$$\Delta U = Q + W$$

$$Q_A = 0$$
$$\Delta H_A = 0$$
$$\Delta U = n C_{v,m} \Delta T$$

$$\Delta U = U_{final} - U_{initial}$$

$$\Delta H = \Delta U + \Delta(PV) = \Delta U + \Delta(nRT) = \Delta U + nR\Delta T$$

$$\Delta U = \Delta H - \Delta(PV)$$

$$\Delta(PV) = \Delta(nRT) = RT\Delta n$$

$$\Delta T = T_{Final} - T_{initial}$$

$$\Delta S = \int \frac{\partial Q_{rev}}{T}$$

$$\Delta G = \Delta H - S\Delta T$$

$$H = U + PV$$

$$\partial H = \partial U + P\partial V + V\partial P$$

$$\Delta H = \int_{T_i}^{T_f} \sum n C_{P,m} \Delta T$$

$$\Delta H_1 + \Delta H_2 = 0$$

$$\Delta H^\circ(x) = \Delta H^\circ(y) + \int_y^x \Delta c_P \partial T$$

$$\Delta H = q_P$$
$$\Delta H = C_{P,m}\Delta T$$

$$C_P = C_V + R$$

$$C_{P,m}^{ideal\ gas} = C_{V,m} + R$$

$$C_{P,m}^{liquid/solid} = C_{P,m} = C_{V,m}$$

$$dP = 0$$
$$q = q_P = \Delta H^\circ$$

$$\frac{\Delta H_r - T\Delta S_r}{T} < 0$$

$$G = H - TS$$

$$\Delta G = \Delta H - \Delta(TS) = \Delta H - T\Delta S$$

$$U = \begin{cases} 3/2\ (nRT) \\ 5/2\ (nRT) + U_{vib}(T) \\ 6/2\ (nRT) + U_{vib}(T) \end{cases}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

$$C_{V,m}^{monotonic} = \frac{3}{2}R$$

$$C_{V,m}^{Diatomic} = \frac{5}{2}R$$

$$C_{V,m}^{Polyatomic} = \frac{6}{2}R = 3R$$

$$Q = \Delta H$$

$$W = -P\Delta V$$

$$\partial W = -P\partial V = \frac{-nRT}{V}\partial V$$

$$W = -nRT\ln\left(\frac{V_2}{V_1}\right)$$

$$P = \frac{1}{\Omega}$$

$$y = E_r$$

$$P_r = \frac{N_r}{N} = \frac{\Omega(E_r)}{\Omega}$$

$$A \leftrightarrow E_r \simeq \quad E^* = E' + E_r$$
$$E_r = E^* - E'$$

$$\Omega'(E') = \Omega'(E^* - E_r)$$

$$P_r = C'\Omega'(E^* - E_r)$$

$$P_r = \underbrace{C'\Omega'(E^*)}\, e^{-\beta E_r}$$

$$P_r = C e^{-\beta E_r}$$

$$\sum_r P_r = 1$$

$$C\sum_r e^{-\beta E_r} = 1$$

$$C = \frac{1}{\sum_r e^{-\beta E_r}}$$

$$P_r = \frac{e^{-\beta E_r}}{\sum_r e^{-\beta E_r}} = \frac{e^{-\beta E_r}}{Z(\beta)}$$

$$E_i(\Omega_i) \simeq P_r, \frac{\Omega_r e^{-\beta E_r}}{\sum_i \Omega_i e^{-\beta E_i}}$$

$$E < \epsilon \simeq \Phi(\epsilon, N, V)$$

$$|\Omega[\epsilon, \epsilon+\Delta\epsilon]| = \Phi(\epsilon+\Delta\epsilon, N, V) - \Phi(\epsilon, N, V)$$

$$\lim_{\Delta\epsilon\to 0} \frac{\Phi(\epsilon+\Delta\epsilon, N, V) - \Phi(\epsilon, N, V)}{\Delta\epsilon} = \left(\frac{\partial\Phi}{\partial\epsilon}\right)_{N,V} = \Omega(\epsilon, N, V)$$

$$\beta = \frac{1}{K_B T},\ T = \infty \simeq \beta = 0$$

$$Z(\beta)_{continuum} = \int_0^\infty \Omega(E)e^{-\beta E}\partial E$$

$$Z(\beta)_{discrete\ states} = \sum_{all\ states} e^{-\beta E_{state}}$$

$$Z(\beta)_{discrete\ levels} = \sum_{levels} \Omega_i e^{-\beta E_i}$$

$$N = N_S + N_L$$
$$\epsilon = \epsilon_S + \epsilon_L + \epsilon_{SL}$$

$$N_S \simeq \epsilon_S \le E_S < \epsilon_S + \partial\epsilon_S$$

$$\Omega_S(\epsilon_S, N_S)\partial\epsilon,\ \Omega_L(\epsilon - \epsilon_S, N - N_S)\partial\epsilon_L$$

$$A = -\frac{1}{\beta}\ln Z, \quad \beta = \frac{1}{K_B T}$$

$$Z_{ind} = \frac{Z_1^n}{n!} \quad A = -K_B T\ln[Z]$$

$$U_1 = \frac{-\partial\ln(Z_1)}{\partial\beta},\ U_N = \frac{-\partial\ln(Z_N)}{\partial\beta}$$

$$Z_{ind} = Z_N = \frac{Z_1^N}{N!}$$

$$\frac{\partial\ln(Z_1)}{\partial\beta} = \frac{1}{Z_1}\frac{\partial Z_1}{\partial\beta}$$

$$Z_{Gas}(N, V, T) = \frac{V^{N_1}}{N_1!\ \lambda_{Gas}^{3N_1}}$$

$$S = K_B(\ln Z + \beta U)$$

$$S = K_B\left(\ln Z + \beta\sum_r P_r E_r\right)$$

$$-\beta E_r = \ln e^{-\beta E_r} = \ln\left(Z\frac{e^{-\beta E_r}}{Z}\right) = \ln(Z P_r)$$

$$S_G = -K_B\sum_r P_r\ln P_r$$

$$\sum_j P_j = 1 \quad P_j = \frac{1}{\Omega}\forall_j$$

$$\langle E\rangle = U = E$$
$$\Omega \equiv \Omega(U, N, V)$$

$$\ln\left(\frac{1}{x}\right) = -\ln(x)$$

$$S(U, N, V) = K_B\ln\Omega(U, N, V)$$

$$S_B = K_B\ln\Omega \simeq NK_B, \quad \ln\Omega \simeq N$$
$$e^N \simeq e^{10^{23}}$$

$$A = -K_B T\ln Z$$

$$K_B\partial\ln\Omega = \partial S = \frac{1}{T}\partial U + \frac{P}{T}\partial V - \sum_\alpha \frac{M_\alpha}{T}\partial N_\alpha$$

$$\frac{1}{K_B T} = \left(\frac{\partial\ln\Omega}{\partial U}\right)_{N,V} \quad \frac{P}{K_B T} = \left(\frac{\partial\ln\Omega}{\partial V}\right)_{U,N}$$

$$\frac{-\mu_i}{K_B T} = \left(\frac{\partial\ln\Omega}{\partial N_i}\right)_{U,V,N_\alpha\neq N_i}$$

$$A = U - TS$$
$$\partial A = \partial U - T\partial S - S\partial T$$
$$\partial U = T\partial S - P\partial V + \mu\partial N$$
$$\partial A = -P\partial V - S\partial T + \mu\partial N$$

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T} = k_B T\left(\frac{\partial\ln Z}{\partial V}\right)_{N,T}$$
$$\mu = \left(\frac{\partial A}{\partial N}\right)_{V,T} = -k_B T\left(\frac{\partial\ln Z}{\partial N}\right)_{V,T}$$
$$S = -\left(\frac{\partial A}{\partial T}\right)_{N,V} = k_B\ln Z + k_B T\left(\frac{\partial\ln Z}{\partial T}\right)_{N,V}$$
$$U = k_B T^2\left(\frac{\partial\ln Z}{\partial T}\right)_{N,V}$$
$$H = U + PV$$
$$G = H - TS$$

$$\Xi(V,T,\mu) = \begin{cases} \sum_N \int_0^\infty \Omega(\epsilon,N)e^{-\beta E}e^{\beta\mu N}\,dE \\ \sum_N \sum_{\text{all states } r} e^{-\beta E_r}e^{\beta\mu N} \\ \sum_N \sum_{\text{levels } i} \Omega_i e^{-\beta E_i}e^{\beta\mu N} \end{cases}$$

$$P = F/A = 2nmv_x^2 = nm\langle v_x^2\rangle$$
$$F = ma = \frac{d(mv)}{dt} = (nv_xA)(2mv_x)$$
$$n = \frac{N}{V}$$
$$PV = \frac{2}{3}N\langle\frac{1}{2}mv^2\rangle = \frac{2}{3}U = (\gamma-1)U$$
$$dW = F(-dx) = -PAdx = -PdV = dU$$
$$PdV + VdP = (\gamma-1)dU \rightarrow PV^\gamma = C$$
$$U_{trans} = \frac{3}{2}Nk_BT = \frac{3}{2}(\frac{N}{N_o})(N_ok_B)T = \frac{3}{2}nRT$$
$$PV = nRT$$
$$\Delta U = Q + W = U_{final} - U_{initial}$$
$$dV = V_{final} - V_{initial} = -Adx$$
$$dw = p_{ext}Adx \rightarrow dw = -p_{ext}dV$$
$$\delta W = -p_{ext}dV$$
$$W = -p_{ext}\int_{V_1}^{V_2} dV = -p_{ext}(V_2 - V_1)$$
$$W = -nRT\int_{V_1}^{V_2}\frac{dV}{V} = -nRTln(\frac{V_2}{V_1})$$
$$W = nRTln(\frac{p_2}{p_1})$$
$$\Delta U = C_V\Delta T \rightarrow dU = C_VdT$$
$$\frac{C_{V,m}}{R}ln\frac{T_2}{T_1} = -ln\frac{V_2}{V_1}$$
$$H = U + PV$$
$$dH = dU + PdV + VdP$$
$$dU = dq - PdV$$
$$dH = dq + VdP$$
$$\Delta H = C_P\Delta T$$
$$dS_{system} = \frac{dq_{rev}}{T}$$
$$\Delta S_{universe} = \Delta S_{system} + \Delta S_{surroundings}$$
$$-\frac{\Delta H_r - T\Delta S_r}{T} > 0$$
$$\Delta G = \Delta H - T\Delta S$$
$$dq_{rev} = C_VdT + \frac{nRT}{V}dV$$
$$dS = \frac{C_V}{T}dT + \frac{nR}{V}dV$$

$$Z_N = Z_{trans} Z_{electronic} Z_{nuclear}$$

$$Z_{trans} = \frac{V}{\Lambda}, \quad Z_{trans,\,indistinguishable} = \frac{\left(\frac{V}{\Lambda}\right)^N}{N!}, \quad \Lambda = \sqrt{\frac{h^2}{2\pi m K_B T}}$$

$$Z_{trans} \approx \left(\frac{eV}{N\Lambda^3}\right)^N \qquad Z_{trans,\,distinguishable} = \left(\frac{V}{\Lambda^3}\right)^N$$

$$Z_{electronic} = Z_{el}(T)^N$$

$$Z_{nuclear} = (W_0^n)^N$$

$$Z_{el}(T) = \left[W_0^e + W_1^e e^{-\beta\Delta\epsilon_1^e} + W_2^e e^{-\beta\Delta\epsilon_2^e} + \ldots\right]$$

$$C_v = \frac{\partial E_0^{nucl}}{\partial T} = 0 \qquad Z_{rot} = \frac{T}{\sigma \cdot \Theta_{rot}} \qquad I = \mu r^2$$

$$\Theta_{rot} = \frac{\hbar^2}{2\mu r^2 K_B}, \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$n_{CB} = \binom{N+g-1}{g-1}$$

$$Z_{trans} = \frac{V}{\left(\frac{h^2}{2\pi m K_B T}\right)} = \frac{V(2\pi m K_B T)^{3/2}}{(h^2)^{3/2}}, \quad Z_{vib} = \frac{e^{-\beta\hbar w/2}}{1 - e^{-\beta\hbar w}}$$

$$W = \sqrt{\frac{K}{\mu}}$$

$$A_{el}(T,N) = -NK_B T \ln\left(\sum_{i=0}^{\infty} w_i^e e^{-\beta\Delta\epsilon_i^e}\right)$$

$$S_{el}(T,N) = \frac{U_{el}(T,N) - A_{el}(T,N)}{T}$$

$N K_B = (\text{mol})(R)$ $\qquad P_i = \dfrac{e^{-\beta\Delta\epsilon_i^e}}{Z_{el}}$

$$C_{v,el}(T,N) = \frac{\partial U_{el}(T,N)}{\partial T} = NK_B\left[\sum_{i=1}^{\infty} P_i\left(\frac{\Delta\epsilon_i^e}{K_B T}\right)^2 - \left(\sum_{i=1}^{\infty} P_i \frac{\Delta\epsilon_i^e}{K_B T}\right)^2\right]$$

$$U_{el} = \frac{\sum_i w_i^e \Delta\epsilon_i e^{-\beta\Delta\epsilon_i}}{\sum_i w_i^e e^{-\beta\Delta\epsilon_i}}$$

$$Z_{vib}(T) = \frac{e^{-\theta_i/2T}}{1 - e^{-\theta_i/T}}, \quad \theta_i = \frac{h\nu_i}{K_B} \qquad U_i = -\frac{\partial \ln(Z_i)}{\partial\beta} = -K_B T^2 \cdot \frac{\partial}{\partial T}\ln(Z_i)$$

$$U = \sum_i U_i \qquad Z^n = (Z_{vib}(T))^N \qquad E_{ground} = \sum_i \frac{\hbar w_i}{2}$$

$$U_i = \frac{K_B\theta_i}{2} + (K_B\theta_i)\frac{e^{-\theta_i/T}}{1 - e^{-\theta_i/T}} \qquad A(T=0) = E_{ground}$$

$$U_{vib}(T) = NK_B\left(\frac{\theta_{vib}}{2} + \frac{\theta_{vib}}{e^{\theta_{vib}/T} - 1}\right) \qquad \hbar w_i = K_B\theta_i, \quad \theta_i = \frac{\hbar w_i}{K_B}$$

$$C_{v,vib}(T) = \frac{\partial U_{vib}}{\partial T} = NK_B\left(\frac{\theta_{vib}}{T}\right)^2 \frac{e^{\theta_{vib}/T}}{(e^{\theta_{vib}/T} - 1)^2} \qquad Z = Z_1 Z_2 \cdots$$

$$S_{vib}(T) = NK_B\left[\left(\frac{\theta_{vib}}{T}\right)\frac{1}{e^{\theta_{vib}/T} - 1} - \ln\left(1 - e^{-\theta_{vib}/T}\right)\right]$$

$$U_{trans} = \frac{3}{2}NK_B T = \frac{3}{2}\left(\frac{N}{N_0}\right)(N_0 K_B T) = \frac{3}{2}(nRT) \qquad U_{rot} = RT$$

$$A = -K_B T \ln(Z) \qquad S_{nuc} = K_B \ln w_0^n$$

$$\beta = \frac{1}{K_B T}$$

$$\binom{n}{k} = \frac{n!}{(n-k)!\,k!}$$

$$C_{V,E} \simeq 3NK_B\left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}$$

$$C_{V,D} \simeq 3NK_B$$

$$\frac{\tilde{Z}^\circ}{N_0} = \frac{(2\pi K_B)^{3/2}}{h^3 N_0^{5/2}} \frac{R}{p^\circ} \tilde{M}^{3/2} T^{5/2} Z_{rot} \tilde{Z}_{vib} W_{e\ell}$$

$$Kp_{diatomic} = \frac{820.519\,(\tilde{M}_x)^3\, T^{3/2}\,(W_{e\ell}^x)^2}{(\tilde{M}_{x_2})^{3/2}\, W_{e\ell}^{x_2}} \cdot \sigma\Theta_{rot}\left(1 - e^{-\theta_{vib}/T}\right)e^{-D_0(x_2)/K_B T}$$

$$Kp_{ionization} = \frac{(2\pi m_e K_B)^{3/2} T^{5/2} R}{h^3 p^\circ} \frac{e^{-I_P/K_B T}}{N_0}$$

$$Kp = \frac{\alpha^2}{1-\alpha}\frac{P}{P^\circ} \simeq \alpha^2 \frac{P}{P^\circ}, \quad \alpha \ll 1$$

$$\alpha = \sqrt{Kp}\left(\frac{P^\circ}{P}\right)^{1/2} \qquad \frac{\alpha^2}{1-\alpha} = \frac{(2\pi m_e)^{3/2}(K_B T)^{5/2}}{h^3 P} e^{-I_P/K_B T}$$

$$\Delta U_T^\circ = \Delta U_0^\circ + 2U_T(X) - U_T(X_2) = \Delta U_0^\circ + \frac{1}{2}RT - \frac{R\theta_{vib}}{e^{\theta_{vib}/T} - 1}$$

$$\ln\left\{\frac{Kp(T_2)}{Kp(T_1)}\right\} = -\frac{\Delta H^\circ}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\Delta H_T^\circ = N_0\left\{\frac{3}{2}K_B T - \frac{K_B\theta_{vib} e^{-\theta_{vib}/T}}{1 - e^{-\theta_{vib}/T}} + D_0\right\}$$

$$\Delta H_T^\circ = \frac{3}{2}RT - R\theta_{vib}\frac{e^{-\theta_{vib}/T}}{1 - e^{-\theta_{vib}/T}} + D_0$$

$$D_0 = \frac{D_0}{K_B} \cdot K_B \cdot N_0, \quad R = K_B \cdot N_0$$

$$Z(T) = \frac{e^{-\tilde{\nu}/(2K_B T)}}{1 - e^{-\tilde{\nu}/(\tilde{K}_B T)}} \qquad P_i(T) = \frac{e^{-\tilde{\nu}((n=i)+1/2)/(\tilde{K}_B T)}}{Z}$$