

# Common Equations Used in Chemistry

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February 22, 2020

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## 1. Basic Conversions and Definitions

Converting °F to °C:

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

Converting °C to °F:

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

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 elevation<sup>1</sup>:

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

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)	$K_{\text{b}}$ (°C/m)	Normal Freezing Point (°C)	$K_{\text{f}}$ (°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:

$$\pi = iMRT$$

Dilution:

$$C_1V_1 = C_2V_2$$

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<sup>1</sup> 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  $\text{CaCl}_2$ , 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  $\chi_i$  = mole fraction of species  $i$  and  $P_T$  is total pressure:

$$P_i = \chi_i P_T$$

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

$$P_T^* = \chi_A P_A^* + \chi_B P_B^* + \dots$$

Alternately,

$$P_i = \chi_i P_i^*$$

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  $\text{L}\cdot\text{atm} = 101.325 \text{ J}$
- $\Delta E = q + w$
- $\Delta H = \Delta E + P\Delta V + V\Delta P$
- $C_P = \frac{5}{2}R$  and  $C_V = \frac{3}{2}R$

**Table 2:** Summary of thermodynamic quantities under different conditions.

Quantity	Constant $P$	Constant $V$	Adiabatic	Isothermal
Heat, $q$	$nC_P\Delta T$	$nC_V\Delta T$	0	$-w$
Work, $w$	$-P\Delta V$	0	$nC_V\Delta T$	$-nRT \ln\left(\frac{V_f}{V_i}\right) = -nRT \ln\left(\frac{P_i}{P_f}\right)$
Energy, $\Delta E$	$q + w$	$q$	$w$	0
Enthalpy, $\Delta H$	$q$	$\Delta E + V\Delta P$	$V\Delta P$	0
Entropy, $\Delta S$	$nC_P \ln\left(\frac{T_f}{T_i}\right)$	$nC_V \ln\left(\frac{T_f}{T_i}\right)$	0	$nR \ln\left(\frac{V_f}{V_i}\right) = nR \ln\left(\frac{P_i}{P_f}\right)$

### 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:

$$T_f = T_i \left( \frac{V_i}{V_f} \right)^{(R/C_V)}$$

### 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:

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

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:

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

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

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

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

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

Change in entropy with  $\Delta V$  or  $\Delta P$  where  $T$  is constant:

$$\Delta S = nR \ln \left( \frac{V_f}{V_i} \right) = nR \ln \left( \frac{P_i}{P_f} \right)$$

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

$$\Delta S = nC_V \ln \left( \frac{T_f}{T_i} \right) - nR \ln \left( \frac{P_f}{P_i} \right)$$

## 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:

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

## 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  $n^{\text{th}}$  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  $n_{\text{i}}$  shell to the  $n_{\text{f}}$  shell:

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

Or, use  $R_{\text{H}} = 10973731.6$  m<sup>-1</sup>:

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

Simplified Rydberg Equation, where  $R_{\infty} = 10973731.6$  m<sup>-1</sup>:

$$\frac{1}{\lambda} = R_{\infty} \left( \frac{1}{n_{\text{lower}}^2} - \frac{1}{n_{\text{upper}}^2} \right)$$

de Broglie wavelength:

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

Formal charge:

$$q_{\text{F}} = N_{\text{i}}e_{\text{V}} - N_{\text{j}}\text{B} - N_{\text{k}}e_{\text{NB}}$$

Dipole moment:

$$\mu = Q \times r$$

Bragg equation:

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

## 6. Quantum Mechanics

Heisenberg Uncertainty Principle:

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

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 ( $5.29 \times 10^{-11}$  m),  $\sigma = Z(r/a_0)$  where  $r$  is the distance (in m) from the nucleus and  $Z$  is the nuclear charge, and  $\theta$  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  $L$ :

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

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:

$$F_{el} = k \frac{q_1 q_2}{r_2}$$

Standard emf of an electrochemical cell:

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

Standard free energy of an electrochemical cell:

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

Nernst equation:

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

Therefore: Standard free energy of an electrochemical cell:

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

## 9. Reaction Kinetics

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

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

First-order decay:

$$[A]_t = [A]_0 (1/2)^n \text{ where } n = t/t_{1/2} \text{ or ln form: } \ln \frac{[A]_t}{[A]_0} = (-\ln 2) \left( \frac{t}{t_{1/2}} \right)$$

Arrhenius equation:

$$k = A \exp \frac{-E_a}{RT} \text{ and ln form: } \ln k = \left( \frac{-E_a}{R} \right) \left( \frac{1}{T} \right) + \ln A$$

Relationships of rate constants at two different temperatures:

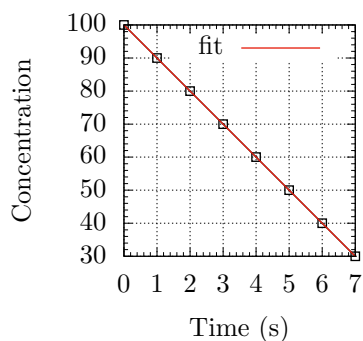
$$\ln \frac{k_1}{k_2} = \frac{E_a}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_a}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$

## 9.1. Kinetics Data

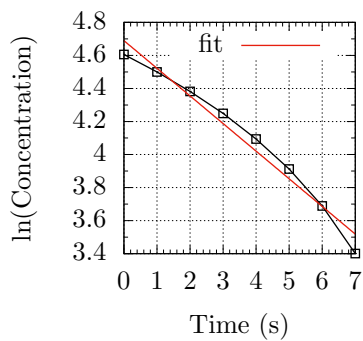
**Table 3:** Kinetics Data — 0th Order

Time	Concentration	$\ln(\text{Concentration})$	$1/(\text{Concentration})$
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

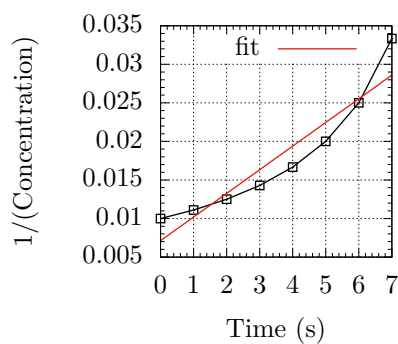
0th Order Plot,  $R^2 = 1$



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

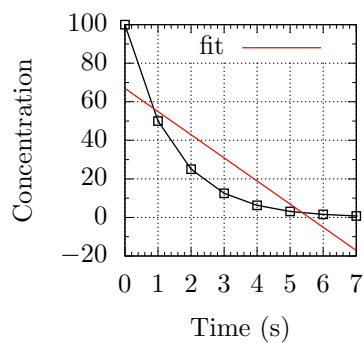
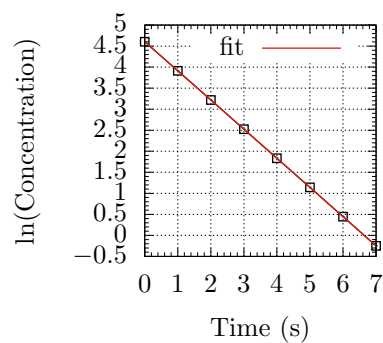
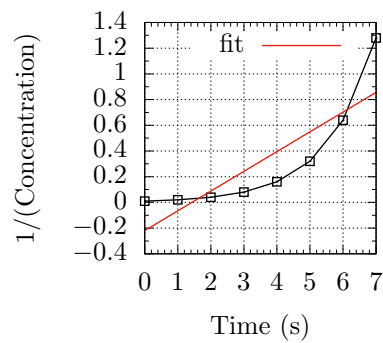


2nd Order Plot,  $R^2 = 0.89$



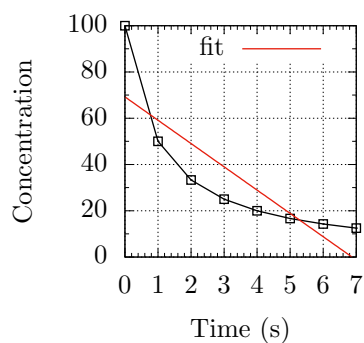
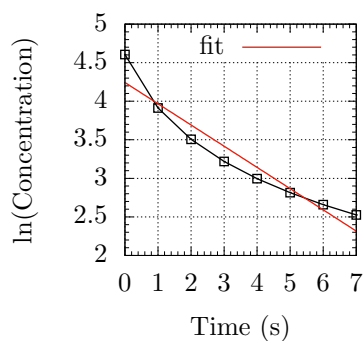
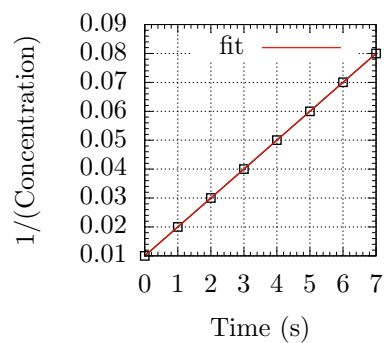
**Table 4:** Kinetics Data — 1st Order

Time	Concentration	$\ln(\text{Concentration})$	$1/(\text{Concentration})$
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	$\ln(\text{Concentration})$	$1/(\text{Concentration})$
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  $aA + bB \longrightarrow cC + dD$ :

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

van't Hoff Equation

$$\ln \left( \frac{K_2}{K_1} \right) = \frac{-\Delta H^\circ}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \text{ or } \ln K_{\text{sp}} = \frac{-\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R}$$

Relationship between equilibrium constants for aqueous systems and for gases:

$$K_p = K_c RT^{\Delta n}$$

Ion product of water:

$$K_w = [\text{H}_3\text{O}^+][\text{OH}^-] = 1 \times 10^{-14}$$

### 10.1. Equilibrium of Acids and Bases

Definition of pH:

$$\text{pH} = -\log[\text{H}_3\text{O}^+]$$

Definition of pOH:

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

For the reaction  $\text{HA} + \text{H}_2\text{O} \longrightarrow \text{H}_3\text{O}^+ + \text{A}^-$ :

$$K_a = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]}$$

For the reaction  $\text{B} + \text{H}_2\text{O} \longrightarrow \text{BH}^+ + \text{OH}^-$ :

$$K_b = \frac{[\text{BH}^+][\text{OH}^-]}{[\text{B}]}$$

Relationship between  $K_a$ ,  $K_b$ , and  $K_w$ :

$$K_w = K_a K_b = 1 \times 10^{-14}$$

Definition of  $\text{p}K_a$ :

$$\text{p}K_a = -\log(K_a)$$

Henderson-Hasselbalch equation:

$$\text{pH} = \text{p}K_a + \log \frac{[\text{base}]}{[\text{acid}]}$$

### 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:

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

van't Hoff Equation:

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

van't Hoff Equation with  $K_{\text{sp}}$  and entropy, plot  $\ln K_{\text{sp}}$  vs.  $1/T$ :

$$\Delta H^\circ - T\Delta S^\circ = \Delta G^\circ = -RT \ln K_{\text{sp}}$$

$$\ln K_{\text{sp}} = \frac{-\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R}$$

### 11.2. Summations

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

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

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

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

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

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

## 12. Other

Mass defect:

$$\Delta m = [Z(m_p + m_e) + (A - Z)m_n] - m_{\text{atom}}$$

**Table 6:** Values for mass defect equation.

Variable	Description	Value
$\Delta m$	mass defect	amu
$m_p$	mass of a proton	1.007277
$m_n$	mass of a neutron	1.008665
$m_e$	mass of an electron	0.000548597
$m_{\text{atom}}$	mass of nuclide	${}^A_ZX$
$Z$	atomic number	number of protons
$A$	mass number	number of nucleons

Relationship between mass defect and energy released:

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