

Common Equations Used in Chemistry

John Terhorst, Ph.D.

February 15, 2019

Contents

1 Basic Conversions and Definitions	2
2 Solutions	2
3 Gases	3
4 Thermodynamics	4
4.1 Heat Exchange	4
4.2 Conditions	4
4.2.1 Definitions	4
4.2.2 In General	4
4.3 The Adiabatic Condition	5
4.4 Enthalpy	5
4.5 Entropy	6
4.6 Gibbs Free Energy	6
5 Electromagnetism	7
6 Quantum Mechanics	8
7 Stoichiometry	8
8 Electrochemistry	9
9 Reaction Kinetics	9
9.1 Kinetics Data	10
10 Equilibrium	13
10.1 Equilibrium of Acids and Bases	13
10.2 Equilibrium and Thermodynamics	13
11 Similarity of Equations	14
11.1 Linear Equations with Different Temperatures	14
11.2 Summations	14

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 elevation¹:

$$\Delta T_b = iK_b b$$

Freezing point depression:

$$\Delta T_f = iK_f b$$

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:

$$\pi = iMRT$$

Dilution:

$$C_1 V_1 = C_2 V_2$$

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:

$$P_i = \chi_i P_T$$

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, ΔE	$q + w$	q	w	0
Enthalpy, ΔH	q	$\Delta E + V\Delta P$	$V\Delta P$	0
Entropy, ΔS	$nC_P \ln\left(\frac{T_f}{T_i}\right)$	$nC_V \ln\left(\frac{T_f}{T_i}\right)$	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 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:

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

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^{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:

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

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

$$\frac{1}{\lambda} = Z^2 R_{\text{H}} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

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:

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

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 (5.29×10^{-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 :

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

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	$t_{1/2} = \frac{1}{k[A]_0}$

Arrhenius equation:

$$k = A \exp \frac{-E_a}{RT}$$

Determining energy of activation:

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

Relationships of rate constants at two different temperatures:

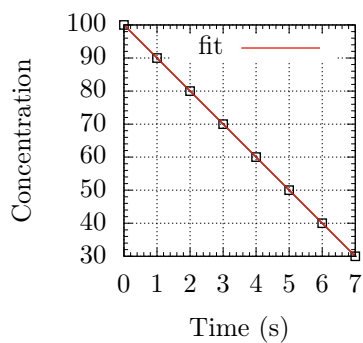
$$\ln \frac{k_1}{k_2} = \frac{E_a}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_a}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

9.1. Kinetics Data

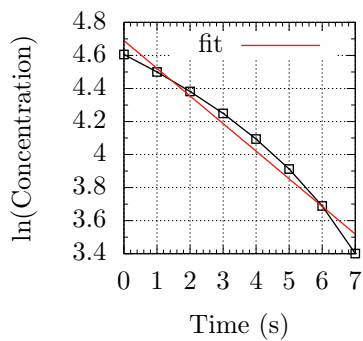
Table 3: Kinetics Data — 0th Order

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, $R^2 = 0.89$

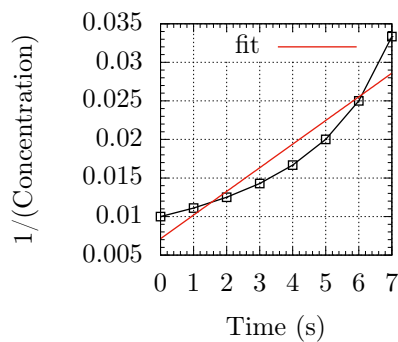


Table 4: Kinetics Data — 1st Order

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

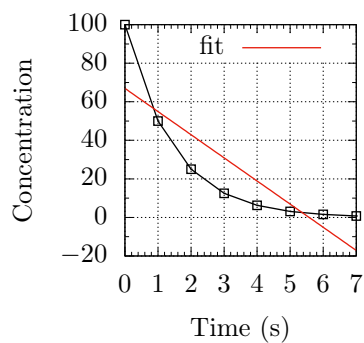
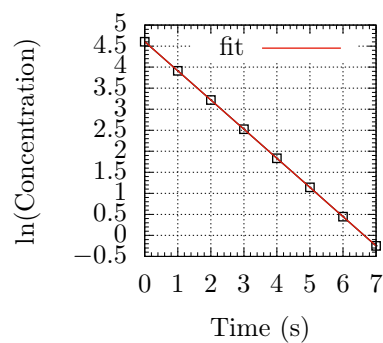
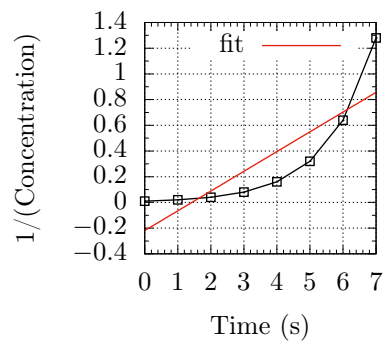
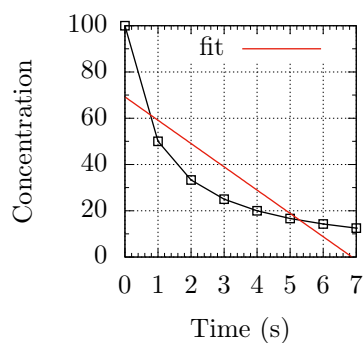
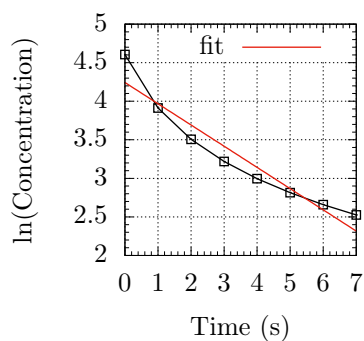
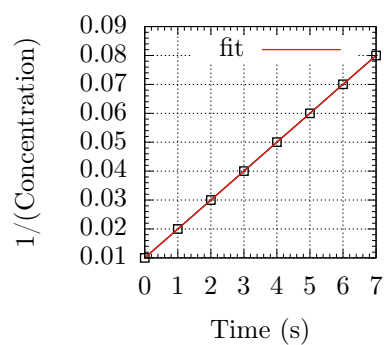
0th Order Plot, $R^2 = 0.73$ 1st Order Plot, $R^2 = 1$ 2nd Order Plot, $R^2 = 0.72$ 

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

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

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

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

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:

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

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

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

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

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