

附公式表:

$$\begin{array}{llll} c = 2.998 \times 10^8 \text{ m} \cdot \text{s}^{-1} & e = 1.602 \times 10^{-19} \text{ C} & N_A = 6.022 \times 10^{23} \text{ mol}^{-1} & h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s} \\ k = 1.381 \times 10^{-23} \text{ J} \cdot \text{K}^{-1} & R = 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} & F = 9.649 \times 10^4 \text{ C} \cdot \text{mol}^{-1} & \end{array}$$

$$E_{n_1, n_2, n_3} = \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right) \frac{h^2}{8m} \quad E_J = J(J+1) \frac{h^2}{8\pi^2 I} \quad E_V = \left(V + \frac{1}{2} \right) h\nu$$

$$P_i = \frac{W_i}{\sum_{i=1}^n W_i} \quad W = \frac{N!}{\prod_{i=1}^n N_i!} \quad \ln(x!) = x \ln x - x \quad S \equiv k \ln W \quad T \equiv \left(\frac{\partial U}{\partial S} \right)_{V, n}$$

$$\frac{P(\varepsilon)}{P(0)} = e^{-\frac{\varepsilon}{kT}} \quad f = \frac{1}{P(0)} \equiv \sum_{i=1}^n e^{-\frac{\varepsilon_i}{kT}} \quad \frac{C(h)}{C(0)} = \frac{P(h)}{P(0)} = e^{-\frac{\Delta \rho V g h}{kT}} \quad \frac{C_i}{C_j} = \frac{P(E_i)}{P(E_j)} \quad \frac{C_i}{C_j} = e^{-\frac{E_i - E_j}{RT}}$$

$$f = \prod_{j=1}^m f_j \quad f_{\text{平动}} = \frac{(2\pi m)^{3/2}}{h^3} (kT)^{3/2} V \quad f_{\text{转动, 线性}} = \frac{8\pi^2 I}{h^2} kT = \frac{1}{hcB} kT \quad f_{\text{转动, 非线性}} = \left(\frac{kT}{hc} \right)^{3/2} \left(\frac{\pi}{ABC} \right)^{1/2}$$

$$f_{\text{振动}j} = \sum_{v=0}^{\infty} e^{-\frac{v h \nu_j}{kT}} = \frac{1}{1 - e^{-\frac{h \nu_j}{kT}}} \quad f_{\text{振动}} = \prod_{j=1}^m f_{\text{振动}j} \quad f_{\text{电子}} = g_{\text{基态}} \quad f_{\text{分子}} = f_{\text{电子}} f_{\text{振动}} f_{\text{转动}} f_{\text{平动}}$$

$$U(T) = NkT^2 \frac{d(\ln f_{\text{总}})}{dT} + U(0) \quad Q_j = U_j(T) - U_j(0) = NkT^2 \frac{d(\ln f_j)}{dT} \quad Q = U(T) - U(0) = NkT^2 \frac{d(\ln f_{\text{总}})}{dT}$$

$$Q_x = \frac{1}{2} NkT = \frac{1}{2} nRT \quad Q_{\text{平动}} = Q_x + Q_y + Q_z = \frac{3}{2} NkT = \frac{3}{2} nRT \quad Q_{\text{转动, 线性}} = NkT = nRT$$

$$Q_{\text{转动, 非线性}} = \frac{3}{2} NkT = \frac{3}{2} nRT \quad Q_{\text{振动}j} = \frac{N h \nu_j}{e^{h \nu_j / kT} - 1} \quad Q_{\text{振动}j, \text{高温}} = NkT = nRT$$

$$S_j = \frac{Q_j}{T} + Nk \ln f_j = Nk \frac{d(T \ln f_j)}{dT} \quad S_{\text{定域}} = \sum_{j=1}^m S_j = Nk \frac{d(T \ln f_{\text{总}})}{dT} \quad S_{\text{离域}} = \frac{Q}{T} + Nk \ln \frac{e f_{\text{总}}}{N}$$

$$S_{\text{平动}} = \frac{5}{2} Nk + Nk \ln \frac{f_{\text{平动}}}{N} \quad S_{\text{转动, 线性}} = Nk \ln \left(\frac{ekT}{hcB} \right) \quad S_{\text{转动, 非线性}} = Nk \ln \left(\frac{\pi e^3 k^3 T^3}{ABCh^3 c^3} \right)^{1/2}$$

$$S_{\text{振动}j} = \frac{Nk h \nu_j}{kT(e^{h \nu_j / kT} - 1)} + Nk \ln \frac{1}{1 - e^{-h \nu_j / kT}} \quad S_{\text{振动}j, \text{高温}} = Nk + Nk \ln \frac{kT}{h \nu_j} = Nk \ln \frac{ekT}{h \nu_j}$$

$$\Delta U = q + w \quad dU = dq + dw \quad dw = -P_{\text{外}} dV \quad C_V \equiv \left(\frac{\partial U}{\partial T} \right)_V \quad dq_V = C_V dT$$

$$H \equiv U + PV \quad C_P \equiv \left(\frac{\partial H}{\partial T} \right)_P \quad dq_P = C_P dT \quad C_P = C_V + nR \quad \frac{T_{\text{终, 绝热}}}{T_{\text{始, 绝热}}} = \left(\frac{V_{\text{终}}}{V_{\text{始}}} \right)^{\frac{nR}{C_V}}$$

$$dS_{\text{孤}} \geq 0 \quad dS_{\text{总}} = dS + dS_{\text{环}} \geq 0 \quad dS \equiv \frac{dq_{\text{可逆}}}{T} \quad dS_{\text{环}} = \frac{dq_{\text{可逆, 环}}}{T_{\text{环}}} = -\frac{dq}{T_{\text{环}}} \quad dS \geq \frac{dq}{T_{\text{环}}}$$

$$\Delta S = \int_{\text{始}}^{\text{终}} \frac{dU}{T} + \int_{\text{始}}^{\text{终}} \frac{PdV}{T} \quad A \equiv U - TS \quad dA = dU - TdS \leq dw_{\text{非}} \quad G \equiv H - TS \quad dG = dH - TdS \leq dw_{\text{非}}$$

$$dB = \left(\frac{\partial B}{\partial X} \right)_{Y, n_1, n_2, \dots, n_C} dX + \left(\frac{\partial B}{\partial Y} \right)_{X, n_1, n_2, \dots, n_C} dY + \sum_{i=1}^C \left(\frac{\partial B}{\partial n_i} \right)_{X, Y, n \neq n_i} dn_i \quad \mu_i \equiv \left(\frac{\partial U}{\partial n_i} \right)_{S, V, n \neq n_i}$$

$$dU = TdS - PdV + \sum_{i=1}^C \mu_i dn_i \quad dH = TdS + VdP + \sum_{i=1}^C \mu_i dn_i \quad dA = -SdT - PdV + \sum_{i=1}^C \mu_i dn_i$$

$$\begin{aligned}
dG &= -SdT + VdP + \sum_{i=1}^C \mu_i dn_i & \frac{1}{2}RT &= E_{k,x} = E_{k,y} = E_{k,z} = \frac{1}{3}E_k & \Phi &= \delta d & \Phi^* &= \alpha' \Sigma \\
\frac{E_{\text{分子}}}{E_{\text{分子}}^0} &= 2 \left(\frac{d}{d^0} \right)^{-6} - \left(\frac{d}{d^0} \right)^{-12} & E_{m,\text{分子}} &= RT_{\text{沸点}} - \Delta H_{m,\text{蒸发,沸点}} = (R - \Delta S_{m,\text{蒸发,沸点}})T_{\text{沸点}} \\
C_{P,m\text{液}} &= 2(C_{P,m\text{气}} - R) & \mu_1 &\equiv \mu_2 \equiv \dots \equiv \mu_j & \frac{dP}{dT} &= \frac{\Delta S_{m\text{平衡}}}{\Delta V_{m\text{平衡}}} = \frac{\Delta H_{m\text{平衡}}}{T\Delta V_{m\text{平衡}}} & \frac{dP^*}{dT} &= \frac{P^* \Delta H_{m\text{平衡, 蒸发}}}{RT^2} \\
\mu_{\text{气,理}} &= \mu^\ominus + RT \ln \frac{P}{P^\ominus} & \mu_{\text{气,实}} &= \mu^\ominus + RT \ln \frac{\xi}{P^\ominus} & \xi &= \gamma P & \mu_{\text{液}} &= \mu^* = \mu^\ominus + RT \ln \frac{P^*}{P^\ominus} \\
\mu_{\text{固}} &= \mu^\ominus + RT \ln \frac{P^*}{P^\ominus} & P_i &= \tau_i P & P &= \frac{RT \sum_{i=1}^C n_i}{V} & \tau_i &\equiv \frac{n_i}{\sum_{i=1}^C n_i} & \mu_i &= \mu_i^\ominus + RT \ln \frac{P_i}{P_i^\ominus} \\
\Delta_{\text{混}}G &= \sum_{i=1}^C n_i RT \ln \tau_i & \Delta_{\text{混}}S &= \sum_{i=1}^C -n_i R \ln \tau_i & \Delta_{\text{混}}H &\equiv 0 & \Delta_{\text{混}}U &\equiv 0 & \Delta_{\text{混}}A &\equiv \Delta_{\text{混}}G \\
\Delta_{\text{混}}G &= \sum_{i=1}^C n_i RT \ln \chi_i & \Delta_{\text{混}}S &= \sum_{i=1}^C -n_i R \ln \chi_i & \Delta_{\text{混}}V &\equiv 0 & \Delta_{\text{混}}H &\equiv 0 & \Delta_{\text{混}}U &\equiv 0 & \Delta_{\text{混}}A &\equiv \Delta_{\text{混}}G \\
\mu_{i,\text{液,理}} &= \mu_i^* + RT \ln \chi_i & P_i &= \chi_i P_i^* & dX &= \left(\frac{\partial X}{\partial T} \right)_{P,n} dT + \left(\frac{\partial X}{\partial P} \right)_{T,n} dP + \sum_{i=1}^C \left(\frac{\partial X}{\partial n_i} \right)_{T,P,n \neq n_i} dn_i \\
mX_i &= \left(\frac{\partial X}{\partial n_i} \right)_{T,P,n \neq n_i} & X &= \sum_{i=1}^C mX_i n_i & \Delta_{\text{混}}X &= X_{\text{混合物}} - \sum_{i=1}^C X_{i,\text{纯}} = \sum_{i=1}^C (mX_i - X_{m,i}) n_i & \sum_{i=1}^C n_i d^m X_i &= 0 \\
P_i &\equiv \alpha_i P_i^* & \alpha_i &\equiv \gamma_i \chi_i & \mu_{i,\text{液}} &= \mu_i^* + RT \ln \alpha_i & \Delta_{\text{混}}G &= \sum_{i=1}^C n_i RT \ln \gamma_i + \sum_{i=1}^C n_i RT \ln \chi_i \\
\Delta_{\text{混}}S &= -RT \sum_{i=1}^C n_i \left(\frac{\partial \ln \gamma_i}{\partial T} \right)_{P,n} - \left(\sum_{i=1}^C n_i R \ln \gamma_i + \sum_{i=1}^C n_i R \ln \chi_i \right) = - \sum_{i=1}^C n_i \left(\frac{\partial (RT \ln \gamma_i)}{\partial T} \right)_{P,n} - \sum_{i=1}^C n_i R \ln \chi_i \\
\Delta_{\text{混}}X_i &\equiv mX_i - X_{m,i} & d(\ln \gamma_i)_n &= \left(\frac{\partial \ln \gamma_i}{\partial T} \right)_{P,n} dT + \left(\frac{\partial \ln \gamma_i}{\partial P} \right)_{T,n} dP = - \frac{\Delta_{\text{混}}H_i}{RT^2} dT + \frac{\Delta_{\text{混}}V_i}{RT} dP \\
\mu_{i,(1)} &= \mu_{i,(2)} = \mu_{i,(3)} = \dots = \mu_{i,(p)} & F &= 2 + C - p & l_{(\text{左})} n_{(\text{左})} &= l_{(\text{右})} n_{(\text{右})} & \frac{\chi_{i(\text{液}A)}}{\chi_{i(\text{液}B)}} &= \frac{\gamma_{i(\text{液}B)}}{\gamma_{i(\text{液}A)}} \\
\frac{1}{\chi_{1(\text{液}B)}} &= \frac{\gamma_{1(\text{液}B)} n_{\text{液}A}}{\gamma_{1(\text{液}A)} n_1} + \frac{n_{\text{液}B}}{n_1} & \gamma_{1(\text{液}B)} &= \lim_{\chi_{1(\text{液}A)} \rightarrow 1} \frac{\chi_{1(\text{液}A)}}{\chi_{1(\text{液}B)}} \gamma_{1(\text{液}A)} = \frac{1}{\chi_{1(\text{液}B)}} & \chi_{A(\text{饱和液})} &= \frac{1}{\gamma_{A(\text{饱和液})}} \\
\mu_{A(\text{溶液})} &= \mu_{A(\text{固})} + RT \ln \frac{P_A}{P_A^*} = \mu_{A(\text{固})} + RT \ln \alpha_A = \mu_{A(\text{饱和液})} + RT \ln \alpha_A & K_{\text{分配}} &= \frac{\chi_{\text{溶质}(\text{液}B)}}{\chi_{\text{溶质}(\text{液}A)}} = \frac{\gamma_{\text{溶质}(\text{液}A)}}{\gamma_{\text{溶质}(\text{液}B)}} \\
(P_{\text{内}} - P_{\text{外}}) &= \frac{2F_{\text{张力}}}{r} & dG &= -SdT + VdP + \sum_{i=1}^C \mu_{i(\infty)} dn_i + \sum_{j=1}^D \sigma_j da_j & \sigma_j &\equiv \left(\frac{\partial G}{\partial a_j} \right)_{T,P,n,a \neq a_j} \\
(P_{\text{内}} - P_{\text{外}}) &= \frac{2\sigma}{r} + \left(\frac{\partial \sigma}{\partial r} \right)_{T,P,n} & h &= \frac{2\sigma_{\text{液-气}}}{r_{\text{管}} \rho_{\text{液}} g} & h &= \frac{4(\sigma_{\text{固-气}} - \sigma_{\text{固-液}} - w_{\text{液}})}{r_{\text{管}} \rho_{\text{液}} g} & \theta &= \frac{KC}{1 + KC}
\end{aligned}$$

$$P^* = P_{(\infty)}^* e^{\frac{V_m(\partial\sigma)}{RT(\partial r)}_{T,P} + \frac{2\sigma V_m}{rRT}} \quad \lim_{r \rightarrow 0} \left(\frac{\partial\sigma}{\partial r} \right)_{T,P} < 0 \quad \chi_{\text{饱和}} = \chi_{\text{饱和}(\infty)} e^{\frac{V_m(\partial\sigma)}{RT(\partial r)}_{T,P} + \frac{2\sigma V_m}{rRT}} \quad \varepsilon_{\text{粒子}} = \frac{\varepsilon_{\text{粒子}}^o}{\kappa_{\text{介质}}} \left(\frac{d}{d^o} \right)^{-\beta}$$

$$d\xi = -\frac{dn_i}{v_i} = \frac{dn_j}{v_j} \quad \left(\frac{\partial G}{\partial \xi} \right)_{T,P} \Big|_{\text{平衡}} = 0 \quad \left(\frac{\partial G}{\partial \xi} \right)_{T,P} = \Delta_r G \equiv \sum_{\text{产物}} \nu_j \mu_j - \sum_{\text{反应物}} \nu_i \mu_i = \Delta_r G^\ominus + RT \ln \Omega$$

$$\Delta_r G^\ominus \equiv \sum_{\text{产物}} \nu_j \mu_j^\ominus - \sum_{\text{反应物}} \nu_i \mu_i^\ominus \quad \Omega \equiv \frac{\prod_{\text{产物}} (\alpha_j)^{\nu_j}}{\prod_{\text{反应物}} (\alpha_i)^{\nu_i}} \quad K \equiv \frac{\prod_{\text{产物}} (\alpha_j)^{\nu_j}}{\prod_{\text{反应物}} (\alpha_i)^{\nu_i}} \Big|_{\text{平衡}} = e^{-\frac{\Delta_r G^\ominus}{RT}} \quad \left[\frac{\partial(\ln K)}{\partial T} \right]_p = \frac{\Delta_r H^\ominus}{RT^2}$$

$$\frac{P_{\text{产物}}}{P_{\text{反应物}}} \equiv \frac{\prod_{\text{产物}} (\chi_j)^{\nu_j}}{\prod_{\text{反应物}} (\chi_i)^{\nu_i}} \Big|_{\text{平衡}} = e^{-\frac{\Delta_r G}{RT}} \quad K_\gamma = \frac{\prod_{\text{产物}} (\gamma_j)^{\nu_j}}{\prod_{\text{反应物}} (\gamma_i)^{\nu_i}} \Big|_{\text{平衡}} \quad -\nu F E = \Delta_r G \quad E^\ominus = -\frac{\Delta_r G^\ominus}{\nu F} = \frac{RT}{\nu F} \ln K$$

$$E = E^\ominus - \frac{RT}{\nu F} \ln \Omega \quad dS_{\text{环}} \equiv -\frac{dq}{T_{\text{环}}} \quad \overrightarrow{A}_B = \frac{dB(x)}{dx} \overrightarrow{x}_o \quad f \equiv \frac{1}{a} \frac{dH}{dt} \quad f = -k_f A = -k_f \frac{dB}{dx} \quad \eta = \kappa \phi$$

$$\phi = \left(\frac{P_{\text{激发态}}}{P_{E_T}} \right)^{-1} = e^{\frac{\Delta E}{RT}} = e^{-\frac{\left[1 - 0.35 \left(\frac{V_m^o}{V_{m,T}} \right)^2 \right] E^o}{RT}} \quad f_{\text{z动量}} = -\eta \frac{dv_z}{dx} \quad f_{\text{物质的量}} = -D \frac{d[i]}{dx} \quad D = \frac{kT}{3\pi d\eta}$$

$$\frac{\partial[i]}{\partial t} = D \frac{\partial^2[i]}{\partial x^2} \quad \frac{\partial[i]}{\partial t} = \frac{2D}{r} \frac{\partial[i]}{\partial r} + D \frac{\partial^2[i]}{\partial r^2} \quad \frac{\partial[i]}{\partial t} = -v \frac{\partial[i]}{\partial x} \quad \frac{\partial[i]}{\partial t} = D \frac{\partial^2[i]}{\partial x^2} - v \frac{\partial[i]}{\partial x} \quad \Delta x = \sqrt{2D\Delta t}$$

$$u = \frac{ze}{3\pi d\eta} \quad t_{i,\text{最短}}^o \gg t_{\text{典型}}^o \Rightarrow L_i \not\ll L \quad \Delta G_{\text{垒}} \equiv (H_{\text{极大值态}} - H_{\text{反应态}}) - T(S_{\text{极大值态}} - S_{\text{反应态}})$$

$$\frac{P_{\text{垒}}}{P_{\text{反应物}}} \equiv \frac{\Omega_{\text{垒}}}{\Omega_{\text{反应物}}} = e^{-\frac{\Delta G_{\text{垒}}^\ominus}{RT}} \frac{1}{t_{\text{上}}^o} \quad \frac{\Delta G_{\text{垒}}^\ominus}{RT} \rightarrow \infty \Rightarrow \text{“电子态I”} \not\subset \text{系统} \quad t_{\text{上}}^o \rightarrow \infty \Rightarrow \text{“电子态I”} \not\subset \text{系统}$$

$$\ln k = \ln A - \frac{B}{T} \quad E_a = RT^2 \frac{d(\ln k)}{dT} \quad \nu = \frac{1}{t_{\text{上}}^o t_{\text{下}}^o} e^{-\frac{\Delta G_{\text{垒}}^\ominus}{RT}} [A][BC] = \left(\frac{1}{t_{\text{上}}^o t_{\text{下}}^o} e^{\frac{\Delta_r S_{\text{垒}}^\ominus}{R}} \right) e^{-\frac{\Delta_r H_{\text{垒}}^\ominus}{RT}} [A][BC]$$

$$n_{\text{步}} = n_{\text{电子态}} - 1 \quad \frac{d[A]_i}{\sum_{i=1}^n d[A]_i} = \frac{\nu_i}{\nu_{\text{总}}} = \frac{k_i}{\sum_{i=1}^n k_i} \quad \frac{d[A]_{\text{主}}}{d[A]_{\text{副}}} = \frac{\nu_{\text{主}}}{\nu_{\text{副}}} = \frac{k_{\text{主}}[B]}{k_{\text{副}}[C]} \quad \frac{d[A]_{\text{主}}}{d[A]} = \frac{\nu_{\text{主}}}{\nu_{\text{总}}} = \frac{k_{\text{主}}[B]}{k_{\text{主}}[B] + k_{\text{副}}[C]}$$

$$\nu = \frac{d[(AB)]}{dt} = 4\pi(r_A + r_B)(D_A + D_B)[A][B] \quad \nu = \frac{1}{V} \frac{\partial \xi}{\partial t} \quad \nu = k[A]^\alpha [B]^\beta [C]^\gamma [D]^\delta \quad [A] = [A]_0 - kt$$

$$[A] = [A]_0 e^{-kt} \quad \frac{1}{[A]^{n-1}} - \frac{1}{[A]_0^{n-1}} = (n-1)kt \quad \mathcal{A} \equiv -\lg \frac{I}{I_0} = \varepsilon [i] d \quad \varepsilon = \frac{n_{\text{溶液}} k \lg e}{c}$$

$$\nu_{t=0} = -\frac{1}{\nu_i} \frac{d[i]}{dt} \Big|_{t=0} = -\frac{a_1}{\nu_i} \quad \nu_{t=0} = \frac{1}{\nu_j} \frac{d[j]}{dt} \Big|_{t=0} = \frac{a_1}{\nu_j} \quad \ln \nu = \ln A - \frac{E_a}{RT} + \alpha \ln [A] + \beta \ln [B] + \gamma \ln [C]$$

$$[A] = \frac{k_{\text{正}}}{k_{\text{正}} + k_{\text{逆}}} [A]_0 e^{-(k_{\text{正}} + k_{\text{逆}})t} + \frac{k_{\text{逆}}}{k_{\text{正}} + k_{\text{逆}}} [A]_0 \quad \tau_{\text{平衡}}^\ominus = \tau_{\text{平衡}} = \frac{\ln 2}{k_{\text{正}} + k_{\text{逆}}} \quad \frac{P_{\text{产物}}}{P_{\text{反应物}}} = \frac{1 - e^{-t \ln 2 / \tau_{\text{平衡}}}}{e^{-t \ln 2 / \tau_{\text{平衡}}} + 1/K}$$

$$\nu = \frac{k_1 k_2 [E]_0 [S]}{k_1' + k_1 [S]}$$