3.8: Cromer–Mann coefficients

The set of nine coefficients a_i, b_i, c $(i = 1, \ldots, 4)$ in a parameterization of the non-dispersive part of the atomic scattering factor for neutral atoms as a function of (sinθ) / λ:

$$f^0(\sin\theta/\lambda) = \sum_{i=1}^{4} a_i \exp[-b_i(\sin\theta/\lambda)^2] + c$$

for $0 < (\sin\theta)/\lambda < 2.0\,\text{Å}^{-1}$.

This expression is convenient for calculation in crystal structure software suites.

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