Common Equations Used in Chemistry

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Contents

1. Basic Conversions and Definitions

Converting °F to °C:

$$°\text{C} = (°\text{F} - 32) \times \frac{5}{9}$$

Converting °C to °F:

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

Converting °C to K:

$$K = °\text{C} + 273.15$$

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 elevation[1]:

$$\Delta T_\text{b} = iK_\text{b}b$$

Freezing point depression:

$$\Delta T_\text{f} = iK_\text{f}b$$

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:

$$\pi = i\text{M}RT$$

Dilution:

$$C_1V_1 = C_2V_2$$

[1] The van't Hoff factor, i, describes the number of particles formed upon solvation. For example, for solvation of sodium chloride, $\text{NaCl}(s) \longrightarrow \text{Na}^+(aq) + \text{Cl}^-(aq)$, $i = 2$. 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 ($\text{CaCl}_2(s) \longrightarrow \text{Ca}^{2+}(aq) + 2\text{Cl}^-(aq)$).

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):

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

Relation of density to molar mass:

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

Dalton's Law of Partial Pressures, where χ_i = mole fraction of species i and P_{T} is total pressure:

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

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

$$P_T^\star = \chi_A P_A^\star + \chi_B P_B^\star + \ldots$$

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

$$\frac{\text{rate}_1}{\text{rate}_2} = \sqrt{\frac{M_2}{M_1}}$$

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:

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

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
- $\Delta E = q + w$
- $\Delta H = \Delta E + P\Delta V + V\Delta P$
- $C_{\text{P}} = \frac{5}{2}R$ and $C_{\text{V}} = \frac{3}{2}R$

Table 2: Summary of thermodynamic quantities under different conditions.

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

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:

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

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:

$$\Delta H^\circ_\mathrm{rxn} = \sum n\Delta H^\circ_\mathrm{f}(\text{products}) - \sum m\Delta H^\circ_\mathrm{f}(\text{reactants}) = \sum D_\text{broken} - \sum D_\text{formed}$$

Clausius–Clapeyron equation:

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

Heat of vaporization based on the Clausius–Clapeyron equation:

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

4.5. Entropy

Second Law of Thermodynamics:

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

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

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

Change in entropy with ΔH_{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:

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

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

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

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:

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

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:

$$\Delta G^\circ_{\text{rxn}} = \sum n\Delta G^\circ_{\text{f}}(\text{products}) - \sum m\Delta G^\circ_{\text{f}}(\text{reactants})$$

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 $h = 6.626 \times 10^{-34}$ J·s:

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

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

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

Energy of a photon emitted as the electron undergoes a transition from the n_{i} shell to the n_{f} shell:

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

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

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

de Broglie wavelength:

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

Formal charge:

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

Dipole moment:

$$\mu = Q \times r$$

Bragg equation:

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

6. Quantum Mechanics

Heisenberg Uncertainty Principle:

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

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 (5.29×10^{-11} 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:

$$\mathscr{E}^\circ_{\text{cell}} = \mathscr{E}^\circ_{\text{ox}} - \mathscr{E}^\circ_{\text{red}} = \frac{RT}{nF}\ln K$$

Standard free energy of an electrochemical cell:

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

Nernst equation:

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

Therefore: Standard free energy of an electrochemical cell:

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

9. Reaction Kinetics

	Rate Laws		
Order	Standard Form	Integrated Form	Line Form
0	rate $= k$	$[\text{A}]_t - [\text{A}]_0 = -kt$	$[\text{A}]_t = -kt + [\text{A}]_0$
1	rate $= k[\text{A}]$	$\ln\frac{[\text{A}]_t}{[\text{A}]_0} = -kt$	$\ln[\text{A}]_t = -kt + \ln[\text{A}]_0$
2	rate $= k[\text{A}]^2$	$\frac{1}{[\text{A}]_t} - \frac{1}{[\text{A}]_0} = kt$	$\frac{1}{[\text{A}]_t} = kt + \frac{1}{[\text{A}]_0}$

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

Arrhenius equation:

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

Determining energy of activation:

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

Relationships of rate constants at two different temperatures:

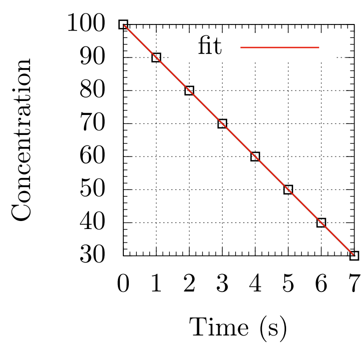
$$\ln\frac{k_1}{k_2} = \frac{E_\text{a}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \frac{-E_\text{a}}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

9.1. Kinetics Data

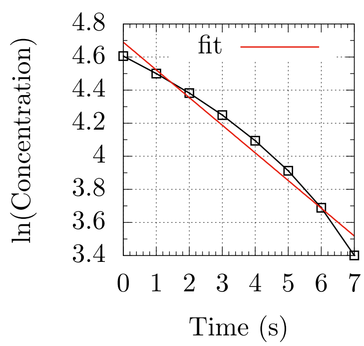
Table 3: Kinetics Data — 0th Order

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, $R^2 = 1$



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



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

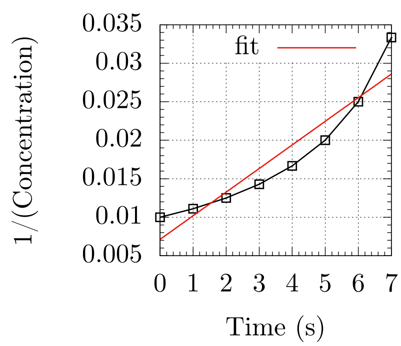
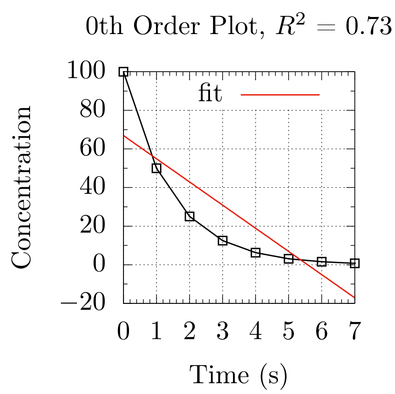
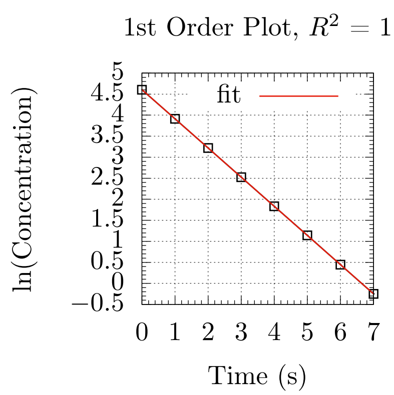


Table 4: Kinetics Data — 1st Order

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





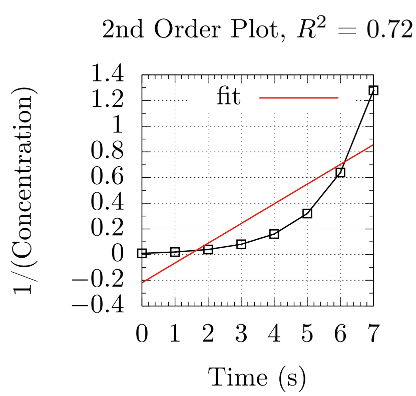
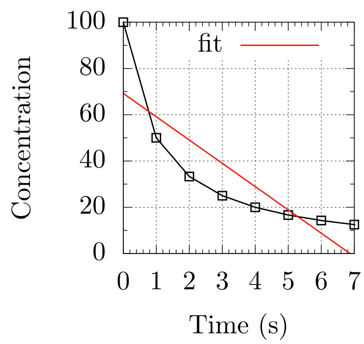


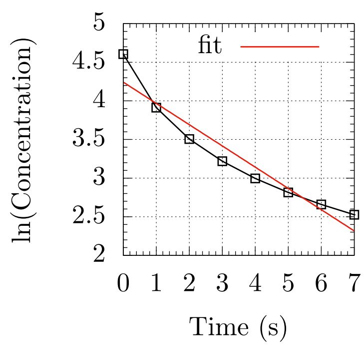
Table 5: Kinetics Data — 2nd Order

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

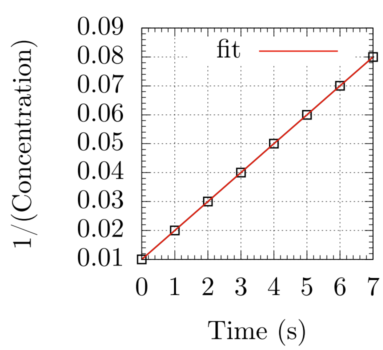
0th Order Plot, $R^2 = 0.70$



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 $a\mathrm{A} + b\mathrm{B} \longrightarrow c\mathrm{C} + d\mathrm{D}$:

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

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:

$$K_{\mathrm{p}} = K_{\mathrm{c}}RT^{\Delta n}$$

Ion product of water:

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

10.1. Equilibrium of Acids and Bases

Definition of pH:

$$\mathrm{pH} = -\log[\mathrm{H_3O^+}]$$

Definition of pOH:

$$\mathrm{pOH} = -\log[^-\mathrm{OH}] = 14 - \mathrm{pH}$$

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

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

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

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

Relationship between K_{a}, K_{b}, and K_{w}:

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

Definition of pK_{a}:

$$\mathrm{p}K_{\mathrm{a}} = -\log(K_{\mathrm{a}})$$

Henderson–Hasselbalch equation:

$$\mathrm{pH} = \mathrm{p}K_{\mathrm{a}} + \log\frac{[\mathrm{base}]}{[\mathrm{acid}]}$$

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 $a\mathrm{A} + b\mathrm{B} \longrightarrow c\mathrm{C} + d\mathrm{D}$, where $Q = \frac{[\mathrm{C}]^c[\mathrm{D}]^d}{[\mathrm{A}]^a[\mathrm{B}]^b}$:

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

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

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

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:

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

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

$$\Delta H^\circ_{\text{rxn}} = \sum n\Delta H^\circ_{\text{f}}(\text{products}) - \sum m\Delta H^\circ_{\text{f}}(\text{reactants})$$

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

$$\Delta G^\circ_{\text{rxn}} = \sum n\Delta G^\circ_{\text{f}}(\text{products}) - \sum m\Delta G^\circ_{\text{f}}(\text{reactants})$$

12. Other

Relationship between mass defect and energy released:

$$\Delta E = (\Delta m)c^2$$