V.B. INTEGRAL QUANTITIES

Although SAMMY was designed for calculating and fitting "differential" quantities such as cross section as a function of energy, nevertheless it often is useful to have the code calculate integral quantities for comparison with integral data. These integral quantities can also be included in the fitting procedure, if desired.* Details of the methods used to calculate these quantities are given in [NL97]. Additional features have been added to the code after publication of that report in order to facilitate direct comparisons between calculations made by SAMMY and those made by NJOY [RM82]; see items 9 and 10 below.

A single SAMMY run is used to calculate a variety of integral quantities. The first four quantities listed below are calculated for x = capture, fission, and absorption (as appropriate for the nuclide under consideration); the others are calculated only for fissile nuclides.

It should be noted that this option works only with the Reich-Moore formalism, not with either of the Breit-Wigner formalisms nor with SAMMY's original implementation of the Reich-Moore formalism. Also, the cross section for the unresolved resonance region is not included here.

1. Thermal cross section,

$$\sigma_{0x} = \sigma_x\left(E_0\right) \quad \text{for } E_0 = 0.0253 \text{ eV} \quad . \tag{V B.1}$$

2. Maxwellian average at thermal energy. This quantity is defined with somewhat different normalization from that used in Section V.D, that is, as

$$\bar{\sigma}_x = \int_{E_1}^{E_2} \sigma_x\left(E\right) \frac{E}{E_0} e^{-E/E_0} dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE \quad , \tag{V B.2}$$

where $E_1 = 10^{-5}$ eV and $E_2 = 3$ eV.

3. Westcott's g-factor,

$$g_x = \frac{2}{\sqrt{\pi}} \frac{\bar{\sigma}_x}{\sigma_{0x}} \quad . \tag{V B.3}$$

* Integral quantities may be calculated and fitted only for the resolved resonance region. In the future, this capability will be made available for the unresolved resonance region as well.

4. Resonance integral,

$$I_x = \int_{E_3}^{E_4} \sigma_x(E)\frac{dE}{E} + X_{4x} \quad , \qquad \text{(V B.4)}$$

in which $E_3 = 0.5$ eV, and E_4 and X_{4x} are specified by the user.

5. Average integral,

$$\hat{\sigma}_x = \int_{E_5}^{E_6} \sigma_x(E)\,dE \Big/ \left(E_6 - E_5\right) \quad . \qquad \text{(V B.5)}$$

6. Watt spectrum average,

$$\bar{\sigma}_{Wf} = \int_{E_1}^{E_7} \sigma_f(E)\Phi(E)\,dE \Big/ \int_{E_1}^{E_7} \Phi(E)\,dE \quad , \qquad \text{(V B.6)}$$

in which the upper limit $E_7 = 20$ MeV. The Watt fission spectrum, $\Phi(E)$, is given by the function

$$\Phi(E) = e^{-E/a}\sinh\left(\sqrt{bE}\right) = e^{-E/a}\left(e^{\sqrt{bE}} - e^{-\sqrt{bE}}\right)/2 \quad . \qquad \text{(V B.7)}$$

Here a and b are constants to be supplied by the user. For ^{235}U, values of a and b are 0.988 MeV and 2.249 MeV^{-1}, respectively.

An alternative formulation to Eq. (V B.7) for the flux is discussed in Section V.B.1.

7. K1,

$$K1 = \nu\,\sigma_{0f}\,g_f - \sigma_{0a}\,g_a = \left(\nu\sigma_f - \sigma_a\right)\frac{2}{\sqrt{\pi}} \quad , \qquad \text{(V B.8)}$$

where ν, the total number of neutrons per fission, is a constant whose value is provided by the user.

8. Alpha, or α,

$$\alpha = I_c / I_f \quad . \qquad \text{(V B.9)}$$

9. Thermal alpha integral (NJOY's α) [RM98],

$$\alpha_{NJOY} = \int_{E_1}^{E_2} \frac{\sigma_c(E)}{\sigma_f(E)} \frac{E}{E_0} e^{-E/E_0} dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE \quad . \tag{V B.10}$$

10. Thermal eta integral (NJOY's η) [RM98],

$$\eta_{NJOY} = \int_{E_1}^{E_2} \frac{\nu\sigma_f(E)}{\sigma_a(E)} \frac{E}{E_0} e^{-E/E_0} dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE \quad . \tag{V B.11}$$

Input to SAMMY for fitting integral quantities is essentially the same as input for fitting differential quantities, with a few minor changes and one additional file. Please see Section VI.D for details. Test cases tr069, tr077, and tr082 have examples of fitting to integral quantities.