III.E.1. Transmission Experiments

The analysis of transmission (or total cross section) data requires an extension to the description given in Section III.A, since what is actually measured (and thus what is to be “fitted”) is not cross section σ but transmission *T*, where

$$T = e^{-n\sigma} \quad . \tag{III E1.1}$$

Here *n* is the sample thickness, measured independently and expressed in units of atoms/barn. In this section we consider the case of uniform thickness; for the case of non-uniform thickness, see the next section (Section III .E.1.a).

Theoretical values of *T* and $\partial T/\partial u$ are generated in SAMMY according to the following procedure:

1. Generate total cross section σ and partial derivatives $\partial\sigma/\partial u$ as described in Section II.

2. Doppler broaden the cross section and derivatives as described in Section III.B.

3. Convert to transmission using Eq. (III E1.1) for the value and

$$\frac{\partial T}{\partial u} = -n\, e^{-n\sigma} \frac{\partial \sigma}{\partial u} \tag{III E1.2}$$

   for the derivatives.

4. If thickness *n* is a varied parameter, generate $\partial T/\partial n$ from

$$\frac{\partial T}{\partial n} = -\sigma e^{-n\sigma} = -\sigma T \quad . \tag{III E1.3}$$

5. Resolution broaden the transmission and derivatives, as described in Section III.C.

6. If total cross sections are to be fitted, rather than transmissions, convert the broadened transmissions and derivatives thereof back to cross section. **NOTE: Experience has shown that fewer numerical difficulties are encountered if transmissions, rather than cross sections, are used for the fitting procedure.**

The total cross section determined using the above procedure corresponds to the actual unbroadened total cross section. It may differ considerably from the “cross section” extracted directly from the measured transmission using the relationship

$$"\sigma" = -\frac{1}{n}\ln\left(T_{\text{measured}}\right) \quad . \tag{III E1.4}$$

In the study of transmission data, the distinction is made between "effective cross section" σ_{eff} and "true cross section" σ_{true}. The effective cross section is defined by first resolution broadening the transmission:

$$\mathrm{Tr}(E) = \int e^{-n\,\sigma_D(E')} R(E-E')\, dE' \quad , \tag{III E1.5}$$

where $\sigma_D(E')$ is the Doppler-broadened total cross section and $R(E-E')$ is the resolution function, and then converting to cross section,

$$\sigma_{\mathrm{eff}}(E) = -\frac{1}{n} \ln\left(\mathrm{Tr}(E)\right) \quad . \tag{III E1.6}$$

The so-called true cross section, on the other hand, is defined by resolution-broadening the Doppler-broadened total cross section directly (i.e., by omitting the conversion to and from transmission):

$$\sigma_{\mathrm{true}}(E) = \int \sigma_D(E') R(E-E')\, dE' \quad . \tag{III E1.7}$$

The difference between σ_{eff} and σ_{true} corresponds to the "self-shielding effect" in transmission measurements.

In SAMMY, the "true cross section" can be generated (i.e., the conversion to and from transmission can be omitted from the calculations) by including the command

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USE TRUE TOTAL CROSS section for resolution broadening
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in the INPut file. With this command invoked, the treatment of transmission and total cross section (as outlined on the previous page) is replaced with the following:

1. Generate total cross section σ and partial derivatives $\partial\sigma/\partial u$ as described in Section II.
2. Doppler broaden the cross section and derivatives, as described in Section III.B.
3. Resolution broaden the cross section and derivatives, as described in Section III.C.

Fitting to experimental data is inappropriate with this command, since Eq. (III E1.7) does not correspond to data measured by any practical experiment.