FORMULAS FOR LIFE

All formulas you'll ever need

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A helpful tool for scientific studies

Contents

1 Statistics

1.1 Mean

1.1.1 Arithmetic mean

$$\overline{x} = \sum_{i=1}^{n} \frac{x_i}{N}$$

1.1.2 Geometric mean

$$\overline{x} = \left(\prod_{i=1}^{n} x_i\right)^{\frac{1}{n}}$$

1.1.3 Harmonic mean

$$\overline{x} = n\left(\sum_{i=1}^{n} \frac{1}{x_i}^{-1}\right)$$

1.2 Standard Deviation

1.2.1 Absolute

$$s = \sqrt{\frac{\sum_{i=1}^{n}(x_i - \overline{x})^2}{N-1}}$$

1.2.2 Relative

$$RSD = \frac{s}{\overline{x}}$$

2 Pure Physics

3 Pure Chemistry

3.1 Concentration

3.1.1 Mole

$$n = \frac{m}{MW}$$

3.1.2 Molarity

$$M = \frac{n}{V}$$

4 Thermodynamics

4.1 Perfect gases

4.1.1 State equation

$$pV = nRT$$
$$pV_m = RT$$

4.1.2 Properties

Molar mass

$$d_{gas} \cdot V_m = MW$$

Boyle's law

$$p_1 V_1 = p_2 V_2 \quad T = const$$

Charle's law

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \quad p = const$$

Gay-Lussac's Law

$$\frac{p_1}{T_1} = \frac{p_2}{T_2} \quad V = const$$

4.1.3 Compression factor

$$Z = \frac{PV}{nRT}$$

Z = 1 for perfect gases

4.2 Real gases

4.2.1 Virial equation

$$pV_m = RT \left(1 + \frac{B}{V_m} + \frac{C}{V_m^2} + \dots \right)$$

4.2.2 van der Waals equation

$$p = \frac{nRT}{V - nb} - a \left(\frac{n}{V} \right)^2$$
$$p = \frac{nRT}{V_m - b} - \frac{a}{V_m^2}$$

4.2.3 Compression factor

$$Z = \frac{V_m}{V_m - b} - \frac{a}{RTV_m}$$
$$\text{if } y = \frac{1}{V_m} \implies \frac{1}{1 - by} - \frac{ay}{RT}$$

4.2.4 Boyle Temperature

$$\lim_{p \to 0} \frac{dZ}{dp} = 0 \quad p \to 0 \implies \frac{1}{V_m} \to 0$$
$$y = \frac{1}{V_m} \quad \lim_{y \to 0} \frac{1}{1 - by} - \frac{ay}{RT} =$$
$$T_b = \frac{a}{Rb}$$

4.2.5 Critical and reduced variables

$$T_c = \frac{8a}{27Rb} \quad p_c = \frac{a}{27b^2} \quad V_c = 3b \quad Z_c = \frac{p_c V_c}{RT_c}$$

The van der Waals equation can be rewritten :

$$p_r = \frac{8T_r}{3V_r - 1} - \frac{3}{V_r^2}$$

4.3 Internal Energy

$$\Delta U = q + w$$
$$dU = \delta w + \delta q$$
$$dU = TdS - pdV$$
$$dU = \left(\frac{\partial U}{\partial S} \right)_V dS + \left(\frac{\partial U}{\partial V} \right)_S dV$$

Is always true that:

$$dU = \int_{T_1}^{T_2} C_V dT$$
$$\Delta U = nC_{v,m} \Delta T$$

4.4 Enthalpy

$$H = U + pV$$
$$\Delta H = \Delta U + \Delta pV$$
$$dH = -SdT + Vdp$$

For the perfect gas is also true that:

$$\Delta H = \Delta U + \Delta(nRT)$$

4.4.1 Temperature dependence

Pure substance

$$\Delta H(T_2) = \Delta H(T_1) + \int_{T_1}^{T_2} C_p dT.$$

Chemical reaction or phase transition

$$\Delta H(T_2) = \Delta H_r T_1 + \Delta C_p (T_2 - T_1)$$
$$\Delta C_p = [cC_{p,C} + dC_{p,D}] - [aC_{p,A} + bC_{p,B}]$$

4.5 Entropy

$$\Delta S_{TOT} \geq 0$$

$$\Delta S = \frac{q}{T} \implies \Delta S = \int_i^f \frac{q_{rev}}{T}$$

For an ideal gas it is always true that:

$$\Delta S = nC_m \ln\left(\frac{T_f}{T_i}\right) + nR \ln\left(\frac{V_f}{V_i}\right)$$

Only mixing two gases results in:

$$\Delta S_{mix} = -R \sum_{i=1}^N n_i \ln \chi_i$$

4.5.1 Trouton's Rules

$$\Delta S_{trs} = \frac{\Delta H_{trs}}{T_{trs}}$$

4.5.2 Temperature dependence

Constant pressure

$$\Delta S = S(T_f) - S(T_i) = C_p \int_i^f \frac{dT}{T} = C_p \ln\left(\frac{T_f}{T_i}\right)$$

Constant volume

$$\Delta S = S(T_f) - S(T_i) = C_v \int_i^f \frac{dT}{T} = C_v \ln\left(\frac{T_f}{T_i}\right)$$

4.5.3 Chemical reaction

$$aA + bB \to cC + dD$$
$$\Delta_r S^0 = (cS_C^0 + dS_D^0) - (aS_A^0 + bS_B^0)$$
$$\Delta_r S^0 = \sum_{i=1}^N \nu_i S_{reagents}^0 - \sum_{i=1}^N \nu_i S_{products}^0$$

If calculating $T \neq 298K$:

$$\Delta_r S(T_2) = \Delta_r S(T_1) + \Delta C_p \ln \frac{T_2}{T_1}$$
$$\Delta C_p = (cC_{c,p} + dC_{d,p}) - (aC_{a,p} + bC_{b,p})$$

4.6 Isothermal Transformations

4.6.1 Free expansion

$$\Delta T = 0 \implies \Delta U = 0 \implies q = w$$
$$w = q = -p_{ext}\Delta V = 0$$
$$\Delta H = \Delta PV \text{ (0 for perfect gas)}$$
$$\Delta S = nR \ln(\frac{V_f}{V_i}) \quad \Delta S' = 0 \quad \Delta S_{tot} = \Delta S$$

4.6.2 Expansion vs. p_{ext}

$$\Delta T = 0 \implies \Delta U = 0 \implies q = w$$
$$w = q = -p_{ext}\Delta V$$
$$\Delta H = \Delta PV \text{ (0 for perfect gas)}$$
$$\Delta S = nR \ln(\frac{V_f}{V_i}) \quad \Delta S' = \frac{-q_{sistema}}{T}$$
$$\Delta S_{tot} = \Delta S + \Delta S'$$

4.6.3 Reversible expansion

$$\Delta T = 0 \implies \Delta U = 0 \implies q = w$$
$$q = w = -nRT \ln(\frac{V_f}{V_i})$$
$$\Delta H = \Delta PV \text{ (0 for perfect gas)}$$
$$\Delta S = nR \ln(\frac{V_f}{V_i}) \quad \Delta S' = -nR \ln(\frac{V_f}{V_i})$$
$$\Delta S_{tot} = 0$$

4.7 Adiabatic Transformations

$$dU = dw$$
$$C_v dT = -pdV$$
$$w_{Adiabatic} = nC_{V,m}\Delta T$$

For an adiabatic process is also true that:

$$\gamma = \frac{C_{p,m}}{C_{V,m}} = \frac{C_p}{C_V} \quad P_1(V_1)^\gamma = P_2(V_2)^\gamma$$

4.7.1 Reversible process

$$C_V dT = \frac{-nRT}{V}dV$$
$$\int_{T_1}^{T_2} \frac{C_V dT}{T} = -nR \int_{T_1}^{T_2} \frac{dV}{V}$$
$$C_V \ln\left(\frac{T_1}{T_2}\right) = -R \ln \frac{V_2}{V_1}$$
$$\frac{T_2}{T_1} = \left[\frac{V_2}{V_1}\right]^{-\frac{R}{C_V}}$$

4.7.2 Irreversible

Take P as constant

$$\int_{T_1}^{T_2} Cv\,dT = -p\int_{V_1}^{V_2} dV$$
$$\text{Assuming } C_V = cost$$
$$C_V \Delta T = -p\Delta V$$

4.7.3 Free expansion

$$q = 0, \ w = -p_{ext}\Delta V = 0 \implies \Delta U = 0$$
$$\Delta H =$$
$$\Delta S = nR\ln(\frac{V_f}{V_i}) \quad \Delta S' = 0 \quad \Delta S_{tot} = 0$$

4.7.4 Expansion vs. p_{ext}

$$q = 0 \implies \Delta U = w$$
$$\Delta U = nC_{V,m}\Delta T = w = -p_{ext}\Delta V$$
$$\Delta T = -\frac{p_{ext}\Delta V}{nC_{v,m}}$$
$$\Delta H = V\Delta p$$
$$\Delta S = nC_{V,m}\ln(\frac{T_f}{T_i}) + nR\ln(\frac{V_f}{V_i})$$
$$\Delta S' = 0 \implies \Delta S_{TOT} = \Delta S$$

4.7.5 Reversible expansion

$$q = 0 \implies \Delta U = w$$
$$\Delta U = nC_{V,m}\Delta T$$
$$\Delta S = \Delta S' = \Delta_{tot} = 0$$

4.8 Isobaric transformations

$$dp = 0$$
$$q = \Delta H = nC_{p,m}\Delta T$$
$$w = -pdV$$
$$\Delta S = nC_{p,m}\ln(\frac{T_f}{T_i}) \quad \Delta S' = -nC_{p,m}\ln\frac{V_f}{V_i}$$
$$\implies \Delta S_{TOT} = 0$$

4.9 Thermodynamic cycles

$$\Delta U = 0, \ \Delta S = 0, \ \Delta H = 0.$$

4.9.1 Carnot cycle

There is 4 stage (ABCD):

AB Reversible Isothermal expansion

$$\Delta U = 0 \implies q_{AB} = -w_{AB}$$
$$w_{AB} = -q_{AB} = -nRT_h\ln\left(\frac{V_B}{V_A}\right)$$

BC Reversible Adiabatic Expansion

$$q_{BC} = 0 \implies \Delta U_{BC} = w_{BC}$$
$$w_{BC} = nC_{V,m}(T_C - T_h)$$

CD Reversible Isothermal compression

$$\Delta U = 0 \implies q_{CD} = -w_{CD}$$
$$w_{CD} = -q_{CD} = -nRT_h\ln\left(\frac{V_D}{V_C}\right)$$

DA Reversible Adiabatic compression

$$q_{DA} = 0 \implies \Delta U_{DA} = w_{DA}$$
$$w_{DA} = nC_{V,m}(T_C - T_h)$$

4.10 Helmholtz's Energy

$$A = U - ST$$
$$\Delta A_V = \Delta U_V - T\Delta S_V$$

ΔA is the maximum (more negative) work that can be done by the system if dT=0.

$$0 \geq w \geq \Delta A$$

It can also be expressed with natural variables:

$$dA = -SdT - pdV$$
$$dA = \left(\frac{\partial A}{\partial T}\right)_V dT + \left(\frac{\partial A}{\partial V}\right)_T dV$$

4.11 Gibbs's Energy

$$G = H - ST$$
$$\Delta G_p = \Delta H_p - T\Delta S_p$$

ΔG is the maximum (more negative) work that can be done by the system if dT=0.

$$0 \geq w_{ne} \geq \Delta G$$

It can also be expressed with natural variables:

$$dG = -SdT + Vdp$$
$$dG = \left(\frac{\partial G}{\partial T}\right)_p dT + \left(\frac{\partial G}{\partial p}\right)_T dp$$

4.11.1 Gibbs-Helmholtz's equation

$$\frac{\partial}{\partial T}\left(\frac{\Delta G}{T}\right)_p = -\frac{\Delta H}{T^2}$$
$$\frac{\Delta G(T_2)}{T_2} - \frac{\Delta G(T_1)}{T_1} = \Delta H\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

4.11.2 Pressure dependence

$$\Delta G = G(p_2) - \Delta G(p_1) = nRT \ln\left(\frac{p_2}{p_1}\right)$$

It can be also used to find $G_m(T_2)$ for a reaction:

$$nA \rightarrow mB$$
$$nG(A, p_2) = nG^0 + nRT \ln p_2$$
$$nG(B, p_2) = mG^0 + mRT \ln p_2$$
$$\Delta G(p_2) = mG(B, p_2) - nG(A, p_2) =$$
$$\Delta G^0 + (m - n)RT \ln p_2$$

4.12 Chemical potential

G is an extensive variable, otherwise a p, T = cost it would be always true that dG = 0. G depends on the composition of the system: $G = G(p, T, n_1, n_2, \ldots)$ The partial derivative of G is the chemical potential:

$$\mu = \left(\frac{\partial G}{\partial n_i}\right)_{p,T,n_j} \implies dG = \sum_{i=1}^{N} \mu_i dn_i$$

4.12.1 Gibbs-Duhem equation

$$\sum_{i=1}^{N} n_i d\mu_i = -SdT + Vdp$$

If temperature and pressure are constant:

$$\sum_{i=1}^{N} n_i d\mu_i = 0$$

4.12.2 Natural variables

$$\left(\frac{d\mu}{dp}\right)_T = V_m \quad \left(\frac{d\mu}{dT}\right)_p = -S_m$$

4.12.3 Perfect gas chemical potential

$$\left(\frac{d\mu}{dp}\right)_T$$
$$\int_{p^0}^{p} = \int_{p_0}^{p} \frac{RT}{p} = dp$$
$$\mu(p, T) = \mu_0(p_0, T) + RT \ln\left(\frac{p}{p_0}\right)$$

4.13 Chemical equilibrium

$\Delta_r G$ is related to G variation at constant temperature and pressure

$$\Delta_r G = \left(\frac{\partial G}{\partial \xi}\right)_{p,T} = \sum_{i=1}^{n} \nu_i \mu_i$$

Is possible to relate $\Delta_r G^0$ and K :

$$K = e^{-\frac{\Delta_r G^0}{RT}}$$

Different K calculation are related easily:

$$K_c = K_n \left(\frac{1}{V}\right)^{\Delta\nu} \quad K_\chi = K_n \left(\frac{1}{n_{tot}}\right)^{\Delta\nu}$$
$$K_p = K_n \left(\frac{p_{tot}}{n_{tot}}\right)^{\Delta\nu}$$

4.13.1 Pressure dependence

$$\frac{\partial \ln K}{\partial p} = -\frac{1}{RT}\left(\frac{\partial \Delta_r G}{\partial p}\right)$$
$$\frac{\partial \ln K}{\partial p} = -\frac{\Delta_r V}{RT}$$
$$\Delta_r V \approx 0 \implies \left(\frac{\partial K}{\partial p}\right)_T = 0$$

Still, the equilibrium's composition is not independent of the pressure.

4.13.2 Temperature dependence

$$\frac{\partial d \ln K}{\partial \frac{1}{T}} = -\frac{\Delta_r H^0}{R}$$
$$\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta_r H^0}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$
$$K_2 = e^{\left(-\frac{\Delta_r H^0}{R}\left(\frac{1}{T_2} - \frac{1}{T_2}\right)\right)} \cdot K_1$$

4.14 Clausius-Clapeyron equation

$$\text{Clausius' equation} \quad \frac{dp}{dT} = \frac{\Delta S_m}{\Delta V_m}$$
$$\text{Clausius-Clapeyron} \quad \frac{dp}{dT} = \frac{\Delta H_m}{T\Delta V_m}$$

4.14.1 Solid-liquid equilibrium

$$\frac{dp}{dT} = \frac{\Delta_{fus}H_m}{\Delta V_{fus}}\frac{dT}{T}$$
$$p_2 = p_1 + \frac{\Delta_{fus}H_m}{\Delta_{fus}V_m}\ln\left(\frac{T_2}{T_1}\right)$$

4.14.2 Liquid-vapor equilibrium

Temperature dependence

$$\frac{dp}{dT} = \frac{\Delta_{vap}H_m}{T\Delta_{vap}V_m}$$
$$d\ln p = \frac{\Delta_{vap}H_m}{RT^2}dT$$
$$p_2 = p_1 \cdot e^{\frac{\Delta_{vap}H_m}{RT^2}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$$

Pressure dependence

$$p = p^* \cdot e^{\left(\frac{V_{m,liq}}{RT}\Delta p\right)}$$

4.14.3 Solid-vapor equilibrium

$$\frac{\mathrm{dp}}{\mathrm{dT}} = \frac{\Delta_{sub}H_m}{T\Delta_{sub}V_m}$$

$$d\ln p = \frac{\Delta_{sub}H_m}{RT^2}dT$$

$$p_2 = p_1 \cdot e^{\frac{\Delta_{sub}H_m}{RT^2}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$$

5 Radiations

5.1 Bragg Equation

$$n\lambda = 2d_{hkl}\sin\theta$$