# Common Equations Used in Chemistry

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# March 5, 2020

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#### 1. Basic Conversions and Definitions

Converting °F to °C:

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

Converting  $^{\circ}$ C to  $^{\circ}$ 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 elevation<sup>1</sup>:

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

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)	$K_{\rm b}~(^{\circ}{\rm C/m})$	Normal Freezing Point (°C)	$K_{\rm f}~(^{\circ}{ m C/m})$
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:

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

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  $\operatorname{CaCl}_2$ , 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:

$$P_T^{\star} = \chi_{\mathcal{A}} P_{\mathcal{A}}^{\star} + \chi_{\mathcal{B}} P_{\mathcal{B}\mathcal{b}}^{\star} + \dots$$

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, $\Delta E$	q+w	q	w	0
Enthalpy, $\Delta H$	q	$\Delta E + V \Delta P$	$V\Delta P$	0
Entropy, $\Delta S$	$nC_{ m P} \ln \left( rac{T_{ m f}}{T_{ m i}}  ight)$	$nC_{ m V} \ln \left( rac{T_{ m f}}{T_{ m i}}  ight)$	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  $\Delta V$  or  $\Delta P$  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  $R_{\rm H} = 10973731.6~{\rm m}^{-1}$ :

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

Simplified Rydberg Equation, where  $R_{\infty} = 10973731.6~\mathrm{m}^{-1}$ :

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

de Broglie wavelength:

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

Formal charge:

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

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  $\theta$  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:

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

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:

% 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:

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

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

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

First-order decay:

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

Arrhenius equation:

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

Relationships of rate constants at two different temperatures:

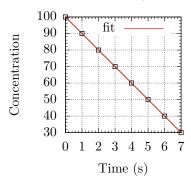
$$\ln \frac{k_1}{k_2} = \frac{E_{\rm a}}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_{\rm a}}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$

#### 9.1. Kinetics Data

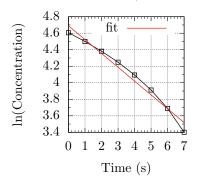
**Table 3:** Kinetics Data — 0th Order

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,  $R^2 = 0.89$ 

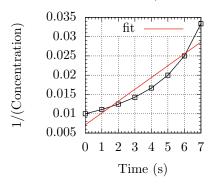
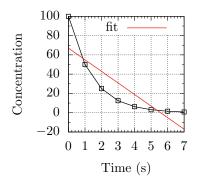


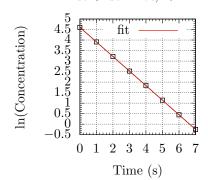
Table 4: Kinetics Data — 1st Order

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,  $R^2 = 0.72$ 

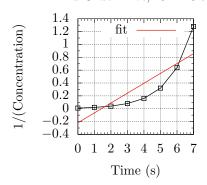
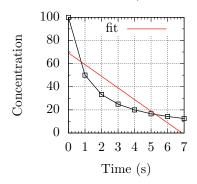


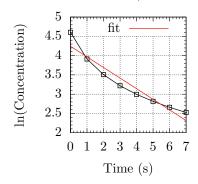
Table 5: Kinetics Data — 2nd Order

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

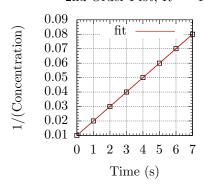
0th Order Plot,  $R^2 = 0.70$ 



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

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

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:

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

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

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

#### 11.2. Summations

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

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

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

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

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

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

# 12. Other

Mass defect:

$$\Delta m = \left[Z(m_{\rm p} + m_{\rm e}) + (A - Z)m_{\rm n}\right] - m_{\rm atom}$$

 Table 6: Values for mass defect equation.

Variable	Description	Value
$\Delta m$	mass defect	amu
$m_{ m p}$	mass of a proton	1.007277
$m_{ m n}$	mass of a neutron	1.008665
$m_{ m e}$	mass of an electron	0.000548597
$m_{ m atom}$	mass of nuclide	$_{Z}^{A}X$
Z	atomic number	number of protons
A	mass number	number of nucleons

Relationship between mass defect and energy released:

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