Appendix A.6. MODIFICATIONS AND ADDITIONS IN REVISION 6

(This section is modified slightly from Appendix A.6 in Revision 6 of this manual, with ~~strikeouts~~ and {inserts} to clarify topics that might otherwise cause confusion.)

Modifications, additions, and improvements to SAMMY subsequent to the publication of Revision 5 of this manual are summarized here.

New Input Options

1. The "obsolete spin group format" is no longer supported. Current formats are described in Table VI.A.1, card sets 10.1 and 10.2. (For help in converting to one of those formats, users can attempt to make a SAMMY run with the obsolete INPut file and then follow the instructions which SAMMY provides.)

2. Key-word-based input is now available as an alternative to the sometimes-confusing earlier possibilities: particle-pair and spin group definitions (See Section VI.A, Table VI A.1, card set ~~4.1~~ {4}), information needed when writing an ENDF File 2 output file (~~VI.F~~ {VI.F.2}), and input to unresolved resonance calculations (VIII).

3. Input for R-matrix parameters has traditionally been provided in two locations, with spin-group definitions in the INPut file and resonance parameters in the PARameter file. Eventually the intent is to have one file for each nuclide, and that file would give all R-matrix information for only that one nuclide. As an intermediate step in that direction, version M6 of SAMMY includes the possibility to store all R-matrix information (for all nuclides) in the PARameter file rather than splitting it between INPut and PARameter files. SAMMY can also provide guidance for making the conversion. See Section VI on input.

4. Mistakes in command lines in the INPut file are now reported "live" as well as in the LPT file. (By "live" is meant "on screen", or "in the file to which the on-screen information is printed.") Command lines may be "commented out" (so that SAMMY ignores them) by inserting a pound sign (#) in the first column. See Table ~~VI.A.2~~ {VI A1.2}.

5. Previous versions of SAMMY permitted at most 50 spin groups, due to restrictions in the input format. An alternate format now makes it possible to use up to 500 spin groups. See Table VI A .1 and ~~VI B.1~~ {VI B.2} for details.

6. When using an ENDF file to obtain resonance parameters for SAMMY, it is no longer necessary to edit and extract File 2; instead, the complete ENDF file may be used as input to SAMMY. See Sections IX ("the ENDF Connection") and ~~VI.G~~ {VI.F.3} (input).

7. Units may be specified by the user for the energies in the plot file (SAMMY.PLT or SAMMY.ODF). See Table ~~VI.A.2~~ {VI A1.2}. A flag indicating which units are used is reported in both versions of the plot file (see the FORTRAN file plt/mplt.f), and can be used for printing column headings for example.

Output Changes

1. An effort has been made to eliminate inconsistencies in output in the SAMMY.LPT file. Users are requested to report any remaining inconsistencies to the author.

2. The formulae used to generate chi-squared values printed in the LPT file have been modified somewhat: When off-diagonal data covariances are given (either explicitly or implicitly), they are now included in the calculation of χ^2.

3. To ease your publication efforts, an option exists for generating a listing of resonance parameters and uncertainties in a format suitable for porting to a spreadsheet program, which can then be used to arrange the information in publishable form. See Table VIA.2 for details.

4. ENDF files can be created for analyses in the unresolved resonance region (URR) as well as in the resolved. See Sections VIII (URR) and IX (ENDF) for details.

New Features

1. Angular distributions for reaction cross sections can be generated; previously, only elastic angular distributions were permitted. See Section ~~III.E~~ {II.B.1.c}.

2. Angular distributions can be angle-averaged; see Section ~~III.E.3~~ {III.E.7}.

3. A crystal-lattice model (CLM) of Doppler broadening has been added, based on the DOPUSH model of Naberejnev [DN99]; see Section ~~IV.B.4~~ {III.B.4}.

4. For testing purposes, fictitious cross sections can be generated (in lieu of actual Reich-Moore cross sections) in the form of constant, linear, quadratic, Dirac-delta, or 1/v functions. Along with these, specific types of energy grids (uniform in energy, time, or velocity) may be used. See Section V.E for details.

5. Enhancements have been made to the RPI resolution function, Section ~~IV.C.3~~ {III.C.3}.

6. A straight-line energy-average resolution function "DEX" has been added; see Section ~~IV.C.4~~ {III.C.4} for details.

7. The resolution function can now be specified numerically; see Section ~~IV.C.5~~ {III.C.5} for a description of this UDR resolution function. (Use with extreme caution, as this is a preliminary implementation and is known to be flawed.)

8. More than one type of resolution function may be used during a single SAMMY run. For details, see Section ~~IV.C~~ {III.C}.

9. Numerous enhancements have been made in the unresolved resonance region, described in Section VIII. "Annotated" input files may be used to increase the legibility and reduce the risk

of input errors; output parameter files are given in annotated format. Output parameters and covariance matrix can be used as input to another run, in similar fashion to that used for sequential runs in the RRR. Parameters and covariance matrix, or point-wise cross sections, can be written in ENDF format.

10. Experience has shown that it is possible to use SAMMY's Reich-Moore approximation in a manner which mimics full (unapproximated) R-matrix behavior. See Section ~~III.I~~ {II.B.2} for details.

11. When appropriate, covariance matrices are now tested to ensure that they are positive-definite. Error messages are written if they are not. (Note: For virtually all the SAMMY test cases, the parameter covariance matrices are positive definite. The notable exceptions are those involving approximate covariance matrices.)

Debugging the Code

1. Bugs were uncovered and resolved in the calculation of the partial derivatives with respect to the resolution parameters, for both the ORR and RPI resolution functions. Attempts to include these parameters in the fitting procedure should now meet with far more success than previously.

2. Other less-obvious bugs have also been corrected; these will not be itemized here. Users are encouraged to contact the author when they suspect their problems to be due to a bug in the code. See Section XI.B for suggested procedures for resolving problems and for contacting the author.

Modifications to the Manual

1. Irrelevant and outdated material from the earlier releases has been eliminated:

   APPENDIX A. FORTRAN LISTING OF SAMMY. A listing of the coding for SAMMY, currently ~ ~~120,000~~ {140,000} lines, is no longer provided in the manual. See Table XIII.C.1 for a description of the various segments of the code.

   APPENDIX B. EXAMPLES. Please see Section XII for a description of the SAMMY tutorial exercises and test cases, which provide examples of input and output for most features of the code.

   APPENDIX C. POSSIBLE JCL FOR IBM VERSION OF SAMMY. This information is no longer relevant.

APPENDIX D. ANALYSES USING SAMMY. Revision 5 (and earlier versions) of this manual contained a listing of publications describing SAMMY analyses. Because it is impossible to maintain an accurate and complete listing, this appendix is discontinued with Revision 6.

Information from the old "APPENDIX E. CONSTANTS" is now included in a new section (Section IX. THE ENDF CONNECTION), which summarizes SAMMY features related to the Evaluated Nuclear Data Files.

APPENDIX F, detailing future plans for restructuring of the SAMMY code and input, ~~has been repositioned to Appendix B~~ {removed}.

2. The structure of much of the manual has been reorganized in a more logical fashion. (~~Sections II and III will be reorganized at a later date.~~ {Sections II, III, and IV are reorganized for Revision 7.})

3. Tables in Section VI (Input) have been redesigned.

4. The page numbering system ~~(for Section IV through the appendix)~~ has been revised to use sequential integer numbers. Some numbers are skipped, to ease future expansion efforts. References to page numbers are generally omitted throughout the manual; instead, the references are to section numbers.

5. The manual is no longer published on paper, but only as a pdf file. Readers wishing to have hard copy of the manual can print from the pdf file.