VIII.B. INPUT FOR ANALYSIS OF DATA IN UNRESOLVED RESONANCE REGION

Two or more input files are required for analysis in the unresolved resonance region (URR). The first is comparable to the usual SAMMY INPut file, which may contain as few as three lines: Card set 1 of Table VIA.1 (the title line), card set 2 (nuclide name, atomic weight, and energy range), and (at least) one line for card set 3 (alphanumeric information). Options for alphanumeric commands in the URR are

```
UNRESOLVED RESONANCE region
EXPERIMENTAL DATA ARe in separate files
ANNOTATED PARAMETER file for urr
NO ANNOTATED PARAMETer file for urr input
ENDF/B-VI FILE 2 IS wanted
PUT COVARIANCE MATRIx into endf file 32
COVARIANCE MATRIX FRom old run is used
GENERATE FILE 3 POINt-wise cross sections
DEBUG
DO NOT SOLVE BAYES Equations
USE ENERGY LIMITS AS given in the input file
PRINT PARTIAL DERIVAtives
INCLUDE MIN & MAX ENergies when creating endf file
```

The first of these is required, as the SAMMY default is the resolved resonance region (RRR). The other alphanumeric commands are optional; their effects are described below.

The second file, the URR PARameter file, contains the unresolved resonance parameters. In the URR, there are several differences from the usual SAMMY conventions: To inform the code that a parameter is to be varied, FITACS assumes that, if the uncertainty is given as zero for a given parameter, then that parameter is not varied. (Hence there is no means of providing a default value for uncertainty.) This procedure is in contrast with the usual SAMMY procedure of assigning a value (generally 1) to a flag for each varied parameter; in the future, the formats for input to the FITACS portion of SAMMY will perhaps be modified to conform to SAMMY standards.

SAMMY permits several types of modifications to the original FITACS-style PARameter file: (1) Experimental data may be kept in separate files. (2) Normalizations can be included (and varied) for each data set. (3) ENDF File 2 and File 32 can be produced. (4) ENDF File 3 can be produced. (5) The PARameter file itself may be "annotated" in order to be more legible to humans. (6) Units may be specified for various quantities. (7) Different parameters may be specified in different energy regions. (8) Direct inelastic and/or direct capture components may be added. (9) Sequential analyses may be performed. (10) The analysis may be restricted to an energy range smaller than that for which the data are defined. Options (6) through (9) are available only with the annotated PARameter file.

Each of the 10 options is described separately below; details are given in Tables VIII B.1 and VIII B.2. Table VIII B.3 provides a guide for the various types of energy ranges encountered during a URR analysis.

(1) When the INPut file contains the phrase

```
EXPERIMENTAL DATA ARe in separate files,
```

experimental data are kept in separate file(s) rather than included as a portion of the URR PARameter file. Files names for individual data sets are given on the lines immediately following the INPut and PARameter file names in the interactive input stream. See, for example, test case tr073 run y.

(2) Normalizations can be included and varied (i.e., fitted) for each data set. That is, the theoretical calculation of the cross section is modified by

$$Theory = norm \times \sigma_{calculated} \quad , \qquad \text{(VIII B.1)}$$

where *norm* is given by the formula

$$norm = a + bE^{c} \qquad \text{(VIII B.2)}$$

and *a*, *b*, and *c* are input parameters, specified in the PARameter file. Note that one set of values for *a*, *b*, and *c* is given for each data set. Note also that there is no possibility to specify *b* and *c* unless

```
EXPERIMENTAL DATA ARe in separate files.
```

See tr073 for examples.

(3) When output in ENDF File 2 format is wanted, the phrase

```
ENDF/B-VI FILE 2 IS wanted
```

must be present in the INPut file. Also include the command

```
DEBUG
```

if you wish to create an annotated file SAMMY.NDX. This annotated file contains comments that define which parameters' values are given; except for the annotations, this file is identical to the SAMMY.NDF.

One additional SAMMY input file must be provided; the name for this file is given in the input stream after the name of the PARameter file (or after the COVariance file if it exists) and before the name(s) of any data files. This NDF file provides information regarding the specifics of the ENDF file to be created. The NDF file is in key word format, and contains only the following parameters:

`Z` = charge
`A` = atomic number
`Mat` = ENDF material number
`NUmber` of energy points = number
`Energy` number 1 = value of energy-point

Only the one or two characters in capitals are required; others are optional. The value is given following the equal sign. One or the other of "NU...=" and "E...=" must be present. (If both are present, "NU...=" will be ignored.)

The number of energy points specifies at how many equally spaced points per energy region the parameter values will be printed into the ENDF file. Values may also be printed at Emin and Emax, the limits of the analysis, if the phrase

```
INCLUDE MIN & MAX ENergies in endf file
```

is given in the INPut file. For example, for 3 points per region and 5 regions, a total of $3 \times 5 + 2 = 17$ sets of values would be given in the ENDF file.

If, instead of having a certain number of points for each energy range, specific values of energy are wanted in the ENDF file, then the alternative "E...=" should be specified. Subsequent energies are given one per line, with or without the key word "E...=" prior to the value. These energy values should be the last entries in this file.

See test cases tr073 and tr127 for examples. Runs a, b, e, and f of tr127 use "NU...=" key word, while run g uses the "E...=" key word.

To also obtain the associated covariance file (ENDF File 32), include the phrase

```
PUT COVARIANCE MATRix into endf file 32
```

in the INPut file. See test case tr128 runs j and k for examples.

(4) ENDF File 3 output (point-wise cross sections, in file SAMMY.FL3) can be generated when the command

```
GENERATE FILE 3 POINt-wise cross sections
```

is included in the INPut file. The energy grid for this cross section is as defined by the input data sets. If the DEBUG command is also used, an annotated ENDF File 3 (SAMMY.FLX) output file is also produced. See test case tr073, runs n through t, for examples.

(5) Two modes, annotated and unannotated, are available for the URR PARameter file:

The unannotated mode is essentially equivalent to Fröhner's original FITACS file (which includes both parameters and data). Formats for this file are described in Table VIII B .1; all numbers, both integer and real, are specified with F10 formats. To use this mode, the INPut file must contain the command

```
NO ANNOTATED PARAMETer file for urr input
```

Test case tr073 has examples of this input mode.

The annotated PARameter file is described in detail in Table VIII B.2; this is the default mode for SAMMY. With this option, some parameters are entered by key word; other parameter lists have headings to define which parameters are in the list. See, for example, test case tr073 run g, or test cases tr128.

(6) Units may be specified for various energy-related quantities by including the phrase "`in eV`", "`in keV`", or "`in MeV`" in the appropriate location in the PARameter file. (Note that, as always with SAMMY input, capitalization is irrelevant.) If units are not specified, defaults are as given in Table VIII B.2 (i.e., MeV for binding energy and pairing energy, eV for all others). The quantities for which units may be specified are as follows:

excitation energies for inelastic states
binding energy
pairing energy
energy maxima for the different ranges (see (7) below)
energies for direct inelastic contribution (see (8) below)

See in particular tr128 run l (letter "l" not number "one") for examples.

(7) Different parameter values may be used in different energy ranges; see Table VIII.B.2, card sets 4-7, for input details. See test case tr128 for examples.

(8) A direct inelastic component may be added to the inelastic and total cross sections, and/or a direct capture component added to the capture and total cross sections. These components are specified numerically on grids chosen by the user; SAMMY interpolates linearly between grid points. See card set 11 of Table VIII B.2 for details. Examples are in tr088 and tr134.

(9) Although many data sets can be analyzed simultaneously in URR, SAMMY also permits sequential runs similar to those used in the RRR. For details, see the description of the SAMMY.COV file in the next section. For examples, see test case tr073 runs a and g.

(10) The default choice for energy range in the URR is to include all energies for which data are available. However, the analysis may be restricted to a smaller energy range by including the command

```
USE ENERGY LIMITS AS given in the input file
```

in the INPut file. See test case tr073 runs j,k,l for examples.