Appendix A.3. MODIFICATIONS AND ADDITIONS IN REVISION 3

(This page is taken from the Introduction to Revision 3 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Major modifications and improvements to SAMMY have been incorporated subsequent to the publication of Revision 2 of this manual; these changes are documented in Revision 3.

Chief among the improvements is the incorporation of self-shielding and multiple-scattering corrections in the calculation of capture yields. Self-shielding is included exactly. Single-scattering is included exactly for specific geometries (a disk or flat rectangular sample inserted perpendicular to the neutron beam), or may be approximated (by pretending the radius of the disk or dimensions of the rectangle are infinite) in order to shorten computer run time. ~~(Double-scattering in approximate form is "on the drawing board" still.)~~ See Section ~~III.F~~ {III.D}for a more complete description of these corrections.

The ability to calculate angular distributions (double differential elastic cross sections) was initially a by-product of the single-scattering correction, but is also useful in its own right. SAMMY can now be used to analyze angular distributions of elastic cross sections for samples of any spin. Separate normalizations, backgrounds, and attenuation factors can be applied to each angle. A formal description of differential elastic scattering {and other angular distributions} is given in ~~Section III.E~~ {Section II.B.1.b}, and input is described in Section VI.

Mixtures of different isotopes or even nuclei with different Z can now be treated properly in SAMMY; thus data from oxides or other chemical combinations, with impurities, and/or samples with natural isotopic abundances can all be analyzed properly. Spins, abundances, masses, and scattering radii are individually given for each separate nucleus. Abundances and radii may be varied if desired. See Section VI for input information and Section ~~V.D~~ {III.E.2} for a description of the options.

"Simultaneous analyses" (i.e., sequential analyses connected via the parameter covariance matrix) of different data sets is often hindered because of slightly offset energy scales for the two data sets. To compensate for this, SAMMY now permits the user to vary t_0 and L. See Section ~~III.A.2.c~~ {III.E.8} for details and Table ~~VIB.1~~ {VI B.2}, card set 11, for input.

Reconstruction of point-wise cross sections from resonance parameters can now be done automatically in SAMMY, without the user having to provide an energy grid. Details are in Section ~~V.G~~ {V.A}.

SAMMY can now accept ENDF/B File 2 as input, replacing part of the usual SAMMY INPut file and all of the PARameter file. Details are given in Section ~~VI.G~~ {VI.F.3}.

An alternative method for calculating the Reich-Moore R-matrix cross sections is described in ~~Section III.D~~ {Section II.B}. This method was programmed for two reasons: First, accurate calculation of low-energy absorption or capture cross sections required revisions of the coding, since the original method produced numerical instabilities. Secondly, restructuring of the coding was

required in order to facilitate incorporation of some of the other new features (multiple-scattering, angular distributions, reconstruction of point-wise cross sections).

Maxwellian (or stellar) averages of capture cross sections may be calculated from resonance parameters alone, or with resonance parameters plus point-wise cross sections for the unresolved region. See Section ~~V.F~~ {V.D} for details and ~~VI.H~~ {VI.F.4} for input.

The Oak Ridge Resolution function was available at the printing Revision 2 of this manual; documentation, however, was not, but is provided here (see Section ~~IV.E~~ {III.C.2}). The implementation of the ORR function within SAMMY has been modified somewhat, notably in changing all input parameters to consistent units, and introducing energy-dependence into the mean free path for the water moderator. In addition, the auxiliary program SAMORT (Section ~~VIII.C~~ {X.H}) was created to view individual components as well as the complete Oak Ridge Resolution function.

The data-reading segment in SAMMY has been modified to (1) take the "even grid for broadening at end points" as the default in designing the auxiliary grid, and (2) streamline the coding. ~~The user retains the option to use the original version should the need arise; however this "original version" (segment DAX) is not being carefully maintained, so is useful only in simple cases.~~ {Segment DAX is no longer available.}

Auxiliary program SAMAMR replaces SAMADD and SAMMIX (see Section ~~VIII.A~~ {X.C}). In addition to those features contained in SAMADD and SAMMIX, SAMAMR also facilitates simultaneous analysis of angular distributions with angle-integrated data by Adding, Mixing, or Removing data-set-dependent varied parameters from the "active" list.

Computer systems which choose not to use the ORELA "ODF" plotting package are encouraged to make use of SAMMY's alternative, which is to write the information into a "generic" binary file and process this file via a modification of the program ~~SAMBIN~~ {SAMPLT}. Details are given in Section ~~VIII.F~~ {X.I}

Finally, the input/output protocols for temporary storage within SAMMY have been extensively altered as a means of improving run time. This is possible because memory on modern computers has vastly increased; it is no longer necessary, e.g., to read derivatives at only one energy while keeping all others in temporary files. This change should be invisible to most users, except as manifested in increased speed of computation.