III.B.1.a. Derivatives with respect to effective temperature *T*

In SAMMY, the Doppler temperature T may be treated as a u-parameter (see Section IV) and varied via Bayes' equations. Thus, it is necessary to determine derivatives of the broadened cross section (or transmission) with respect to T.

The Doppler-broadening integral of Eq. (III B1.7) depends on effective temperature T only through the Doppler width Δ_D of Eq. (III B1.2). Using the chain rule we find

$$\frac{\partial \sigma_D}{\partial T} = \frac{\partial \Delta_D}{\partial T} \frac{\partial \sigma_D}{\partial \Delta_D} \quad , \qquad \text{(III B1 a.1)}$$

where the first of these partial derivatives is found from Eq. (III B1.2) to be

$$\frac{\partial \Delta_D}{\partial T} = \frac{\Delta_D}{2T} \quad . \qquad \text{(III B1 a.2)}$$

The partial derivative of the cross section with respect to the Doppler width is evaluated numerically in SAMMY, via

$$\frac{\partial \sigma_D}{\partial \Delta_D} = \frac{\sigma_D\left(\Delta_D + d\right) - \sigma_D\left(\Delta_D - d\right)}{2d} \quad . \qquad \text{(III B1 a.3)}$$

The value of d to use in this expression is somewhat arbitrary, subject to the restrictions that (1) d be small enough that $\sigma\left(\Delta\right)$ is approximately a linear function of Δ in the region $\Delta_D - d \le \Delta \le \Delta_D + d$ and (2) d be big enough that sufficient significant digits are retained by the computer in generating the numerical difference in $\sigma_D\left(\Delta_D + d\right) - \sigma_D\left(\Delta_D - d\right)$. Through trial and error, it was determined that setting d equal to $\Delta_D q$, with $q = 0.02$, gives reasonable results for those cases tested. Since the value of this parameter q is not subject to direct user control, anyone experiencing difficulty when varying the effective temperature should contact the author.