III.E.2. Combining Several Nuclides in a Single Sample

Because the samples used in neutron experiments are often made from natural materials rather than isotopically pure materials and may contain chemical combinations of elements and/or impurities, the SAMMY INPut and PARameter files may need to describe resonances corresponding to several different nuclides. A number of features of SAMMY have evolved to deal with this consideration; these features are described below. In addition, users are referred to test case tr060, which treats multiple isotopes of barium as well as oxygen and carbon. The user must provide abundances for each nuclide; however, if the exact composition of a diluent is unknown, abundances may be flagged (varied) so that SAMMY can determine the optimal values to fit the experimental data.

The SAMMY features relevant to multiple nuclides in a single sample are as follows:

1. Spin groups may be specified in one of two ways, either of which may contain information about abundances of isotopes or elements. See Section VI.A, Table VI A.1, card sets 10.1 and 10.2, for details. The nuclear spin (as well as mass and isotopic abundance) can be specified for each nuclide separately.

2. When using a multi-nuclide PARameter file, flags on the appropriate spin groups in the INPut file will eliminate the use of those spin groups in performing the calculation of cross sections; thus, the same PARameter file may be used both for the analysis of data from an isotopically pure sample and for the analysis of data from a "natural" sample, or for data from a specific nuclide and for a chemical combination. Input details are again given in Table VIA.1.

3. Channel radii (see Section II.A.1) for the different nuclei (and for different spin groups) may be specified separately. In addition, the channel radius (PAREFF) used in evaluation of the potential-scattering phase shift φ_l may differ from the channel radius (PARTRU) used in evaluation of penetration factor P_l and level shift factor S_l,; this is included for compatibility with ENDF [ENDF-102]. Input details are given in card set 7a of Table VI B.2; alternatively, one may use the older and more cumbersome card set 7. Any or all of these radii may be varied in a SAMMY run.

4. To specify a single abundance and the correct mass for all spin groups corresponding to a given nucleus, use card set 10 of the PARameter file (see Section VI.B.). Abundances, but not masses, may be varied.

SAMMY will confirm that the sets of spin groups corresponding to a given nuclide are defined consistently between the INPut and the PARameter files.

SAMMY is no longer restricted to a small number of spin groups. Previously, there were two limitations:

1. Only two digits are permitted for the spin group number in the format for the resonance parameters (card set 1 of Table VI B.2). Furthermore, spin group numbers greater than 50 (or negative) are used to designate resonances to be omitted from the calculation. When more than 50 spin groups are needed, an alternative (4-digit) format can now be used; see Table VI B.2 for details. (The maximum permitted number of spin groups is now 500, because the format in the INPut file permits only 3 digits.)

2. The second limitation relates to the itemization of spin groups associated with channel radii or with nuclide abundance in the PARameter file. Originally, this itemization used a two-digit format and required that all spin groups be listed on one line. It is now possible to use a five-digit format (when there are more than 99 spin groups) and to continue the itemization on other lines if needed. Details are given in Table VI B.2. (A better method of input for channel radii is available in card set 7a of the PARameter file, which uses key-word-based input without fixed format.)