

VI.B. THE PARAmeter FILE

The PARAmeter file contains initial values for all those parameters that are to be varied, as well as others that may be held fixed or treated as propagated-uncertainty parameters (see Section IV.D.2 for details concerning PUPs). In addition, this file may contain *a priori* uncertainties or covariances for the varied parameters.

Various types of data can be included in the PARAmeter file. These are organized into “card sets,” with each card set consisting of one or more lines of information. Most card sets begin with a header line and end with a blank line. The header lines are listed in Table VI B.1, along with key words for some of the card sets. Details about each card set are given in Table VI B.2 and summarized here.

Card set 1 contains resonance parameters, ending in a blank line.

Beginning with Revision 8 of this document and Release sammy-7.0.2, the square-root of resonance energies and reduced-width amplitudes may be used for input in place of resonance energies and partial widths. Input for this option is described in card set 1a. To use this option, include the command “REDUCED WIDTH AMPLITudes are used for input” in card set 2 of the INPut file.

For all SAMMY runs for which resolved-resonance-region parameters are fitted, two output parameter files are created. The first, SAMMY.PAR, is in the original format with resonance energies and partial widths; units are eV for energies and meV for partial widths. The second, SAMMY.RED, contains the square-root of resonance energies and reduced-width amplitudes; units for both types of parameters are square-root of eV.

Card set 2 contains a single number, called FUDGE, which is the “fudge factor” by which a parameter is multiplied to give the initial uncertainty for that parameter, unless that uncertainty is specified elsewhere.

Only card set 1 is required to be in the file. If any of card sets 3 through “Last” are present, then card set 2 must also be present.

Card set 3 gives values for parameters of the external R-function (see Section II.B.1.d). Two alternate formats are available for this.

Card set 4 gives values for some broadening (and other) parameters.

Card set 5 gives values of “unused” parameters, that is, of those data-reduction parameters that are not directly affected by the data set to be analyzed but that are coupled via the covariance matrix to other parameters that *are* directly affected. An example of such a parameter would be the thickness of a thin sample, for which the data have already been analyzed via SAMMY, while the current data set is from a measurement with a thick sample. The auxiliary code SAMAMR must be used between the two SAMMY runs to ensure that the correct thickness is used with the appropriate data set (see Section X.C).

Card set 6 gives values for normalization and background parameters, as described in Eqs. (III E3a.1) and (III E3 a.2) of Section III.E.3.a

Card set 7 contains values for the two channel radii (as used for potential scattering and for penetrability and shift factor). Key-word format for the channel radii is described in card set 7a. See item 3 in Section III.E.2 for discussion of effective vs. true radius.

Card set 8 gives names and values for data reduction parameters, as described in Section III.E.3.b.

Card set 9 gives values of parameters for the Oak Ridge resolution function (ORR) parameters, as described in Section III.C.2.

Card set 10 contains isotopic mass and abundance values, as described in Section III.E.2.

Card set 11 contains values for miscellaneous parameters, described in various locations throughout this manual.

Card set 12 provides parameter values for paramagnetic cross sections; see Section III.E.4.

Card set 13 contains values for parameters of the background functions described in Section III.E.3.a.

Card set 14 gives parameters of the RPI resolution function, Section III.C.3.

Card set 15 provides values for l - and isotope-dependent detector efficiencies, Section III.E.5.

Card set 16 gives input for the numerical user-defined resolution function. This is described in more detail in Section III.C.5.

The last card set defines the prior covariance matrix for the parameters. Three alternative methods are given: Card set *Last A* assumes a covariance matrix has been prepared by a previous SAMMY run; the presence of this card set eliminates the possibility of any others being used. Card sets *Last B* (“explicit uncertainties”) and *Last C* (“relative uncertainties”) may be interchanged at will, as long as each occurs at most once in any given PARAmeter file. A fourth alternative is available for resonance energies only (see card set 1, columns 68-80, option 3). A fifth is to omit this card set entirely, in which case, default uncertainties are used for every parameter.

Note that each card set in the PAR file (except for card sets 1 and 2) begins with an alphanumeric description of what follows. Note also that each card set (except card set 2) terminates with a blank card. A blank line at the very end of the file may be omitted, but all others must be present.

Quantum numbers included in PARAmeter file

Beginning with Release M6 of the SAMMY code, it is possible to include all information relevant to the R-matrix within the PARAmeter file rather than have partial information (spin group definitions) in the INPUT file. Details are given in Table VI B.3.