=1261     MTS=18       NT=6       NE=2126433 18 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433 18 <dYi×dYj>
0.00000+0 0.00000+0  LT=0LB=1      NY=14       NE=7           126433 18 LIST
1.00000-5 0.00000+0 1.00000+0 2.50000-3 3.00000+2 3.60000-3126433 18 <dAi×dAj>
3.00000+4 4.90000-3 1.00000+5 6.40000-3 2.00000+5 0.00000+0126433 18
2.00000+7 0.00000+0                                        126433 18
0.00000+0 0.00000+0       LT=0       LB=1       NT=6       NE=3126433 18 LIST
1.00000-5 0.00000+0 2.00000+5 4.00000-4 2.00000+7 0.00000+0126433 18 <dRi×dRj>
      (1264,18;0.102)
0.00000+0 0.00000+0 MAT1=1261     MT1=18       NC=1       NI=0126433 18 CONT
0.00000+0 0.00000+0          0      LTY=2          0         0126433 18 CONT
2.00000+5 2.00000+7 MATS=1261     MTS=18       NT=6       NE=2126433 18 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433 19 <dYi×dYj>
0.00000+0 0.00000+0          0          0         0         0126433  0 SEND
      (1264,102;0,102)
```

Example 33.2. (continued) **File 33 with "NC-type" LTY=1 sub-subsections.**

```
9.42390+4 2.36999+2          0          0          0      NL=2126433102 HEAD
0.00000+0 0.00000+0     MAT=0   MT1=102       NC=1       NI=2126433 18 CONT
0.00000+0 0.00000+0          0     LTY=1          0          0126433 18 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18       NT=6       NE=2126433 18 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433 18 <dY_i×dY_j>
0.00000+0 0.00000+0       LT=0       LB=1     NT=14       NE=7126433 18 LIST
1.00000-5 0.00000+0 1.00000+0 2.50000-3 3.00000+2 3.60000-3126433 18 <dA_i×dA_j>
3.00000+4 4.90000-3 1.00000+5 6.40000-3 2.00000+5 0.00000+0126433 18
2.00000+7 0.00000+0                                          126433 18
0.00000+0 0.00000+0       LT=0       LB=1       NT=6       NE=3126433 18 LIST
1.00000-5 0.00000+0 2.00000+5 4.00000-4 2.00000+7 0.00000+0126433 18 <dR_i×dR_j>
      (1264,18;1261,18)
0.00000+0 0.00000+0    MAT1=0   MT1=102       NC=1       NI=3126433102 CONT
0.00000+0 0.00000+0          0     LTY=1          0          0126433102 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18       NT=6       NE=2126433102 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433102 <dY_i×dY_j>
0.00000+0 0.00000+0       LT=0       LB=1     NT=14       NE=7126433102 LIST
1.00000-5 0.00000+0 1.00000+0 2.50000-3 3.00000+2 3.60000-3126433102 <dA_i×dA_j>
3.00000+4 4.90000-3 1.00000+5 6.40000-3 2.00000+5 0.00000+0126433102
2.00000+7 0.00000+0                                          126433102
0.00000+0 0.00000+0       LT=0       LB=1       NT=6       NE=3126433102 LIST
1.00000-5 0.00000+5 2.00000+5 4.00000-4 2.00000+7 0.00000+0126433102 <dR_i×dR_j>
0.00000+0 0.00000+0       LS=1       LB=5     NT=21       NE=61254331-2 LIST
1.00000-5 2.53000-2 9.00000-2 2.50000-1 1.00000+0 2.00000+7126433102 <da_i×da_j>
2.21000-3 4.84000-4 3.62000-4 3.56000-4 0.00000+0 4.84000-4126433102
3.10000-4 3.04000-4 0.00000+0 6.25000-4 2.30000-4 0.00000+0126433102
2.21000-3 0.00000+0 0.00000+0 0.00000+0 0.00000+0 0.00000+0126433102
      (1264,102;1261,18)
0.00000+0 0.00000+0 MAT1=1261    MT1=18       NL=1       NI=0126433102 CONT
0.00000+0 0.00000+0          0     LTY=2          0          0126433102 CONT
2.00000+5 2.00000+7 MATS=1261    MTS=18       NT=6       NE=2126433102 LIST
0.00000+0 0.00000+0 2.00000+5 1.00000+0 2.00000+7 0.00000+0126433102 <dY_i×dY_j>
0.00000+0 0.00000+0          0          0          0          0126433  0 SEND
```

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

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

1. Total cross sections (MT=1), σ_i^T, were evaluated over the complete energy range, with the covariance matrix obtained, and:

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

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

2. Elastic cross sections (MT=2), σ_i^E, were "derived" up to 8.5 MeV from the "evaluated: cross sections:

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

Above 8.5 MeV the elastic cross sections were evaluated and:

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

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

3. Inelastic cross sections (MT=4), σ_i^I, were evaluated from threshold, 4.8 MeV, to 8.5 MeV and:

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

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

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

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

4. Capture cross sections (MT=102), σ_i^C, were evaluated over the complete energy range and:

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

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

5. The (n,α) cross sections (MT=107), σ_i^α, were evaluated from threshold, 6.18 MeV to 20 MeV and:

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

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

In the listing given in Example 33.2 for File 33 of MAT=1274, corresponding to our example, we have shown only one "NI-type" sub-subsection for each evaluated covariance matrix. Again it is assumed that there are no correlations among the directly evaluated quantities.

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

a. MT=51

The inelastic scattering to the first excited state, σ_1^{51}, up to 8.5 MeV is identical to σ_i^I. Therefore, we may consider up to 8.5 MeV that σ_i^{51} is a "derived" cross section with: $\sigma_i^{51} = \sigma_1^I$. This is permissible because MT=4 has only "NI-type" sub-subsection in this energy range.

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

$$<d\sigma_i^{51} \cdot d\sigma_j^{51}> \rightarrow \{E_k^{51}, F_k^{51}\} ,$$

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

b. MT=91

From 8.5 to 20 MeV, the continuum inelastic, σ_1^{91}, was "derived" as: $\sigma_i^{91} = \sigma_i^{I} - \sigma_i^{51}$. However, we cannot use this relationship for purposes of File 33 because in this energy range σ_i^{I} is indicated in the file as being already "derived."

Therefore, for purposes of File 33, we must write: $\sigma_i^{91} = \sigma_i^{T} - \sigma_i^{E} - \sigma_i^{51} - \sigma_i^{C} - \sigma_i^{\alpha}$, which now only refers to cross sections having exclusively "NI-type" sub-subsections. Therefore, we may now add the sections to the File 33, MAT=1274, shown in Example 33.3, to have a more complete File 33.

Example 33.2. File 33 with "NC-type" LTY=0 sub-subsection.

```
      (1274.1;0.1)
 6.01200+3 1.18969+1          0          0          0          1112733  1 HEAD
 0.00000+0 0.00000+0          0          1          0          1112733  1 CONT
 0.00000+0 0.00000+0          0          1          6          3112733  1 LIST
 1.00000-5 5.00000-5 2.00000+6 2.50000-5 2.00000+7 0.00000+0112733  1
 0.00000+0 0.00000+0          0          0          0          0112733  0 SEND
      (1274,2;0,2)
 6.01200+3 1.18969+1          0          0           0         1112733  2 HEAD
 0.00000+0 0.00000+0          0          2           1         1112733  2 CONT
 0.00000+0 0.00000+0          0          0           0         0112733  2 CONT
 1.00000-5 8.50000+6          0          0           8         4112733  2 LIST
 1.00000+0 1.00000+0 1.00000+0 4.00000+0-1.00000+0 1.02000+2112733  2
-1.00000+0 1.07000+0                                           112733  2
 0.00000+0 0.00000+0          0          1          8         4112733  2 LIST
 1.00000-5 0.00000-0 8.50000+6 8.00000-6 1.50000+6 2.50000-5112733  2
 2.00000+7 0.00000+0                                           112733  2
 0.00000+0 0.00000+0          0          0          0         0112733  0 SEND
      (1274,4;0,4)
 6.01200+3 1.18970+1          0          0          0         1112733  4 HEAD
 0.00000+0 0.00000+0          0          4          1         1112733  4 CONT
 0.00000+0 0.00000+0          0          0          0         0112733  4 CONT
LIST
 1.00000+0 1.00000+0-1.00000+0 2.00000+0-1.00000+0 1.02000+2112733  4
-1.00000+0 1.07000+2                                           112733  4
 0.00000+0 0.00000+0          0          1          8         4112733  4 LIST
 4.80000+6 1.00000-3 6.00000+6 1.00000-4 8.50000+6 0.00000-0112733  4
  8.50000+6 2.00000+7          0          0          8         4112733  4
2.00000+7 0.00000+0                                            112733  4
 0.00000+0 0.00000+0          0          0          0         0112733  0 SEND
      (1274,102;0,102)
 6.01200+3 1.18969+1          0          0          0         1112733102 HEAD
 0.00000+0 0.00000+0          0        102          0         1112733102 CONT
 0.00000+0 0.00000+0          0          1          6         3112733102 LIST
 1.00000-5 3.60000-3 1.00000+3 4.00000-2 2.00000+7 0.00000+0112733102
 0.00000+0 0.00000+0          0          0          0         0112733  0 SEND
      (1274,107;0,107)
 6.01200+3 1.18969+1          0          0          0         1112733107 HEAD
 0.00000+0 0.00000+0          0        107          0         1112733107 CONT
 0.00000+0 0.00000+0          0          0          8         4112733107 LIST
 6.18000+6 1.00000-5 6.32000+6 1.00000-4 7.36000+6 2.00000-4112733107
 2.00000+7 0.00000+0                                           112733107
 0.00000+0 0.00000+0          0          0          0         0112733  0 SEND
```

Example 33.3. Additional sections of File 33 which could be added to File 33 given in Example 33.3

```
      (1274,51;0.51)
 6.01200+3 1.18969+1          0          0          0          1127433 51 HEAD
 0.00000+0 0.00000+0          0         51          1          1127433 51 CONT
 0.00000+0 0.00000+0          0          0          0          0127433 51 CONT
 1.00000-5 8.50000+6          0          0          2          1127433 51 LIST
 1.00000+0 4.00000+0                                           127433 51
 0.00000+0 0.00000+0          0          1          6          3127433 51 LIST
 1.00000-5 0.00000+0 8.50000+6 2.50000-3 2.00000+7 0.00000+0127433 51
 0.00000+0 0.00000+0          0          0          0          0127433  0 SEND
      (1274,91;0,91)
 6.01200+3 1.18969+1          0          0          0          1127433 91 HEAD
 0.00000+0 0.00000+0          0         91          1          0127433 91 CONT
 0.00000+0 0.00000+0          0          0          0          0127433 51 CONT
 8.50000+6 2.00000+7          0          0         10          5127433 51 LIST
 1.00000+0 1.00000+0-1.00000+0 2.00000+0-1.00000+0 5.10000+1127433 51
-1.00000+0 1.02000+2-1.00000+0 1.07000+2                     127433 51
 0.00000+0 0.00000+0          0          0          0          0127433  0 SEND
```