Common Equations Used in Chemistry

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Contents

1. Basic Conversions and Definitions

Converting °F to °C:

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

Converting °C to °F:

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

Converting °C to K:

$$K = °\mathrm{C} + 273.15$$

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]:

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

Freezing point depression:

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

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

Solvent	Normal Boiling (°C)	K_b (°C/m)	Normal Freezing (°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
Carbon tetrachloride	76.8	5.26	−22.62	31.4
Carbon disulfide	46.2	2.42	−112.1	3.74
Nitrobenzene	210.9	5.24	5.67	6.87
D-Camphor	207.4	4.91	178.8	37.8

Osmotic pressure:

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

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, $NaCl(s) \longrightarrow Na^+(aq) + Cl^-(aq)$, $i = 2$. 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 ($CaCl_2(s) \longrightarrow Ca^{2+}(aq) + 2Cl^-(aq)$).

3. Gases

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

$$PV = nRT$$

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:

$$P_{\mathrm{Tot}} = \chi_{\mathrm{A}} P_{\mathrm{A}}^{\star} + \chi_{\mathrm{B}} P_{\mathrm{Bb}}^{\star} + \ldots$$

For ionic solutes we include the van't Hoff factor i:

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

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

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

Rates of Effusion by Molar Mass

$$\frac{\mathrm{rate}_1}{\mathrm{rate}_2} = \sqrt{\frac{\mathcal{M}_2}{\mathcal{M}_1}}$$

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:

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

$$P = \frac{an^2(V - nb) - RTV^2}{V^2(nb - V)}$$

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:

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

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

Table 2: Summary of thermodynamic quantities under different conditions.

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

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

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:

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

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 $R_\infty = 2.18 \times 10^{-18}$ J:

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

Energy of a photon corresponding to an electron transition from the n_{i} shell to the n_{f} shell:

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

Or, using $R_\infty = 10973731.6$ m^{-1}:

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

de Broglie wavelength; if the particle size is much smaller than λ, then quantum rules are needed:

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

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:

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

Coulomb's law, where k_{e} is Coulomb's constant $k_{\text{e}} \approx 8.99 \times 10^9 \ \text{N}\,\text{m}^2\,\text{C}^{-2}$

$$F = k_{\text{e}}\frac{q_1 q_2}{r^2}$$

cf. Newton's law of gravitation, where G is the universal gravitational constant, $6.674 \times 10^{-11} \ \text{m}^3\,\text{kg}^{-1}\,\text{s}^{-2}$

$$F = G\frac{m_1 m_2}{r^2}$$

6. Quantum Mechanics

Heisenberg Uncertainty Principle, Δx is the minimum "size of a box" for a particle:

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

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:

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

Potential energy between two charged bodies:

$$V = k\frac{q_1q_2}{r}$$

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 $F = 96485$ coulomb/mol:

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

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 $= k$	$[\mathrm{A}]_t - [\mathrm{A}]_0 = -kt$	$[\mathrm{A}]_t = -kt + [\mathrm{A}]_0$
1	rate $= k[\mathrm{A}]$	$\ln \frac{[\mathrm{A}]_t}{[\mathrm{A}]_0} = -kt$	$\ln [\mathrm{A}]_t = -kt + \ln [\mathrm{A}]_0$
2	rate $= k[\mathrm{A}]^2$	$\frac{1}{[\mathrm{A}]_t} - \frac{1}{[\mathrm{A}]_0} = kt$	$\frac{1}{[\mathrm{A}]_t} = kt + \frac{1}{[\mathrm{A}]_0}$

Order	Half-life	Alternate Form
0	$t_{1/2} = \frac{[\mathrm{A}]_0}{2k}$	
1	$t_{1/2} = \frac{\ln 2}{k}$	$\ln \frac{[\mathrm{A}]_t}{[\mathrm{A}]_0} = (-\ln 2)\left(\frac{t}{t_{1/2}}\right)$
2	$t_{1/2} = \frac{1}{k[\mathrm{A}]_0}$	

Arrhenius equation:

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

Arrhenius equation for different rate constants for different E_a at constant T:

$$\ln\left(\frac{k_2}{k_1}\right) = \left(\frac{1}{RT}\right)(-E_{\mathrm{a}_2} + E_{\mathrm{a}_1})$$

Relationships of rate constants at two different temperatures:

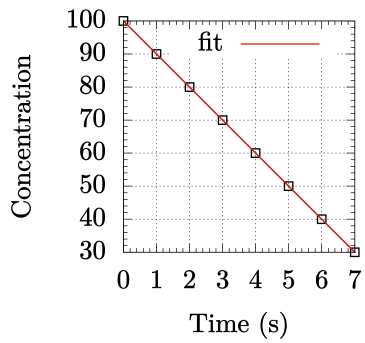
$$\ln \frac{k_1}{k_2} = \frac{E_\mathrm{a}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \frac{-E_\mathrm{a}}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

9.1. Kinetics Data

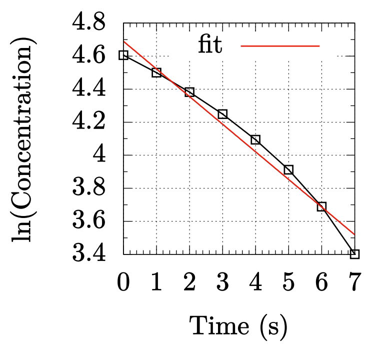
Table 3: Kinetics Data — 0th Order

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, $R^2 = 0.89$

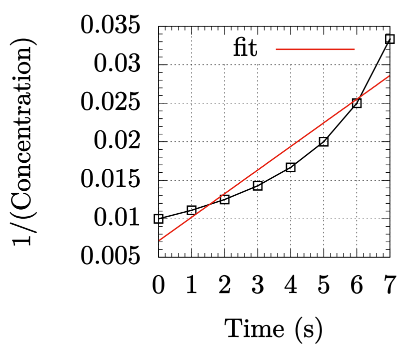
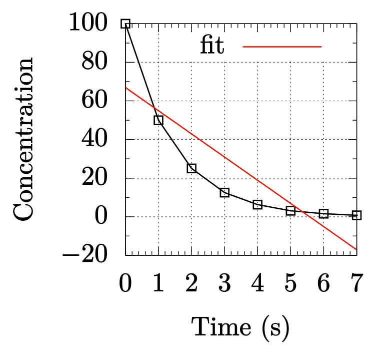


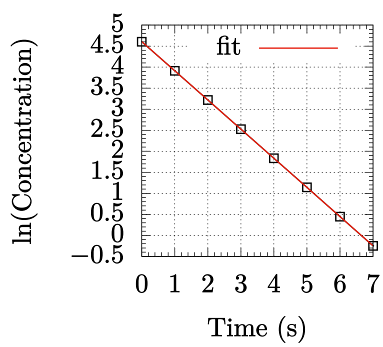
Table 4: Kinetics Data — 1st Order

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

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



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



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

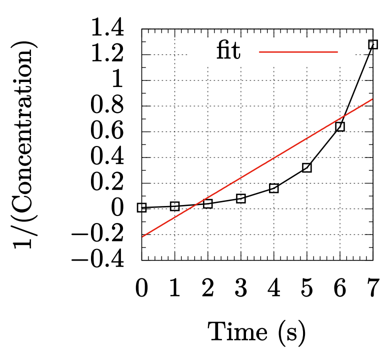
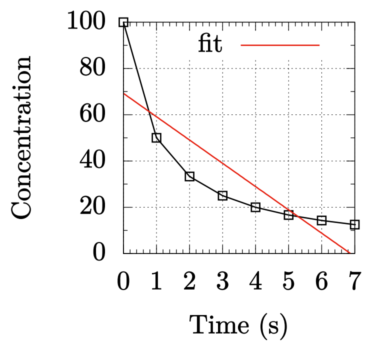


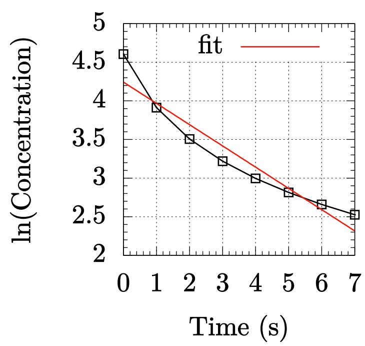
Table 5: Kinetics Data — 2nd Order

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

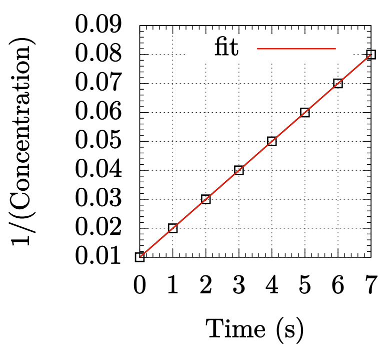
0th Order Plot, $R^2 = 0.70$



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

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

van't Hoff Equation

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

Relationship between equilibrium constants for aqueous systems and for gases:

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

Ion product of water:

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

The Quadratic Formula: for a quadratic equation $ax^2 + bx + c = 0$, the solutions x are:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

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:

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

Arrhenius Equation:

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

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_{sp} and entropy, plot $\ln K_{\mathrm{sp}}$ vs. $1/T$:

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

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

11.2. Summations

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

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

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

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

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

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

12. Statistics

Arithmetic mean (average):

$$\overline{x} = \frac{\sum_i (x_i)}{n}$$

Standard deviation:

$$\sigma = \sqrt{\frac{\sum_i (x_i - \overline{x})^2}{n-1}}$$

x_i	$x_i - \overline{x}$	$(x_i - \overline{x})^2$	$\sum(x_i - \overline{x})^2$	σ
0.685	0.003	0.000009		
0.676	−0.006	0.000036		
0.669	−0.013	0.000169		
0.688	0.006	0.000036		
0.692	0.010	0.000100		
$n = 5$			0.00035	0.0094

Confidence interval (true mean), see end of document for t values.

$$\mu = \overline{x} \pm \frac{t\sigma}{\sqrt{n}}$$

Outliers (Grubbs' Test): If $G > G_{\text{ref}}$ then x_i can be considered an outlier. See end of document for G values.

$$G = \frac{|x_i - \overline{x}|}{\sigma}$$

13. Nuclear Decay and Mass Defect

Mass defect:

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

Table 6: Values for mass defect equation.

Variable	Description	Value
Δm	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_{atom}	mass of nuclide	${}^{A}_{Z}X$
Z	atomic number	number of protons
A	mass number	number of nucleons

Relationship between mass defect and energy released:

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

14. Acidities

Acid	Conj. Base	pK_a	Remarks	
HI	I^-	-10	hydroiodic acid	strong acids
HBr	Br^-	-9	hydrobromic acid	
H_2SO_4	HSO_4^-	-9	sulfuric acid	
HCl	Cl^-	-7	hydrochloric acid	
H_3O^+	H_2O	-2	hydronium	
HNO_3	NO_3^-	-1	nitric acid	
HSO_4^-	SO_4^{2-}	2	2nd H of sulfuric acid	weak acids
HF	F^-	3	hydrofluoric acid	
$RCOOH$	$RCOO^-$	4	carboxylic acids	
H_2S	HS^-	7	compare to H_2O	
NH_4^+	NH_3	9	ammonium	
HCN	NC^-	9.2	nitriles	
$PhOH$	PhO^-	10	phenols[a]	
H_2O	HO^-	15.7	water[b]	
ROH	RO^-	16	aliphatic alcohols[c]	
$RC(O)NH_2$	$RC(O)NH^-$	17	amides	
$RC(O)CH_3$	$RC(O)CH_2^-$	20	α H of ketones	
$PhNH_2$	$PHNH^-$	25	aniline[d]	
$RC{\equiv}CH$	$RC{\equiv}C^-$	25	terminal alkyne (*sp* C—H)	
H_2	H^-	36	hydrogen gas	
NH_3	NH_2^-	38	ammonia	
RNH_2	RNH^-	40	aliphatic amines	
$PhCH_3$	$PhCH_2^-$	41	benzylic (sp^3 C—H)	
C_6H_6	$C_6H_5^-$	42	aryl (sp^2 C—H)	
$H_2C{=}CHCH_3$	$H_2C{=}CHCH_2^-$	43	allylic (sp^3 C—H)	
$RCH{=}CH_2$	$RCH{=}CH^-$	47	vinylic (sp^2 C—H)	
RCH_3	RCH_2^-	50	alkanes (sp^3 C—H)	

Footnotes:

[a] depending on the substitution of Ph, pK_a can vary from 4–11

[b] water is amphoteric, so anything less acidic than water can act as a base in aqueous solution

[c] depending on the substitution of R, pK_a can vary from 15–17

[d] depending on the substitution of Ph, pK_a can vary from 18–28

A conjugate base can deprotonate any acid higher than it on this table.

15. Compound Units

- joule = coulomb $\times$ volt
- joule = kg $\times$ m^2 / s^2
- watt = joule / sec
- kilowatt = 1000 joules / sec
- kilowatt-hour = (1000 joules / sec) $\times$ 3600 sec = 3.6×10^6 joules
- amp = coulomb / second
- 1000 milliamp-hour = 1 amp-hour = 3600 amp-seconds = 3600 coulombs

Standand Enthalpies of Formation & Standard Entropies of Common Compounds

Substance	*State*	ΔH_f° $\left(\frac{\text{kJ}}{\text{mol}}\right)$	S° $\left(\frac{\text{J}}{\text{mol}\cdot\text{K}}\right)$
Ag	s	0	42.6
Ag^{+}	aq	105.79	72.7
AgCl	s	−127.01	96.2
AgBr	s	−100.4	107.1
$AgNO_3$	s	−124.4	140.9
Al	s	0	28.3
Al^{+3}	aq	−538.4	−321.7
$AlCl_3$	s	−704	110.7
Al_2O_3	s	−1675.7	50.9
Ba	s	0	62.8
$BaCl_2$	s	−858.6	123.7
$BaCO_3$	s	−1216.3	112.1
$Ba(NO_3)_2$	s	−992	214
BaO	s	−553.5	70.4
$Ba(OH)_2$	s	−998.2	112
$BaSO_4$	s	−1473.2	132.2
Br_2	ℓ	0	152.2
C	s	0	5.7
CCl_4	ℓ	−135.4	216.4
$CHCl_3$	ℓ	−134.5	201.7
CH_4	g	−74.8	186.2
C_2H_2	g	+226.7	200.8
C_2H_4	g	+52.3	219.5
C_2H_6	g	−84.7	229.5
C_3H_8	g	−103.8	269.9
CH_3OH	ℓ	−238.7	126.8
C_2H_5OH	ℓ	−277.7	160.7
CO	g	−110.53	197.6
CO_2	g	−393.51	213.6
${CO_3}^{-2}$	aq	−675.23	−56.9
Ca	s	0	41.4
Ca^{+2}	aq	−543.0	−53.1
$CaCl_2$	s	−795.8	104.6
$CaCO_3$	s	−1206.9	92.9
CaO	s	−634.92	39.8
$Ca(OH)_2$	s	−986.1	83.4
$CaSO_4$	s	−1434.1	106.7
Cd	s	0	51.8
Cd^{+2}	aq	−75.92	−73.2
$CdCl_2$	s	−391.5	115.3
CdO	s	−258.35	54.8

Substance	*State*	ΔH_f° $\left(\frac{\text{kJ}}{\text{mol}}\right)$	S° $\left(\frac{\text{J}}{\text{mol}\cdot\text{K}}\right)$
Cl_2	g	0	223.0
Cl^{-}	aq	−167.080	56.5
${ClO_4}^{-}$	aq	−128.10	182.0
Cr	s	0	23.8
Cr_2O_3	g	−1139.7	81.2
Cu	s	0	33.2
Cu^{+}	aq	+71.7	40.6
Cu^{+2}	aq	+64.8	−99.6
CuO	s	−157.3	42.6
Cu_2O	s	−168.6	93.1
CuS	s	−53.1	66.5
Cu_2S	s	−79.5	120.9
$CuSO_4$	s	−771.4	107.6
F^{-}	aq	−335.35	−13.8
F_2	g	0	202.7
Fe	s	0	27.3
$Fe(OH)_3$	s	−823.0	106.7
Fe_2O_3	s	−824.2	87.4
Fe_3O_4	s	−1118.4	146.4
H_2	g	0	130.6
H^{+}	aq	0	0.0*
HBr	g	−36.29	198.6
${HCO_3}^{-}$	aq	−689.93	91.2
HCl	g	−92.31	186.8
HF	g	−273.30	173.7
HI	g	26.50	206.5
HNO_3	ℓ	−174.1	155.6
${HPO_4}^{-2}$	aq	−1299.0	−33.5
${HSO_4}^{-}$	aq	−886.9	131.8
H_2O	ℓ	−285.830	69.9
H_2O	g	−241.826	188.7
$H_2{PO_4}^{-}$	aq	−1302.6	90.4
H_2S	g	−20.6	205.7
Hg	ℓ	0	76.0
Hg^{+2}	aq	170.21	−32.2
HgO	cr,red	−90.79	70.3

*The standard entropy of the $H^{+}(aq)$ ion is defined to be 0.

Substance	*State*	ΔH_f° $\left(\frac{kJ}{mol}\right)$	S° $\left(\frac{J}{mol \cdot K}\right)$
I^-	aq	−56.78	111.3
I_2	s	0	116.1
K	s	0	64.2
K^+	aq	−252.14	102.5
KBr	s	−393.8	95.9
KCl	s	−436.7	82.6
$KClO_3$	s	−397.7	143.1
$KClO_4$	s	−432.8	151.0
KNO_3	s	−494.6	133.0
Mg	s	0	32.7
Mg^{+2}	aq	−467.0	−138.1
$MgCl_2$	s	−641.3	89.6
$MgCO_3$	s	−1095.8	65.7
MgO	s	−601.60	26.9
$Mg(OH)_2$	s	−924.5	63.2
$MgSO_4$	s	−1284.9	91.6
Mn	s	0	32.0
Mn^{+2}	aq	−220.8	−73.6
MnO	s	−385.2	59.7
MnO_2	s	−520.0	53.0
N_2	g	0	191.5
NH_3	g	−45.94	192.3
${NH_4}^+$	aq	−133.26	113.4
${NO_2}^-$	aq	−104.6	123.0
${NO_3}^-$	aq	−206.85	146.4
N_2H_4	ℓ	+50.6	121.2
NH_4Cl	s	−314.4	94.6
NH_4NO_3	s	−365.6	151.1
NO	g	+90.2	210.7
NO_2	g	+33.2	240.0
N_2O_4	g	+9.2	304.2
Na	s	0	51.2
Na^+	aq	−240.34	59.0
NaCl	s	−411.2	72.1
NaF	s	−573.6	51.5
NaOH	s	425.6	64.5

Substance	*State*	ΔH_f° $\left(\frac{kJ}{mol}\right)$	S° $\frac{J}{mol\ K}$
Ni	s	0	29.9
NiO	s	−239.7	38.0
OH^-	aq	−230.015	−10.8
O_2	g	0	205.0
P_4	s	0	164.4
PCl_3	g	−287.0	311.7
PCl_5	g	−374.9	364.5
${PO_4}^{-3}$	aq	−1277.4	−222
Pb	s	0	64.8
Pb^{+2}	aq	0.92	10.5
$PbBr_2$	s	−278.7	161.5
$PbCl_2$	s	−359.4	136.0
PbO	s	−219.0	66.5
PbO_2	s	−277.4	68.6
S	s	0	31.8
SO_2	g	−296.81	248.1
SO_3	g	−395.7	256.7
${SO_4}^{-2}$	aq	−909.34	20.1
${S_2}^-$	aq	+33.1	−14.6
Si	s	0	18.8
SiO_2	s	−910.7	41.8
Sn	s	0	51.6
Sn^{+2}	aq	−8.9	−17.4
SnO_2	s	−577.63	52.3
Zn	s	0	41.6
Zn^{+2}	aq	−153.39	−112.1
ZnI_2	s	−208.0	161.1
ZnO	s	−350.46	43.6
ZnS	s	−206.0	57.7

TABLE 9.3 Average Bond Energies

Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)
H—H	436	N—N	163	Br—F	237
H—C	414	N=N	418	Br—Cl	218
H—N	389	N≡N	946	Br—Br	193
H—O	464	N—O	222	I—Cl	208
H—S	368	N=O	590	I—Br	175
H—F	565	N—F	272	I—I	151
H—Cl	431	N—Cl	200	Si—H	323
H—Br	364	N—Br	243	Si—Si	226
H—I	297	N—I	159	Si—C	301
C—C	347	O—O	142	S—O	265
C=C	611	O=O	498	Si=O	368
C≡C	837	O—F	190	S=O	523
C—N	305	O—Cl	203	Si—Cl	464
C=N	615	O—I	234	S=S	418
C≡N	891	F—F	159	S—F	327
C—O	360	Cl—F	253	S—Cl	253
C=O	736*	Cl—Cl	243	S—Br	218
C≡O	1072			S—S	266
C—Cl	339				

*799 in CO_2

TABLE 10.4 Van der Waals Constants for Common Gases

Gas	a ($L^2 \cdot atm/mol^2$)	b (L/mol)
He	0.0342	0.02370
Ne	0.211	0.0171
Ar	1.35	0.0322
Kr	2.32	0.0398
Xe	4.19	0.0511
H_2	0.244	0.0266
N_2	1.39	0.0391
O_2	1.36	0.0318
Cl_2	6.49	0.0562
H_2O	5.46	0.0305
CH_4	2.25	0.0428
CO_2	3.59	0.0427
CCl_4	20.4	0.1383

Values of Grubbs Statistic (G)

Number of Observations n	Confidence Level (%)					
	99.9	99.5	99	97.5	95	90
3	1.155	1.155	1.155	1.155	1.153	1.148
4	1.499	1.496	1.492	1.481	1.463	1.425
5	1.780	1.764	1.749	1.715	1.672	1.602
6	2.011	1.973	1.944	1.887	1.822	1.729
7	2.201	2.139	2.097	2.020	1.938	1.828
8	2.358	2.274	2.221	2.126	2.032	1.909
9	2.492	2.387	2.323	2.215	2.110	1.977
10	2.606	2.482	2.410	2.290	2.176	2.036
11	2.705	2.564	2.485	2.355	2.234	2.088
12	2.791	2.636	2.550	2.412	2.285	2.134
13	2.867	2.699	2.607	2.462	2.331	2.175
14	2.935	2.755	2.659	2.507	2.371	2.213
15	2.997	2.806	2.705	2.549	2.409	2.247
16	3.052	2.852	2.747	2.585	2.443	2.279
17	3.103	2.894	2.785	2.620	2.475	2.309
18	3.149	2.932	2.821	2.651	2.504	2.335
19	3.191	2.968	2.854	2.681	2.532	2.361
20	3.230	3.001	2.884	2.709	2.557	2.385
30	3.507	3.236	3.103	2.908	2.745	2.563
40	3.673	3.381	3.240	3.036	2.866	2.682
50	3.789	3.483	3.336	3.128	2.956	2.768
60	3.874	3.560	3.411	3.199	3.025	2.837
70	3.942	3.622	3.471	3.257	3.082	2.893
80	3.998	3.673	3.521	3.305	3.130	2.940
90	4.044	3.716	3.563	3.347	3.171	2.981
100	4.084	3.754	3.600	3.383	3.207	3.017

Source: ASTM E178-00, “Standard Practice for Dealing with Outlying Observations”

Values of Student's t

Degrees of Freedom	Confidence Level (%)						
	50	90	95	97.5	99	99.5	99.9
1	1.000	6.314	12.706	25.452	63.657	127.321	636.619
2	0.816	2.920	4.303	6.205	9.925	14.089	31.599
3	0.765	2.353	3.182	4.177	5.841	7.453	12.924
4	0.741	2.132	2.776	3.495	4.604	5.598	8.610
5	0.727	2.015	2.571	3.163	4.032	4.773	6.869
6	0.718	1.943	2.447	2.969	3.707	4.317	5.959
7	0.711	1.895	2.365	2.841	3.499	4.029	5.408
8	0.706	1.860	2.306	2.752	3.355	3.833	5.041
9	0.703	1.833	2.262	2.685	3.250	3.690	4.781
10	0.700	1.812	2.228	2.634	3.169	3.581	4.587
11	0.697	1.796	2.201	2.593	3.106	3.497	4.437
12	0.695	1.782	2.179	2.560	3.055	3.428	4.318
13	0.694	1.771	2.160	2.533	3.012	3.372	4.221
14	0.692	1.761	2.145	2.510	2.977	3.326	4.140
15	0.691	1.753	2.131	2.490	2.947	3.286	4.073
16	0.690	1.746	2.120	2.473	2.921	3.252	4.015
17	0.689	1.740	2.110	2.458	2.898	3.222	3.965
18	0.688	1.734	2.101	2.445	2.878	3.197	3.922
19	0.688	1.729	2.093	2.433	2.861	3.174	3.883
20	0.687	1.725	2.086	2.423	2.845	3.153	3.850
30	0.683	1.697	2.042	2.360	2.750	3.030	3.646
40	0.681	1.684	2.021	2.329	2.704	2.971	3.551
50	0.679	1.676	2.009	2.311	2.678	2.937	3.496
60	0.679	1.671	2.000	2.299	2.660	2.915	3.460
70	0.678	1.667	1.994	2.291	2.648	2.899	3.435
80	0.678	1.664	1.990	2.284	2.639	2.887	3.416
90	0.677	1.662	1.987	2.280	2.632	2.878	3.402
100	0.677	1.660	1.984	2.276	2.626	2.871	3.390
∞	0.674	1.645	1.960	2.241	2.576	2.807	3.291

Values for the F Statistic at the 95% Confidence Level

Degrees of Freedom (denominator)	Degrees of Freedom (numerator)										
	2	3	4	5	6	7	8	9	10	20	∞
2	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.45	19.50
3	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.66	8.53
4	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.80	5.63
5	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74	4.56	4.36
6	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06	3.87	3.67
7	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64	3.44	3.23
8	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35	3.15	2.93
9	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14	2.94	2.71
10	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98	2.77	2.54
20	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35	2.12	1.84
∞	3.00	2.60	2.37	2.21	2.10	2.01	1.94	1.88	1.83	1.57	1.00

Values for the F Statistic at the 90% Confidence Level

Degrees of Freedom (denominator)	Degrees of Freedom (numerator)										
	2	3	4	5	6	7	8	9	10	20	∞
2	9.00	9.16	9.24	9.29	9.33	9.35	9.37	9.38	9.39	9.44	9.49
3	5.46	5.39	5.34	5.31	5.28	5.27	5.25	5.24	5.23	5.18	5.13
4	4.32	4.19	4.11	4.05	4.01	3.98	3.95	3.94	3.92	3.84	3.76
5	3.78	3.62	3.52	3.45	3.40	3.37	3.34	3.32	3.30	3.21	3.10
6	3.46	3.29	3.18	3.11	3.05	3.01	2.98	2.96	2.94	2.84	2.72
7	3.26	3.07	2.96	2.88	2.83	2.78	2.75	2.72	2.70	2.59	2.47
8	3.11	2.92	2.81	2.73	2.67	2.62	2.59	2.56	2.54	2.42	2.29
9	3.01	2.81	2.69	2.61	2.55	2.51	2.47	2.44	2.42	2.30	2.16
10	2.92	2.73	2.61	2.52	2.46	2.41	2.38	2.35	2.32	2.20	2.06
20	2.59	2.38	2.25	2.16	2.09	2.04	2.00	1.96	1.94	1.79	1.61
∞	2.30	2.08	1.94	1.85	1.77	1.72	1.67	1.63	1.60	1.42	1.00