Table 6.3.3.1. *Transmission coefficients*

(1) Reflection from a crystal slab with negligible transmission; the crystal planes are inclined at an angle φ to the extended face, and the normal in the plane of the incident and diffracted beams $$A = \frac{\sin(\theta - \varphi)}{\mu\{\sin(\theta - \varphi) + \sin(\theta + \varphi)\}}$$ (1*a*) $\varphi = 0$ $$A = 1/2\mu$$
(2) Reflection from a crystal slab of thickness t, with planes parallel to the extended face $$A = \{1 - \exp(-2\mu t \operatorname{cosec} \theta)\}/2\mu$$
(3) Transmission through a crystal slab of thickness t; the crystal planes are at $\pi/2 - \varphi$ to the surface, with the normal in the plane of the incident and reflected beams $$A = \frac{\exp\{-\mu t \sec(\theta + \varphi)\} - \exp\{-\mu t \sec(\theta - \varphi)\}}{\mu\left[1 - \frac{\sec(\theta + \varphi)}{\sec(\theta - \varphi)}\right]}$$ (3*a*) $\varphi = 0$ $$A = t \sec\theta \exp(-\mu t \sec\theta)$$
(4) Transmission through a sphere of radius R (*i.e.* for a uniform X-ray beam and $\theta = 0^\circ$) $$A = \frac{3}{2(\mu R)^3}[1/2 - e^{-2\mu R}\{1/2 + \mu R + (\mu R)^2\}]$$
(5) Reflection from a sphere of radius R (*i.e.* for a uniform X-ray beam, and $\theta = 90^\circ$) $$A = \frac{3}{4\mu R}\left\{1/2 - \frac{1}{16(\mu R)^2}\,[1 - (1 + 4\mu R)\,e^{-4\mu R}]\right\}$$

Values of the absorption correction A^* obtained by numerical integration by Dwiggins (1975*a*) are listed in Table 6.3.3.2.

The reduced expression for a spherical crystal of radius R is

$$\begin{aligned} A = \frac{3}{4\pi R^3} \int\limits_0^R \int\limits_{-1}^1 \int\limits_0^{2\pi} \exp\Big(&-\mu\{[R^2 - r^2\cos^2\alpha \\ &- r^2\sin^2\alpha\sin^2(\theta+\varphi)]^{1/2} \\ &+ [R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta-\varphi)]^{1/2} \\ &- 2r\sin\theta\sin\alpha\sin\varphi\}\Big) r^2\,\mathrm{d}r\,\mathrm{d}(\cos\alpha)\,\mathrm{d}\varphi. \end{aligned} \quad (6.3.3.5)$$

Values of A^* obtained using numerical integration by Dwiggins (1975*b*) are listed in Table 6.3.3.3. An estimate of the accuracy of the numerical integration is given by comparison with the results for special values of θ at which equations (6.3.3.4) and (6.3.3.5) may be integrated analytically, which are included in Table 6.3.3.1. The comparison indicates a reliability for the tabulated values of better than 0.1%. Tables at finer intervals for cylinders and spheres for $\mu R < 1.0$ are given by Rouse, Cooper, York & Chakera (1970). A tabulation up to $\mu R < 5.0$ for spheres is given by Weber (1969). Interpolation for μR may be effected by the formula

$$A^*(\mu R) = \exp\left\{\sum_{m=1}^{M} K_m(\mu R)^m\right\}, \quad (6.3.3.6)$$

where the K_m are determined, for fixed θ, from the values in Tables 6.3.3.2 and 6.3.3.3.

Subsequent interpolation as a function of θ may be effected by the interpolation formula

$$A^*\{\theta\} = \sum_{n=1}^{N} L_n \sin^{2n}(\theta). \quad (6.3.3.7)$$

Interpolation is accurate to 0.1% with $N = M = 3$.

For cylinders and spheres, $\bar{T}$ may be obtained by means of the expression

$$\bar{T} = \frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}\mu} = R\left[\frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}(\mu R)}\right] \quad (6.3.3.8)$$

using the values listed in Tables 6.3.3.2 and 6.3.3.3.

Values of $(1/A^*)[\mathrm{d}A^*/\mathrm{d}(\mu R)]$ obtained by numerical integration by Flack & Vincent (1978) for spheres with $\mu R < 2.5$ are listed in Table 6.3.3.4. An equivalent table of $\mu(R/A^*)/[\mathrm{d}A^*/\mathrm{d}(\mu R)]$ for $\mu R < 4.0$ is given by Rigoult & Guidi-Morosini (1980).

Alternatively, one can differentiate the interpolation formula (6.3.3.6), yielding

$$\bar{T}(\mu R, \theta) = \frac{1}{\mu}\sum_{m=1}^{M} mK_m(\mu R)^m. \quad (6.3.3.9)$$

In this case, however, the maximum index $M = 7$ is required to obtain convergence for $\mu R \leq 2.5$. Numerical values of the coefficients K_m for cylinders and spheres evaluated by Tibballs (1982) are listed in Table 6.3.3.5.

Interpolation between the tabulated θ values is obtained from the θ interpolation formula, noting that

$$L_m = \sum_{j=1}^{7} (C^{-1})_{mj} A_j^*, \quad (6.3.3.10)$$

where

$$C_{mj} = \sin^{2m}\theta_j. \quad (6.3.3.11)$$

The elements $(C^{-1})_{mj}$ and the $K_m(\theta_j)$ for θ_j at 15° intervals in the range $0 < \theta_j < 90^\circ$ are listed in Table 6.3.3.5. Differentiating (6.3.3.7) yields

$$A^*(\mu R, \theta)\bar{T}(\mu R, \theta) = \sum_{m=0}^{M} P_m \sin^{2m}\theta, \quad (6.3.3.12)$$

where

$$P_m = R\frac{\partial L_m}{\partial(\mu R)} = \sum_{j=1}^{7}(C^{-1})_{mj} A_j^* \bar{T}_j. \quad (6.3.3.13)$$

Equation (6.3.3.12) for path lengths is the analogue of equation (6.3.3.7) for the transmission factors. It provides the basis for an interpolation formula.

In the case of a cylindrical crystal much larger than the X-ray beam, the absorption correction has been determined by Coyle (1972), in an extension of earlier work by Coyle & Schroeder (1971). The absorption correction for the case of the cylinder axis coincident with the φ axis of a Eulerian cradle, shown in Fig. 6.3.3.1, reduces to the line integral

$$\frac{1}{2\tau}\int\limits_0^{2\tau} \exp\{-\mu[(z) + T(z)]\}\,\mathrm{d}z, \quad (6.3.3.14)$$

 references