Equation Sheet for Exam 1, CHE 371

Constants:

$h = 6.626 \times 10^{-34}$ J·s $\quad N_A = 6.02 \times 10^{23}$ molecules/mol

$c = 2.9979 \times 10^{8}$ m/s $\quad k_B = 1.38 \times 10^{-23}$ J/K = 0.695 cm^{-1}·K^{-1}

$R = 0.0820$ L·atm·mol^{-1}·K^{-1} = 8.314 J·mol^{-1}·K^{-1} = 0.08314 L·bar·mol^{-1}·K^{-1}

Quantum Mechanics Equations:

$$E = h\upsilon \qquad E = \frac{hc}{\lambda} \qquad E = hc\tilde{\upsilon} \qquad \hbar = \frac{h}{2\pi} \qquad D_e = D_0 + \frac{h\upsilon}{2} \qquad \varepsilon_{vib} = \sum_{j=1}^{n_{vib}} h\upsilon_j\left(v_j + \tfrac{1}{2}\right)$$

$$\varepsilon_{n_x,n_y,n_z} = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right) \qquad \boxed{\begin{array}{c}\varepsilon_v = h\upsilon(v+\tfrac{1}{2}) \\ v = 0,1,2,\ldots\end{array}} \qquad \boxed{\varepsilon_J = \frac{\hbar^2}{2I}J(J+1) \quad \begin{array}{c} J = 0,1,2,\ldots \\ g_J = 2J+1\end{array}}$$

Gas Laws Equations:

$$Z = \frac{P\overline{V}}{RT} \qquad P = \frac{RT}{\overline{V} - b} - \frac{a}{\overline{V}^2} \qquad P = \frac{RT}{\overline{V} - B} - \frac{A}{T^{1/2}\overline{V}(\overline{V} + B)} \qquad T_R = \frac{T}{T_c} \qquad P_R = \frac{P}{P_c}$$

$$P = \frac{RT}{\overline{V} - \beta} - \frac{\alpha}{\overline{V}(\overline{V} + \beta) + \beta(\overline{V} - \beta)} \qquad \overline{V}_c = 3b \quad P_c = \frac{a}{27b^2} \qquad T_c = \frac{8a}{27bR} \qquad \overline{V}_R = \frac{\overline{V}}{\overline{V}_c}$$

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

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

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

Statistical Mechanics Equations (BZ and PFIG):

$nR = k_BN \qquad N = nN_A \qquad R = k_BN_A$

$$Q(N,V,\beta) = \frac{q(V,\beta)^N}{N!} \qquad Q(N,V,\beta) = \sum_j e^{-\beta E_j} \qquad \beta = \frac{1}{k_BT} \qquad \langle E\rangle = k_BT^2\left(\frac{\partial \ln Q}{\partial T}\right)_{N,V}$$

$$\overline{C}_V = \left(\frac{\partial \overline{U}}{\partial T}\right)_V = \left(\frac{\partial\langle E\rangle}{\partial T}\right)_V \qquad \langle P\rangle = k_BT\left(\frac{\partial \ln Q}{\partial V}\right)_{N,\beta} \qquad \frac{N}{V}\left(\frac{h^2}{8mk_BT}\right)^{\frac{3}{2}} << 1 \qquad p_j = \frac{e^{-E_j/k_BT}}{\sum_i e^{-E_i/k_BT}}$$

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

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

$$f_J = \left(\frac{\Theta_{rot}}{T}\right)(2J+1)e^{-\Theta_{rot}J(J+1)/T}$$

$$\overline{U} = \frac{3}{2}RT + RT + R\frac{\Theta_{vib}}{2} + R\frac{\Theta_{vib}e^{-\Theta_{vib}/T}}{1 - e^{-\Theta_{vib}/T}} - N_AD_e$$