Electron-phonon : let us define

$$g_{\mathbf{q}\nu}(\mathbf{k},i,j) = \left(\frac{\hbar}{2M\omega_{\mathbf{q}\nu}}\right)^{1/2} \langle\psi_{i,\mathbf{k}}|\frac{dV_{SCF}}{d\hat{u}_{\mathbf{q}\nu}} \cdot \hat{\epsilon}_{\mathbf{q}\nu}|\psi_{j,\mathbf{k}+\mathbf{q}}\rangle. \tag{1}$$

The phonon linewidth $\gamma_{\mathbf{q}\nu}$ is defined by

$$\gamma_{\mathbf{q}\nu} = 2\pi\omega_{\mathbf{q}\nu} \sum_{ij} \int \frac{d^3k}{\Omega_{BZ}} |g_{\mathbf{q}\nu}(\mathbf{k},i,j)|^2 \delta(e_{\mathbf{q},i} - e_F)\delta(e_{\mathbf{k}+\mathbf{q},j} - e_F), \tag{2}$$

while the electron-phonon coupling constant $\lambda_{\mathbf{q}\nu}$ for mode ν at wavevector $\mathbf{q}$ is defined as

$$\lambda_{\mathbf{q}\nu} = \frac{\gamma_{\mathbf{q}\nu}}{\pi\hbar N(e_F)\omega^2_{\mathbf{q}\nu}} \tag{3}$$

where $N(e_F)$ is the DOS at the Fermi level. The spectral function is defined as

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(e_F)} \sum_{\mathbf{q}\nu} \delta(\omega - \omega_{\mathbf{q}\nu}) \frac{\gamma_{\mathbf{q}\nu}}{\hbar\omega_{\mathbf{q}\nu}}. \tag{4}$$

The electron-phonon mass enhancement parameter λ can also be defined as the first reciprocal momentum of the spectral function:

$$\lambda = \sum_{\mathbf{q}\nu} \lambda_{\mathbf{q}\nu} = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega. \tag{5}$$

Note that a factor $M^{-1/2}$ is hidden in the definition of normal modes as used in the code.

McMillan:

$$T_c = \frac{\Theta_D}{1.45} \exp\left[\frac{-1.04(1+\lambda)}{\lambda(1-0.62\mu^*) - \mu^*}\right] \tag{6}$$

or (better?)

$$T_c = \frac{\omega_{log}}{1.2} \exp\left[\frac{-1.04(1+\lambda)}{\lambda(1-0.62\mu^*) - \mu^*}\right] \tag{7}$$

where

$$\omega_{log} = \exp\left[\frac{2}{\lambda} \int \frac{d\omega}{\omega} \alpha^2 F(\omega) \log\omega\right] \tag{8}$$