# Guidance on Generating Neutron Reaction Data Covariances for the ENDF/B Library

Prepared by the CSEWG Covariance Committee

**Notice**: The recommendations in this document are intended to apply primarily to evaluated neutron cross-sections, neutron spectra, and nu-bar data in the neutron sub-library of ENDF/B for all new evaluations as well as those that have undergone major revisions since the release of ENDF/B-VII.1. Evaluations that are grandfathered from earlier versions of ENDF/B or that have undergone only minor revisions are exempted.

## 1. Basic Mathematical Properties

**1.1** The numerical data and recipes provided in an evaluated covariance file should enable complete, square, and symmetric covariance matrices, that provide both correlations and standard deviations (uncertainties), to be generated from the included values by the most widely used contemporary evaluated data processing codes.

**1.2** Complete correlation matrices that are derived from the evaluated covariance data should have unity values along the matrix diagonal and off-diagonal elements with magnitudes generally less than unity, to the extent allowed by the numerical precision of the file and consistent with limitations of the ENDF formats.

**1.3** Covariance matrices for evaluated normalized neutron-emission spectra (MF = 35) should satisfy the mathematically mandatory "sum-to-zero" property for rows and columns of the matrix, to the extent allowed by the numerical precision of the file and consistent with limitations of the ENDF formats.

## 2. Matrix Eigenvalues

**2.1** Full covariance matrices generated from information provided by the evaluator should be at least positive semi-definite (*i.e.*, involve only non-negative eigenvalues) on the evaluator's original energy grid, to the extent allowed by the numerical precision of the file and consistent with limitations of the ENDF formats. However, the presence of zero eigenvalues may be mandated by physical constraints such as normalization (see Section 1.3), the need for consistency of partial reaction channel data, or other conditions that apply to sums or differences of data for two or more reaction channels. Zero eigenvalues may also be introduced as an unavoidable consequence of having to represent evaluator-generated covariance information using the available ENDF covariance formats.

## 3. "Realistic" Covariances

**3.1** Covariance data should be sufficiently detailed and complete so as to satisfy the needs of the intended users of these data for applications. The magnitude of the uncertainties provided in a particular evaluation may be found to be inconsistent with the normal expectations of most experienced nuclear data evaluators. However, if these uncertainty magnitudes are not consistent with such expectations, then an explanation should be supplied in File 1 and in printed documentation to substantiate the claimed values (see Section 6.1).

**3.2** For evaluated energy-dependent cross sections that exceed 1% of the total cross section in magnitude, uncertainties greater than 50% predicted by the provided covariance data should be treated by reviewers as potentially unrealistic and flagged for possible rejection unless they can be amply substantiated by the evaluator. However, for cross sections smaller than 1% of the total cross section, a specified uncertainty that is greater than 50% (but always less than 100%) can be considered as representing a flag that signifies that the evaluator believes that the evaluated data should be viewed as qualitatively very uncertain. Reviewers should then treat such large assigned uncertainties as acceptable under these circumstances.

**3.3** Uncertainties which are very small, *e.g.*, smaller than those assigned to neutron reaction cross-section standards for the same process types, should be treated by reviewers as potentially unrealistic and flagged for possible rejection unless they can be amply substantiated by the evaluator.* Reviewers can also refer to the following table for general guidance in making these judgments, with the understanding that there may be legitimate exceptions that need to be considered. These exceptions may be based on certain physical considerations or on the characteristics of the experimental and theoretical information that is available to the evaluator.

| Reaction Process | Minimum Uncertainty |
|---|---|
| (n,tot) | 1% |
| (n,el) | 2% |
| (n,γ) | 2% |
| (n,inel) | 3% |
| (n,f) | 1% |
| (n,p) | 3% |
| (n,α) | 3% |
| nu-bar | 1% |
| Other | 3% |

*Guidance concerning the uncertainties claimed for the neutron reaction cross-section standards can be found in the following reference: A.D. Carlson *et al.*, “International Neutron Cross Sections Standards”, *Nuclear Data Sheets* **110**, No. 2, 3215 (2009). In particular, the plots in Figs. 66 – 78, which can be found on pages 3280 – 3283, can be examined for this purpose.

## 4. Covariance Evaluation Consistency, Completeness, and Methodology

**4.1** <u>Consistency</u>: The provided uncertainties for an evaluation should be reasonably consistent in magnitude with the uncertainties encountered with all relevant experimental data, as well as with the evaluator’s estimates of the uncertainties associated with nuclear modeling practices employed for the evaluation in question (see Section 3).

**4.2** Completeness: It is suggested that whenever it is feasible and/or practical to do so, covariance data should be provided for each evaluated cross section, neutron spectrum, or nu-bar representation that is included in the ENDF/B Library.

**4.3** Methodology: It is advisable, whenever it is feasible and/or practical to do so, that the covariance data for an evaluated physical process be generated as a direct consequence of the evaluation procedures that produce the central values. Some data users expect that this criterion will be satisfied as a requisite for their acceptance of these data for their particular applications.

## 5. Covariance Formats

**5.1** Covariance information in the ENDF/B Library should be specified using only those formats that are defined in the contemporary ENDF Formats Manual. The National Nuclear Data Center applies computerized checking procedures to examine this point for any evaluation that is submitted for inclusion in the ENDF/B Library.

## 6. Documentation

**6.1** It is strongly encouraged that descriptive information be provided within an evaluated data file. This information should be included in the category "Descriptive Comments" (MF = 1; MT = 451). It should indicate how the provided covariance information was generated and also document justifications for any uncertainty values that appear to be unrealistic in magnitude, *i.e.*, either unusually small or large (see Section 3). References to the literature and other available documents that provide more detailed descriptions of the procedures used to generate the provided covariance information, including links to information available from the Internet, should also be specified in this section.

## 7. Checking Procedures and Visual Inspections

**7.1** Evaluated central value and corresponding covariance data files should pass all numerical and physical consistency tests that can be performed by the ENDF/B file checking procedures that are applied by the National Nuclear Data Center before an evaluation is accepted for inclusion in the ENDF/B Library.

**7.2** An evaluated covariance file should be subjected to a visual inspection of plots of uncertainties and correlation matrices by at least one independent reviewer, in order to weed out obvious errors and nonsensical values and to identify those instances where the results appear to be otherwise unrealistic. Identified anomalies should subsequently be examined further by the evaluator, and the issues in question resolved or explained before the file is accepted for the ENDF/B Library (see Section 3).

## 8. Processing Requirements

**8.1** The covariance data included in ENDF/B evaluations should be capable of being processed by the most widely used contemporary evaluated nuclear data processing codes (*e.g.*, by the current versions of NJOY and PUFF) for common group structures that are employed in contemporary nuclear applications.

**8.2** The covariance data generated from the processing of ENDF/B files by codes such as NJOY and PUFF in comparable situations should agree numerically to within precisions that are consistent with limitations associated with the ENDF formats as well as acceptable differences in the computational methodologies employed by these codes.

*December 7, 2012*
*Reviewed on October 1, 2013. by the CSEWG Covariance Committee Chair*