IX. THE ENDF CONNECTION

Analyses accomplished with SAMMY often find their way into one or more of the evaluated nuclear data files [ENDF (United States), JEFF (European), CENDL (Chinese), JENDL (Japanese), BROND (Russian), FOND (Russian), ...]. Resonance parameters from the evaluated nuclear data files or experimental data from the EXFOR files are sometimes used as input for SAMMY analyses. Many options are available within SAMMY to expedite this information interchange. Some of these are described in various places throughout this document and summarized here. Others are described in more detail in this section. See also Section XI.C for miscellaneous comments regarding ENDF format conventions. Details of ENDF formats are given in [ENDF-102]; SAMMY users can more readily obtain information about resolved-resonance ENDF formats from [NL07b].

SAMMY command statements related to using ENDF formats as either input or output are summarized in Table VI A1.2 under the categories "ENDF as input" or "ENDF output." See also Sections VI.F.2 and VI.F.3 for other input requirements.

(In the following comments, "endf" in lowercase letters refers to "evaluated nuclear data files" in general, and "ENDF" in capital letters refers to the United States' Evaluated Nuclear Data Files [ENDFw] as housed at the National Nuclear Data Center [NNDC] at Brookhaven National Laboratory.)

In 1998 the Cross Section Evaluation Working Group (CSEWG), an advisory group for the ENDF, appointed a "constants" task force subcommittee whose purpose was to ensure that each code contributing to or using data from the evaluated files would use the same values for mathematical and physical constants. The final report of that subcommittee is found in Section IX.A of this document. Also included there is Table IXA.1, which gives values for the physical constants used in the current version of SAMMY.

In the resolved resonance region (RRR), SAMMY can read resonance parameters directly from File 2 (extracted from an endf file), or from an entire endf file if the MAT (material) number is provided. Test cases tr049, tr050, tr086, tr102, and tr129 provide examples of this use of endf files. See Section VI.F.3 for details.

SAMMY can also write the R-matrix parameters into endf file 2 formats. For the RRR, see Section VI.F.2 for details. For the unresolved resonance region (URR), see Section VIII.D. Note that SAMMY can produce two output files corresponding to endf File 2, named SAMMY.NDF and SAMMY.NDX. The first of these is suitable for direct use within a complete endf file. The second (which is produced if the command "DEBUG" is included in the INPut file) contains the identical information but also includes comment lines (beginning with ####) that may be helpful in understanding the contents of the file.

When creating File 2, it is also possible to create File 32, which contains covariance information for the resonance parameters. The necessary command line is "`PUT COVARIANCE MATRIx into endf file 32`". The output file is named SAMMY.N32, and the corresponding annotated file (containing comment lines) is SAMMY.N3X. Test case tr126 has numerous examples with LCOMP = 0, 1, and 2. Test case tr128 gives examples in the URR.

When the input resonance parameters are in endf File 2 format (RRR), and the intent is to generate an estimated covariance matrix for endf File 32, SAMMY can automatically generate the input *.ndf file for that purpose. To invoke, include the command "AUTOMATIC NDF FILE Creation" in the INPut file. See test case tr137 (k and l) for examples. Note that other commands are also necessary:

```
AUTOMATIC NDF FILE Creation
INPUT IS ENDF/B FILE  MAT=9446
FLAG ALL RESONANCE Parameters
ENDF/B-VI FILE 2 IS wanted
NDF FILE IS IN KEY Word format (optional)
PUT COVARIANCE MATRIx into endf file 32
```

It is important to note that the resonance parameter covariance matrix alone is not capable of conveying complete information regarding the evaluated cross section covariance matrix, as discussed in Section IV.E.6. Additional information (normalization or background uncertainty) can be introduced via the use of endf File 33, which can be created using auxiliary code XXXXXX discussed in Section X.S.

Point-wise cross sections can be printed in endf File 3 formats, in both the RRR and the URR. To invoke this option, include the phrase "GENERATE FILE 3 POINt-wise cross section", or "FILE 3", in the INPut file. An annotated "ndf" file, similar to that described in Section VI.F.2 for File 2, is also needed; see Table IX.1 for details. (Note that most entries in this table are optional.) The output file is named SAMMY.FL3, and the corresponding annotated file is SAMMY.FLX. For examples, see test case tr086 (w) in the RRR, and test case tr073 (n) in the URR.

It is possible to use ENDF File 3 as the "experimental data file". To do so, include one of these commands in the INPut file: "DATA ARE ENDF/B FILE MAT=1234" or "USE ENDF/B ENERGIES MAT=1234", where the spacing before "MAT=" is not important (but there must be at least one space), and the endf MAT (material) number is used instead of "1234".

When calculating group averages, results can be reported in an endf-like format, similar to File 3, and the associated covariance matrix into a file with format similar to File 33. Include the command "FILE 33 LB=1 COVARIAnce is wanted" (or just "FILE 33") to write the average cross sections into file SAMMY.CRS and covariance information into file SAMMY.N33. See test case tr089 (h and i) for examples. (Historical note: SAMMY.N33 was once called SAMMY.NDF, but the name has been changed to avoid confusion with other files of the same name.) It is important to note that this is not the standard use for File 3 and 33; these files should not be used for inclusion in official ENDF files.

Legendre coefficients for angular distributions may be reported in endf File 4 format by including the command "PREPARE LEGENDRE COEfficients in endf format". The output file is called endf_legendre.dat. (File SAMJNK.DAT contains the same information in an expanded format, which some people may find useful.) The version of File 4 used here is that described in Section 4.2.2 of [ENDF-102], LTT = 1, LVT = 0, and LI = 0 (that is to say, the

Legendre expansion coefficients Al(E) are given, no transformation matrix is given, and the angular distributions are not all isotropic). See test case tr112 for examples.

CAVEAT: As with all SAMMY options, it is the responsibility of the analyst (and not only of the SAMMY author) to ensure that these features are correct. In particular, when endf output files are generated, SAMMY users are strongly encouraged to compare those files with the requirements of the endf formats. When endf files are used for input to SAMMY, users are urged to look carefully at all output to be sure that SAMMY is properly interpreting the input. When discrepancies are found, please notify the SAMMY author so that adjustments can be made.

Table IX.1. Key-word-based file needed for generating ENDF File 3 output

Card Set	Key-word variable	Notes
1	`Z`	Z for target nucleus.
	`A`	Atomic mass number.
	`ZA`	If different from (1000 * Z + A), then value must be inserted directly.
	`AW`	Ratio of the mass of the sample nucleus to the neutron mass (if absent, will be calculated from the SAMMY input).
	`MAT`	ENDF MAT number (default = 9999).
	(blank)	
2	`NUclide` or `ISOtope`	No value need be given here; this word simply indicates that information for the next nuclide will follow. For the URR, card sets 2 and 3 are not used, as the present implementation of the URR in SAMMY permits only one nuclide at a time.
3	`Z`	Z for target nucleus (this isotope); not needed here if same as above.
	`A`	Atomic mass number (this isotope); not needed if same as above.
	`ZA`	If different from (1000 * Z + A), then value must be inserted directly.
	`AW`	Ratio of mass of sample nucleus (this isotope) to neutron mass.
	`ABN`	Abundance for this isotope, if different from unity.
	`SPIN`	Spin of this isotope.
	(blank)	