

Equation Sheet for Exam 1, CHE 371

Constants:

$$\begin{aligned}
 h &= 6.626 \times 10^{-34} \text{ J}\cdot\text{s} & N_A &= 6.02 \times 10^{23} \text{ molecules/mol} \\
 c &= 2.9979 \times 10^8 \text{ m/s} & k_B &= 1.38 \times 10^{-23} \text{ J/K} = 0.695 \text{ cm}^{-1}\cdot\text{K}^{-1} \\
 R &= 0.0820 \text{ L}\cdot\text{atm}\cdot\text{mol}^{-1}\cdot\text{K}^{-1} = 8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1} = 0.08314 \text{ L}\cdot\text{bar}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}
 \end{aligned}$$

Quantum Mechanics Equations:

$$\begin{aligned}
 E &= h\nu & E &= \frac{hc}{\lambda} & E &= hc\tilde{\nu} & \hbar &= \frac{h}{2\pi} & D_e &= D_0 + \frac{h\nu}{2} & \varepsilon_{\text{vib}} &= \sum_{j=1}^{n_{\text{vib}}} h\nu_j \left(v_j + \frac{1}{2} \right) \\
 \varepsilon_{n_x, n_y, n_z} &= \frac{h^2}{8m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right) & \varepsilon_v &= h\nu \left(v + \frac{1}{2} \right) & v &= 0, 1, 2, \dots & \varepsilon_J &= \frac{\hbar^2}{2I} J(J+1) & J &= 0, 1, 2, \dots & g_J &= 2J+1
 \end{aligned}$$

Gas Laws Equations:

$$\begin{aligned}
 Z &= \frac{P\bar{V}}{RT} & \left(P + \frac{a}{\bar{V}^2} \right) (\bar{V} - b) &= RT & P &= \frac{RT}{\bar{V} - B} - \frac{A}{T^{1/2}\bar{V}(\bar{V} + B)} & T_R &= \frac{T}{T_c} & P_R &= \frac{P}{P_c} \\
 P &= \frac{RT}{\bar{V} - \beta} - \frac{\alpha}{\bar{V}(\bar{V} + \beta) + \beta(\bar{V} - \beta)} & \bar{V}_c &= 3b & P_c &= \frac{a}{27b^2} & T_c &= \frac{8a}{27bR} & \bar{V}_R &= \frac{\bar{V}}{V_c}
 \end{aligned}$$

$$\left(P_R + \frac{3}{\bar{V}_R^2} \right) \left(\bar{V}_R - \frac{1}{3} \right) = \frac{8}{3} T_R \quad Z = \frac{P\bar{V}}{RT} = 1 + \frac{B_{2V}(T)}{\bar{V}} + \frac{B_{3V}(T)}{\bar{V}^2} + \frac{B_{4V}(T)}{\bar{V}^3} \dots \quad P\bar{V} = RT$$

$$Z = \frac{P\bar{V}}{RT} = 1 + B_{2P}(T)P + B_{3P}(T)P^2 + B_{4P}(T)P^3 + \dots \quad u(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

$$B_{2V}(T) = -2\pi N_A \int_0^\infty \left[e^{-\frac{u(r)}{k_B T}} - 1 \right] r^2 dr \quad B_{2V}(T) = \bar{V} - \bar{V}_{\text{ideal}}$$

Statistical Mechanics Equations (BZ and PFIG):

$$R = k_B N/n \quad p_j = \frac{e^{-E_j/k_B T}}{\sum_i e^{-E_i/k_B T}} \quad Q(N, V, \beta) = \sum_j e^{-\beta E_j} \quad \beta = \frac{1}{k_B T} \quad \langle E \rangle = k_B T^2 \left(\frac{\partial \ln Q}{\partial T} \right)_{N, V}$$

$$\bar{C}_V = \left(\frac{\partial \bar{U}}{\partial T} \right)_V = \left(\frac{\partial \langle \bar{E} \rangle}{\partial T} \right)_V \quad \langle P \rangle = k_B T \left(\frac{\partial \ln Q}{\partial V} \right)_{N, \beta} \quad \frac{N}{V} \left(\frac{h^2}{8mk_B T} \right)^{3/2} \ll 1$$

$$q(V, T) = \sum_{j, \text{states}} e^{-\beta \varepsilon_j} \quad q(V, T) = \sum_{j, \text{levels}} g_j e^{-\beta \varepsilon_j} \quad \Theta_{\text{vib}} = \frac{h\nu}{k_B} \quad \Theta_{\text{rot}} = \frac{\hbar^2}{2Ik_B}$$

$$\frac{\bar{C}_{V, \text{vib}}}{R} = \left(\frac{\Theta_{\text{vib}}}{T} \right)^2 \frac{e^{-\Theta_{\text{vib}}/T}}{(1 - e^{-\Theta_{\text{vib}}/T})^2} \quad f_v = (1 - e^{-\Theta_{\text{vib}}/T}) e^{-\Theta_{\text{vib}}/T} \quad f_{v>0} = e^{-\Theta_{\text{vib}}/T}$$

$$\bar{U} = \frac{3}{2} RT + RT + R \frac{\Theta_{\text{vib}}}{2} + R \frac{\Theta_{\text{vib}} e^{-\Theta_{\text{vib}}/T}}{1 - e^{-\Theta_{\text{vib}}/T}} - N_A D_e \quad f_J = \left(\frac{\Theta_{\text{rot}}}{T} \right) (2J+1) e^{-\Theta_{\text{rot}} J(J+1)/T}$$