

## Chem 534: Problem Set #6

Due in class: Tues, Nov. 3rd

From McQuarrie, Statistical Mechanics:

A modification of the Debye theory was introduced by Born, who proposed a different cutoff for the spectrum of vibrational modes. He proposed that the cutoff be made such that both the longitudinal and transverse modes have a common minimum wavelength. If we denote this common minimum wavelength by  $\lambda_m$ , then  $\lambda_m \nu_{\text{long}} = c_{\text{long}}$  and  $\lambda_m \nu_{\text{trans}} = c_{\text{trans}}$ , the normalization of  $g(\nu)$  becomes:

$$4\pi V \left\{ \int_0^{\nu_t} \frac{2}{c_{\text{trans}}^3} \nu^2 d\nu + \int_0^{\nu_l} \frac{1}{c_{\text{long}}^3} \nu^2 d\nu \right\} = 3N$$

Show that this leads to the following expression for the heat capacity:

$$C_v = R \left[ D\left(\frac{\Theta_l}{T}\right) + 2D\left(\frac{\Theta_t}{T}\right) \right] \quad \text{where } D(z) \text{ is the Debye function: } D(z) = \frac{3}{z^3} \int_0^z \frac{x^4 e^x dx}{(e^x - 1)^2}, \text{ where}$$

$$x = \frac{h\nu}{kT}$$