III. A. THEORETICAL FOUNDATION FOR NUMERICAL BROADENING

The primary method used in SAMMY for evaluating the integrals required in Doppler and resolution broadening involves several operations for which details are given in the subsequent subsections. The method was borrowed originally from the MULTI code [GA74] and subsequently modified as the need arose. Note that in SAMMY, broadening is applied both to the cross sections and to the partial derivatives, while in MULTI, it was applied only to the cross sections. A summary of the operations is given here.

1. Choose an appropriate "auxiliary energy grid" at which to evaluate the integrands. The auxiliary grid consists of (a) the original energy grid (i.e., the energies at which experimental data are given), (b) points below the minimum energy of the experimental data and above the maximum energy, and (c) additional points sufficient to describe the structure of any "narrow" resonance. See Section III.A.2 for more details regarding the choice of auxiliary grid and Section III.A.3 for details regarding the integration scheme. (Different criteria are required for Leal-Hwang Doppler broadening; see Section III.B.2.)

2. A discussion of pitfalls that can arise when insufficient care is devoted to the choice of auxiliary grid is given in Section III.A.1. While Sections III.A.2 and III.A.3 may safely be regarded as "black boxes" by some analysts, all SAMMY users are encouraged to pay careful attention to issues raised in Section III.A.1.

3. For each energy in the auxiliary grid, evaluate the theoretical cross sections and derivatives thereof, as described in Section II.

4. Determine Doppler-broadened cross section and derivatives wherever possible (i.e., for all but the highest and the lowest energies in the auxiliary grid). Generate derivatives with respect to Doppler temperature. See Section III.B for details.

5. Transform from cross section to transmission as needed; apply transformation to derivatives also. See Section III.E.1. Generate derivative with respect to sample thickness.

6. Apply self-shielding and multiple-scattering corrections as needed, both to cross sections and to derivatives. See Section III.D for details.

7. For each energy in the original (experimental) grid, determine the resolution-broadened cross section (or transmission) and derivatives thereof. Also generate derivatives with respect to resolution-broadening parameters. See Section III.C.

8. If needed, transform from transmission back to cross section; transform derivatives also.

9. Multiply by normalization and add backgrounds, as needed. Generate derivatives with respect to normalization and background. See Section III.E.3.a.