Constants and units

$$
\begin{aligned}
R &= 8.3145\,\mathrm{J\,K^{-1}\,mol^{-1}} \\
&= 0.082\,06\,\mathrm{L\,atm\,mol^{-1}\,K^{-1}} \\
k_B &= 1.381\times10^{-23}\,\mathrm{J\,K^{-1}} \\
&= 1.381\times10^{-16}\,\mathrm{g\,cm^2\,s^{-2}\,K^{-1}} \\
N_A &= 6.022\times10^{23}\,\mathrm{mol^{-1}} \\
c &= 2.998\times10^{8}\,\mathrm{m\,s^{-1}} \\
h &= 6.626\times10^{-34}\,\mathrm{J\,s} \\
\hbar &= \frac{h}{2\pi} = 1.055\times10^{-34}\,\mathrm{J\,s} \\
1\,\mathrm{N} &= 1\,\mathrm{kg\,m\,s^{-2}} \\
1\,\mathrm{J} &= 1\,\mathrm{N\,m} = 1\,\mathrm{kg\,m^2\,s^{-2}} \\
1000\,\mathrm{L} &= 1\,\mathrm{m^3}
\end{aligned}
$$

$$
\begin{aligned}
\ln N! &\approx N\ln N - N \\
\ln\left(M-N\right) &\approx \ln M \text{ if } M \gg N
\end{aligned}
$$

Quantum mechanics

$$
\begin{aligned}
E &= h\nu = \frac{hc}{\lambda} \\
E_{\text{1D PIB}} &= \frac{n^2h^2}{8mL^2}, n = 1,2,3,\cdots \\
E_{\text{RR}} &= \frac{\hbar^2 J\left(J+1\right)}{2I}, J = 0,1,2,\cdots \\
E_{\text{HO}} &= \hbar\left(\frac{k}{\mu}\right)^{1/2}\left(v+\frac{1}{2}\right), v = 0,1,2,\cdots
\end{aligned}
$$

Molecular transport

$$
\begin{aligned}
J(x) &= -D\left[\frac{\partial c(x)}{\partial x}\right] \\
\frac{\partial c(x,t)}{\partial t} &= D\frac{\partial^2 c(x,t)}{\partial x^2} \\
D &= \frac{k_BT}{f} \\
f_{\text{sphere}} &= 6\pi\eta r \\
f_{\text{disk, random}} &= 12\eta r \\
\left\langle r^2\right\rangle_{3D}^{1/2} &= \sqrt{6Dt}
\end{aligned}
$$

Kinetic molecular theory, gas collisions

$$
\begin{aligned}
\sigma &= \pi d^2; z_{AA} = \sqrt{2}\rho\sigma\left\langle v\right\rangle; t = \frac{1}{z_{AA}} \\
l &= \frac{\left\langle v\right\rangle}{z} = \frac{1}{\sqrt{2}\rho\sigma} \\
Z_{AA} &= \frac{\sigma\left\langle v\right\rangle\rho^2}{\sqrt{2}} \\
\mu &= \frac{m_1m_2}{m_1+m_2}
\end{aligned}
$$

Maxwell-Boltzmann speed distribution

$$
\begin{aligned}
P(v) &= 4\pi\left(\frac{M}{2\pi RT}\right)^{3/2} v^2e^{-Mv^2/2RT} \\
\left\langle v\right\rangle &= \left(\frac{8RT}{\pi M}\right)^{1/2} \\
\left\langle v^2\right\rangle^{1/2} &= \left(\frac{3RT}{M}\right)^{1/2} \\
\left\langle v_{mp}\right\rangle &= \left(\frac{2RT}{M}\right)^{1/2}
\end{aligned}
$$

Kinetics

$$
\begin{aligned}
k &= Ae^{-\frac{E_a}{RT}} \\
t_{1/2} &= \frac{\ln 2}{k} \text{ first-order only} \\
v(t) &= -\frac{1}{a}\frac{d\left[A\right]}{dt} = \cdots \\
&= -\frac{1}{V}\frac{d\xi}{dt} \\
K_c &= \frac{k_1}{k_{-1}} = \frac{\left[B\right]_{eq}}{\left[A\right]_{eq}} \\
\Delta\left[B\right] &= \Delta\left[B\right]_0 e^{-t/\tau}; \tau = \frac{1}{k_1+k_{-1}} \\
k &= \frac{k_BT}{hc^\circ}e^{\frac{\Delta^\ddagger S^\circ}{R}}e^{-\frac{\Delta^\ddagger H^\circ}{RT}} \\
&= \frac{k_BT}{hc^\circ}e^2\cdot e^{\frac{\Delta^\ddagger S^\circ}{R}}e^{-\frac{E_a}{RT}} \\
E_a &= \Delta^\ddagger H^\circ + 2RT \\
\text{yield}_i &= \frac{k_i}{\sum_n k_n} \\
\frac{d\left[I\right]}{dt}_{ss} &= 0; \left[I\right]_{ss} = \frac{k_1}{k_2}\left[A\right]_0 e^{-k_1t} \\
\left[ES\right]_{ss} &= \frac{k_1\left[E\right]\left[S\right]}{k_{-1}+k_2} \\
&= \frac{\left[E\right]_0\left[S\right]}{K_M+\left[S\right]} \\
K_M &= \frac{k_{-1}+k_2}{k_1} \\
\frac{d\left[P\right]}{dt} &= k_2\left[ES\right]_{ss} \\
&= k_2\left[E\right]_0\frac{\left[S\right]}{K_M+\left[S\right]} \\
&= v_{max}\frac{\left[S\right]}{K_M+\left[S\right]} \\
\frac{1}{d\left[P\right]/dt} &= \frac{1}{v_{max}} + \frac{K_M}{v_{max}\left[S\right]} \\
v &= \frac{v_{max}\left[S\right]}{K_M+\left[S\right]}
\end{aligned}
$$

Chemical and phase equilibria

$$\mu = \left(\frac{\partial G}{\partial n}\right)_{p,T}$$

$$\frac{dp}{dT} = \frac{\Delta S}{\Delta V} = \frac{\Delta H}{T\Delta V}$$

$$\ln\frac{p_2}{p_1} = -\frac{\Delta_{vap}H}{R}\left(\frac{1}{T_2}-\frac{1}{T_1}\right)$$

$$\ln\frac{K_p(T_2)}{K_p(T_1)} = -\frac{\Delta_{rxn}H}{R}\left(\frac{1}{T_2}-\frac{1}{T_1}\right)$$

$$\Delta_{rxn}G^\circ(T) = -RT\ln K_p(T)$$

$$\Delta_{rxn}G = \Delta_{rxn}G^\circ + RT\ln Q$$

$$Q = \frac{p_Y^{\nu_Y}p_Z^{\nu_Z}\cdots}{p_A^{\nu_A}p_B^{\nu_B}\cdots}$$

$$K_p = \left(\frac{p_Y^{\nu_Y}p_Z^{\nu_Z}\cdots}{p_A^{\nu_A}p_B^{\nu_B}\cdots}\right)_{eq}$$

$$K_c = \left(\frac{c_Y^{\nu_Y}c_Z^{\nu_Z}\cdots}{c_A^{\nu_A}c_B^{\nu_B}\cdots}\right)_{eq} = \frac{\left(\frac{q_Y}{V}\right)^{\nu_Y}\left(\frac{q_Z}{V}\right)^{\nu_Z}\cdots}{\left(\frac{q_A}{V}\right)^{\nu_A}\left(\frac{q_A}{V}\right)^{\nu_A}\cdots}$$

$$K_p = K_c\left(\frac{c^\circ}{p^\circ}RT\right)^{\nu_Y+\nu_Z+\cdots-\nu_A-\nu_B-\cdots}$$

$$\frac{q}{V} = \frac{q_{trans}}{V}q_{rot}q_{vib}q_{elec} = \frac{q^\circ}{V}e^{D_0/k_BT}$$

$$q_{vib}q_{elec} = \frac{1}{1-e^{-\theta/T}}\cdot g\cdot e^{D_0/RT}$$

$$\frac{q^\circ}{V} = \frac{N_Ap^\circ}{RT}e^{-\left(G^\circ-H_0^\circ\right)/RT}$$

Thermodynamics

$$\delta w = -p_{ext}dV; w = -p_{ext}\Delta V$$

$$w_{\text{iso-T}} = -\int_{V_1}^{V_2}\frac{nRT}{V}dV = -nRT\ln\frac{V_2}{V_1}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V; C_p = \left(\frac{\partial H}{\partial T}\right)_p$$

$$\Delta H = \int dH = \int C_p(T)dT$$

$$C_p = C_V + nR$$

$$\Delta U = w + q$$

$$\Delta S = \frac{q_{rev}}{T} = nR\ln\frac{V_2}{V_1} + C_V\ln\frac{T_2}{T_1}$$

$$\Delta S = \int\frac{C_p}{T}dT + \sum_i\frac{\Delta_{trs}H}{T}$$

$$\ulcorner\frac{S}{R} = \frac{7}{2} + \ln\left[\left(\frac{2\pi mk_BT}{h^2}\right)^{3/2}\frac{V}{N}\right] + \ln\left[\frac{T}{\sigma\theta_{rot}}\right]\ldots$$

$$\ldots + \frac{\theta_{vib}}{T}\left(\frac{1}{e^{\theta_{vib}/T}-1}\right) - \ln\left[1-e^{-\theta_{vib}/T}\right] + \ln\left[g_{e1}\right]\lrcorner$$

$$\frac{p_2}{p_1} = \left(\frac{V_1}{V_2}\right)^\gamma$$

$$V_2 = \frac{V_1}{\gamma}\left[\gamma - 1 + \frac{p_1}{p_2}\right]$$

$$\gamma = C_p/C_V$$

$$H = U + pV; A = U - TS$$

$$G = U - TS + pV = H - TS = A + pV$$

$$dU = TdS - pdV; \left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V$$

$$dH = TdS + Vdp; \left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p$$

$$dA = -SdT - pdV; \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V$$

$$dG = -SdT + Vdp; \left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p$$

$$\left(\frac{\partial\left(\Delta G/T\right)}{\partial T}\right)_p = -\frac{\Delta H}{T^2}$$

$$\mu_{JT} = \left(\frac{\partial T}{\partial p}\right)_H = \frac{T\left(\frac{\partial V}{\partial T}\right)_p - V}{C_p}$$

Statistical mechanics

$$\frac{a_n}{a_m} = e^{-\beta\Delta E}; \beta = \frac{1}{k_BT}$$

$$p_j = \frac{e^{-\beta E_j}}{\sum_i e^{-\beta E_j}} = \frac{e^{-\beta E_j}}{Q}$$

$$Q(N,V,\beta) = \sum_i e^{-\beta E_i} = \frac{q^N}{N!}$$

$$q_{trans} = \left(\frac{2\pi mk_BT}{h^2}\right)^{3/2}V$$

$$q_{rot} \approx \frac{T}{\sigma\theta_{ROT}}; \theta_{ROT} = \frac{\hbar^2}{2Ik_B}, I = \mu r^2$$

$$q_{vib} = \frac{e^{-\theta_{VIB}/2T}}{1-e^{-\theta_{VIB}/T}}$$

$$\theta_{VIB} = \frac{\hbar\left(\frac{k}{\mu}\right)^{1/2}}{k_B} = \frac{h\nu}{k_B}$$

$$\langle E\rangle = U = -\left(\frac{\partial\ln Q}{\partial\beta}\right)_{N,V} = k_BT^2\left(\frac{\partial\ln Q}{\partial T}\right)_{N,V}$$

$$\langle p\rangle = \frac{1}{Q\beta}\left(\frac{\partial Q}{\partial V}\right)_{N,T} = k_BT\left(\frac{\partial\ln Q}{\partial V}\right)_{N,T}$$

$$S = k_B\ln W = -k_B\sum_i p_i\ln p_i$$

$$S = k_BT\left(\frac{\partial\ln Q}{\partial T}\right)_{N,V} + k_B\ln Q$$

$$H = k_BT\left[T\left(\frac{\partial\ln Q}{\partial T}\right)_{N,V} + V\left(\frac{\partial\ln Q}{\partial V}\right)_{N,T}\right]$$

$$A = -k_BT\ln Q$$

$$G = k_BT\left[V\left(\frac{\partial\ln Q}{\partial V}\right)_{N,T} - \ln Q\right]$$

$$\mu = -RT\left(\frac{\partial\ln Q}{\partial N}\right)_{V,T}$$

$$W(M,N) = \frac{M!}{N!(M-N)!}$$