Common Equations Used in Chemistry

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1. Basic Conversions and Definitions

Converting °F to °C:

$$^{\circ}$$
C = $(^{\circ}$ F $- 32) \times \frac{5}{9}$

Converting °C to °F:

$$^{\circ}F = \left(^{\circ}C \times \frac{9}{5}\right) + 32$$

Converting °C to K:

$$K = {}^{\circ}\text{C} + 273.15$$

2. Solutions

Density:

$$d = \frac{m}{V}$$

Molarity:

$$C = \frac{\text{moles of solute}}{\text{liters of solution}}$$

Molality:

$$b = \frac{\text{moles of solute}}{\text{kg of solvent}}$$

Boiling point elevation¹:

$$\Delta T_{\rm b} = i K_{\rm b} b$$

Freezing point depression:

$$\Delta T_{\rm f} = i K_{\rm f} b$$

Table 1: Boiling point elevation and freezing point depression constants for different solvents.

Solvent	Normal Boiling Point (°C)	K_{b} (°C/m)	Normal Freezing Point (°C)	K_{f} (°C/m)
Water	100.0	0.512	0.0	1.86
Acetic acid	118.1	3.04	16.6	3.90
Benzene	80.1	2.53	5.5	5.12
Chloroform	61.3	3.63	-63.5	4.86
Nitrobenzene	210.9	5.24	5.67	8.1

Osmotic pressure:

$$\pi = i \mathbf{M} R T$$

Dilution:

$$C_1V_1 = C_2V_2$$

The van't Hoff factor, i, describes the number of particles formed upon solvation. For example, for solvation of sodium chloride, $\operatorname{NaCl}(s) \longrightarrow \operatorname{Na}^+(aq) + \operatorname{Cl}^-(aq)$, i=2. For a nonelectrolyte (like glucose or benzene), i=1. This factor can deviate from ideality for highly charged ions, where ion-pairing occurs (incomplete dissociation), as is seen with CaCl_2 , where i=2.6 instead of 3.0 ($\operatorname{CaCl}_2(s) \longrightarrow \operatorname{Ca}^{2+}(aq) + 2\operatorname{Cl}^-(aq)$).

3. Gases

Ideal Gas Law, $R = 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{K} \cdot \text{mol}}$

$$PV = nRT$$

Boyle's Law (n, T constant):

$$P_1V_1 = P_2V_2$$

Charles' Law (n, P constant):

$$\frac{V_1}{V_2} = \frac{T_1}{T_2}$$

Avogadro's Law (P, T constant):

$$\frac{V_1}{V_2} = \frac{n_1}{n_2}$$

Gay-Lussac's Law (P, T constant):

$$\frac{P_1}{P_2} = \frac{T_1}{T_2}$$

Combined Gas Law (n is constant):

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

Relation of density to molar mass:

$$M = \frac{dRT}{P}$$

Dalton's Law of Partial Pressures, where $\chi_i =$ mole fraction of species i and P_T is total pressure:

$$P_i = \chi_i P_{\rm T}$$

Raoult's Law, where P_i^{\star} is the vapor pressure of pure substance i:

$$P_T^{\star} = \chi_A P_A^{\star} + \chi_B P_B^{\star} + \dots$$

Alternately,

$$P_i = \chi_i P_i^{\star}$$

Root-mean-square (RMS) speed of a gas particle:

$$\mu = \sqrt{\frac{3RT}{M}}$$

Rates of Effusion by Molar Mass

$$\frac{\mathrm{rate_1}}{\mathrm{rate_2}} = \sqrt{\frac{M_2}{M_1}}$$

van der Waals equation for pressure of a non-ideal gas, where a corrects for the attractive forces between gas particles, and b corrects for the volume occupied by gas particles:

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

4. Thermodynamics

4.1. Heat Exchange

Heat exchange, where C_s is specific heat capacity:

$$q = mC_s\Delta T$$

Calorimetry in an imperfect calorimeter:

$$q_{\rm rxn} = mC_s\Delta T + C_{\rm cal}\Delta T$$

Heat exchange, where C_V is molar heat capacity at constant volume:

$$q = nC_V \Delta T$$

Heat exchange, where C_P is molar heat capacity at constant pressure:

$$q = nC_P \Delta T$$

4.2. Conditions

4.2.1. Definitions

• Isothermal: $\Delta T = 0$, $\Delta E = 0$, q = -w

• Adiabatic: $q = 0, \Delta E = w$

• Isobaric: $\Delta P = 0$ (constant pressure)

4.2.2. In General

• $q = nC\Delta T$

• $w = -P\Delta V$ where L·atm = 101.325 J

• $\Delta E = q + w$

• $\Delta H = \Delta E + P\Delta V + V\Delta P$

• $C_{\rm P} = \frac{5}{2}R$ and $C_{\rm V} = \frac{3}{2}R$

Table 2: Summary of thermodynamic quantities under different conditions.

Quantity	Constant P	Constant V	Adiabatic	Isothermal
Heat, q	$nC_{\mathrm{P}}\Delta T$	$nC_{ m V}\Delta T$	0	-w
Work, w	$-P\Delta V$	0	$nC_V\Delta T$	$-nRT\ln\left(\frac{V_{\rm f}}{V_{\rm i}}\right) = -nRT\ln\left(\frac{P_{\rm i}}{P_{\rm f}}\right)$
Energy, ΔE	q+w	q	w	0
Enthalpy, ΔH	q	$\Delta E + V \Delta P$	$V\Delta P$	0
Entropy, ΔS	$nC_{ m P} \ln \left(rac{T_{ m f}}{T_{ m i}} ight)$	$nC_{ m V} \ln \left(rac{T_{ m f}}{T_{ m i}} ight)$	0	$nR\ln\left(\frac{V_{\mathrm{f}}}{V_{\mathrm{i}}}\right) = nR\ln\left(\frac{P_{\mathrm{i}}}{P_{\mathrm{f}}}\right)$

4.3. The Adiabatic Condition

Given a rapid change in volume where q = 0, both P and T change to accommodate the compression or expansion.

$$\gamma = \frac{C_P}{C_V} = \frac{5}{3}$$

$$(P_1)(V_1)^{\gamma} = (P_2)(V_2)^{\gamma}$$

$$w = nC_V \Delta T$$

Temperature change in adiabatic compression or expansion:

$$T_{\rm f} = T_{\rm i} \left(\frac{V_{\rm i}}{V_{\rm f}}\right)^{(R/C_V)}$$

4.4. Enthalpy

Enthalpy is the energy required to create a system, plus the amount of energy required to make room for the system by displacing its environment by the system's volume at a given pressure.

$$H = E + PV$$

Enthalpy change for a reaction:

$$\Delta H = \Delta E + \Delta (PV) = \Delta E + P\Delta V + V\Delta P$$

Standard enthalpy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta H_{\rm rxn}^{\circ} = \sum n \Delta H_{\rm f}^{\circ}({\rm products}) - \sum m \Delta H_{\rm f}^{\circ}({\rm reactants}) = \sum D_{\rm broken} - \sum D_{\rm formed}$$

Clausius-Clapeyron equation:

$$\ln P = \frac{-\Delta H_{\text{vap}}}{RT} + C$$

Heat of vaporization based on the Clausius–Clapeyron equation:

$$\ln \frac{P_1}{P_2} = \frac{\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

4.5. Entropy

Second Law of Thermodynamics:

$$\Delta S_{\rm universe} = \Delta S_{\rm system} + \Delta S_{\rm surroundings} > 0$$

Standard entropy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta S_{\rm rxn}^{\circ} = \sum n \Delta S^{\circ}({\rm products}) - \sum m \Delta S^{\circ}({\rm reactants})$$

Change in entropy with $\Delta H_{\rm vap}$ or q where T is constant:

$$\Delta S = \frac{\Delta H_{\text{vap}}}{T} = \frac{q}{T}$$

Change in entropy with ΔV or ΔP where T is constant:

$$\Delta S = nR \ln \left(\frac{V_{\rm f}}{V_{\rm i}}\right) = nR \ln \left(\frac{P_{\rm i}}{P_{\rm f}}\right)$$

Change in entropy for a thermodynamic process where T and/or P are varied:

$$\Delta S = nC_V \ln \left(\frac{T_{\rm f}}{T_{\rm i}}\right) - nR \ln \left(\frac{P_{\rm f}}{P_{\rm i}}\right)$$

4.6. Gibbs Free Energy

Free energy change at constant temperature:

$$\Delta G^{\circ} = \Delta H^{\circ} - T \Delta S^{\circ}$$

Or for an equilibrium reaction:

$$\Delta G^{\circ} = -RT \ln K_{\rm eq}$$

Non-standard free energy:

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

Standard free energy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta G_{\rm rxn}^{\circ} = \sum n \Delta G_{\rm f}^{\circ}({\rm products}) - \sum m \Delta G_{\rm f}^{\circ}({\rm reactants})$$

5. Electromagnetism

Relationship of wavelength and frequency, where $c=2.99\times 10^8$ m/s:

$$c = \lambda \nu$$

Energy of a photon, where Planck's constant $h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s}$:

$$E = h\nu = \frac{hc}{\lambda}$$

Energy of an electron in the $n^{\rm th}$ shell in a hydrogen atom, where $R_{\rm H}=2.18\times 10^{-18}$ J:

$$E_n = -Z^2 R_{\rm H} \left(\frac{1}{n^2}\right)$$

Energy of a photon emitted as the electron undergoes a transition from the n_i shell to the n_f shell:

$$\Delta E = Z^2 R_{\rm H} \left(\frac{1}{n_{\rm f}^2} - \frac{1}{n_{\rm i}^2} \right)$$

Or, use $R_{\rm H} = 10973731.6~{\rm m}^{-1}$:

$$\frac{1}{\lambda} = Z^2 R_{\rm H} \left(\frac{1}{n_{\rm f}^2} - \frac{1}{n_{\rm i}^2} \right)$$

de Broglie wavelength:

$$\lambda = \frac{h}{mv}$$

Formal charge:

$$q_{\rm F} = N_i e_{\rm V} - N_j B - N_k e_{\rm NB}$$

Dipole moment:

$$\mu = Q \times r$$

Bragg equation:

$$\lambda\nu = 2d\sin\theta$$

6. Quantum Mechanics

Heisenberg Uncertainty Principle:

$$\Delta x \Delta \rho \ge \frac{h}{4\pi}$$

The time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle=\hat{H}|\Psi(t)\rangle$$

The time-independent Schrödinger equation for a particle of mass m moving in one direction with energy E where $\hbar = h/2\pi$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

Wavefunction for the 1s orbital:

$$\psi_{1s} = \frac{1}{\sqrt{\pi}}e^{-r}$$

Wavefunction for the 2s orbital:

$$\psi_{2s} = \frac{1}{2\sqrt{2\pi}} \left(1 - \frac{r}{2} \right) e^{-r/2}$$

Wavefunction for the $2p_z$ orbital, where a_0 is the radius of the first Bohr orbit $(5.29 \times 10^{-11} \text{ m})$, $\sigma = Z(r/a_0)$ where r is the distance (in m) from the nucleus and Z is the nuclear charge, and θ is an angle:

$$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$$

Wavefunction for a particle in a 1-dimensional box of length L:

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right) x$$

Energy for a particle in a 1-dimensional box of length L:

$$E = \frac{n^2 h^2}{8mL^2}$$

Potential energy between two charged bodies:

$$V = k \frac{q_1 q_2}{r}$$

7. Stoichiometry

Percent composition of an element in a compound, where n = the number of moles of the element in one mole of the compound:

$$\% = \left(\frac{n \times \text{molar mass of element}}{\text{molar mass of compound}}\right) \times 100\%$$

Percent yield:

$$\% \text{ yield} = \left(\frac{\text{actual yield}}{\text{theoretical yield}}\right) \times 100\%$$

8. Electrochemistry

Electrical force between two charged bodies:

$$F_{e\ell} = k \frac{q_1 q_2}{r_2}$$

Standard emf of an electrochemical cell:

$$\mathscr{E}_{\mathrm{cell}}^{\circ} = \mathscr{E}_{\mathrm{ox}}^{\circ} - \mathscr{E}_{\mathrm{red}}^{\circ} = \frac{RT}{nF} \ln K$$

Standard free energy of an electrochemical cell:

$$\Delta G^{\circ} = -nF\mathscr{E}_{\text{cell}}^{\circ}$$

Nernst equation:

$$\mathscr{E}_{\text{cell}} = \mathscr{E}_{\text{cell}}^{\circ} - \frac{RT}{nF} \ln Q$$

Therefore: Standard free energy of an electrochemical cell:

$$\Delta G = -nF\mathscr{E}_{\text{cell}}$$

9. Reaction Kinetics

Order	Standard Form	Integrated Form	Line Form
0	rate = k	$[\mathbf{A}]_t - [\mathbf{A}]_0 = -kt$	$[\mathbf{A}]_t = -kt + [\mathbf{A}]_0$
1	$\mathrm{rate} = k[\mathbf{A}]$	$\ln\frac{[\mathbf{A}]_t}{[\mathbf{A}]_0} = -kt$	$\ln\left[\mathbf{A}\right]_t = -kt + \ln\left[\mathbf{A}\right]_0$
2	$rate = k[A]^2$	$\frac{1}{[\mathbf{A}]_t} - \frac{1}{[\mathbf{A}]_0} = kt$	$\frac{1}{[\mathbf{A}]_t} = kt + \frac{1}{[\mathbf{A}]_0}$

Order	Half-life	
0	$t_{1/2} = \frac{[\mathbf{A}]_0}{2k}$	
1	$t_{1/2} = \frac{\ln 2}{k}$	
2	$t_{1/2} = \frac{1}{k[\mathbf{A}]_0}$	

Arrhenius equation:

$$k = A \exp \frac{-E_{\rm a}}{RT}$$

Determining energy of activation:

$$\ln k = \left(\frac{-E_{\rm a}}{R}\right) \left(\frac{1}{T}\right) + \ln A$$

Relationships of rate constants at two different temperatures:

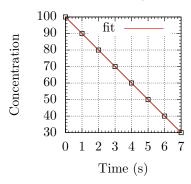
$$\ln \frac{k_1}{k_2} = \frac{E_{\rm a}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_{\rm a}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

9.1. Kinetics Data

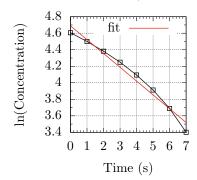
Table 3: Kinetics Data — 0th Order

Time	Concentration	ln(Concentration)	1/(Concentration)
0	100	4.605	0.0100
1	90	4.499	0.0110
2	80	4.382	0.0125
3	70	4.248	0.0141
4	60	4.094	0.0166
5	50	3.912	0.0200
6	40	3.688	0.0250
7	30	3.401	0.0333

0th Order Plot, $\mathbb{R}^2 = 1$



1st Order Plot, $R^2 = 0.97$



2nd Order Plot, $R^2 = 0.89$

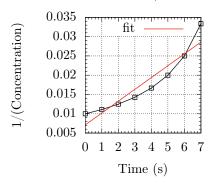
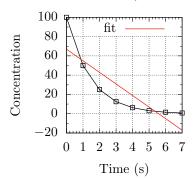


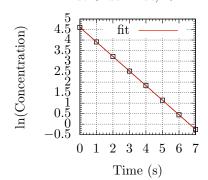
Table 4: Kinetics Data — 1st Order

Time	Concentration	ln(Concentration)	1/(Concentration)
0	100	4.605	0.01
1	50	3.912	0.02
2	25	3.218	0.04
3	12.5	2.525	0.08
4	6.25	1.832	0.16
5	3.13	1.141	0.32
6	1.56	0.444	0.64
7	0.78	-0.248	1.28

0th Order Plot, $R^2 = 0.73$



1st Order Plot, $R^2 = 1$



2nd Order Plot, $R^2 = 0.72$

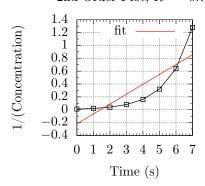
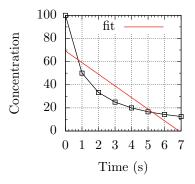


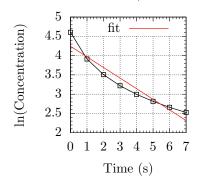
Table 5: Kinetics Data — 2nd Order

Time	Concentration	ln(Concentration)	1/(Concentration)
0	100	4.605	0.01
1	50	3.912	0.02
2	33.3	3.505	0.03
3	25	3.218	0.04
4	20	2.995	0.05
5	16.67	2.813	0.06
6	14.28	2.658	0.07
7	12.5	2.525	0.08

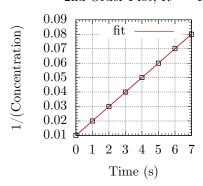
0th Order Plot, $R^2 = 0.70$



1st Order Plot, $R^2 = 0.92$



2nd Order Plot, $R^2 = 1$



10. Equilibrium

Law of Mass Action (equilibrium constant) for a reaction of form $aA + bB \longrightarrow cC + dD$:

$$K_{\text{eq}} = \frac{[\mathbf{C}]^c[\mathbf{D}]^d}{[\mathbf{A}]^a[\mathbf{B}]^b}$$

van't Hoff Equation

$$\ln\left(\frac{K_2}{K_1}\right) = \frac{-\Delta H^{\circ}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Relationship between equilibrium constants for aqueous systems and for gases:

$$K_{\rm p} = K_{\rm c} R T^{\Delta n}$$

Ion product of water:

$$K_{\rm w} = [{\rm H_3O^+}][{\rm ^-OH}] = 1 \times 10^{-14}$$

10.1. Equilibrium of Acids and Bases

Definition of pH:

$$pH = -\log[H_3O^+]$$

Definition of pOH:

$$pOH = -\log[-OH] = 14 - pH$$

For the reaction $HA + H_2O \longrightarrow H_3O^+ + A^-$:

$$K_{\rm a} = \frac{[{\rm H_3O^+}][{\rm A^-}]}{[{\rm HA}]}$$

For the reaction B + $H_2O \longrightarrow BH^+ + {}^-OH$:

$$K_{\rm b} = \frac{[{\rm BH}^+][-{\rm OH}]}{[{\rm B}]}$$

Relationship between K_a , K_b , and K_w :

$$K_{\rm w} = K_{\rm a} K_{\rm b} = 1 \times 10^{-14}$$

Definition of pK_a :

$$pK_a = -\log(K_a)$$

Henderson-Hasselbalch equation:

$$pH = pK_a + \log \frac{[base]}{[acid]}$$

10.2. Equilibrium and Thermodynamics

Relationship between standard free-energy change and the equilibrium constant:

$$\Delta G^{\circ} = -RT \ln K$$

Non-standard free energy for a reaction of form $aA + bB \longrightarrow cC + dD$, where $Q = \frac{[C]^c[D]^d}{[A]^a[B]^b}$:

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

11. Similarity of Equations

11.1. Linear Equations with Different Temperatures

Clausius-Clapeyron equation:

$$\ln \frac{P_1}{P_2} = \frac{\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

Arrhenius Equation

$$\ln \frac{k_1}{k_2} = \frac{E_{\rm a}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_{\rm a}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

van't Hoff Equation

$$\ln \frac{K_1}{K_2} = \frac{\Delta H^{\circ}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-\Delta H^{\circ}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

11.2. Summations

Standard entropy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta S_{\rm rxn}^{\circ} = \sum n \Delta S^{\circ}({\rm products}) - \sum m \Delta S^{\circ}({\rm reactants})$$

Standard enthalpy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta H_{\rm rxn}^{\circ} = \sum n \Delta H_{\rm f}^{\circ}({\rm products}) - \sum m \Delta H_{\rm f}^{\circ}({\rm reactants})$$

Standard free energy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta G_{\rm rxn}^{\circ} = \sum n \Delta G_{\rm f}^{\circ}({\rm products}) - \sum m \Delta G_{\rm f}^{\circ}({\rm reactants})$$