1 Stoichiometry

Proposition 1.1: Solubility Rules

- 1. Alkali metal/ammonium (NH_4^+) salts, and nitrate $(NO_3^-)/acetate$ (CH_3COO^-) salts are always soluble.
- 2. Chlorides, bromides, iodides are soluble except those of silver, mercury, and lead.
- 3. Sulfates $(SO_4^{\ 2^-})$ are soluble except those of silver, mercury, lead, calcium, strontrium, and barium.

Proposition 1.2: Strong Acids/Bases

-	Acids	Bases
	HCl	Group 1 hydroxides
	HBr	Group 2 hydroxides
	HI	NH_3
F	HClO ₄	${\rm Hydride}\ {\rm H}^-$
F	HBrO_4	Oxide O_2^-
F	H_2SO_4	
I	HNO_3	

2 The Periodic Table and Green Chemistry

Definition 2.1: Atomic Masses

The **atomic mass interval** is used for certain elements to indicate the range of values expected for the atomic mass because of observed variations in the isotopic abundances of these elements.

The **conventional atomic mass** is provided for elements having their atomic masses defined in terms of an atomic mass interval and may be used in situations when a representative value of the atomic mass is required.

Definition 2.2: Atom Economy

$$\%$$
 atom economy = $\frac{\text{stoichiometric mass of desired product}}{\text{stoichiometric mass of reactants}} \times 100\%$

Definition 2.3: E-factor

$$E-factor = \frac{mass\ of\ waste\ produced}{mass\ of\ product\ produced}$$

Remark. Water is not considered waste.

3 The H-Atom

Theorem 3.1: Wavelength-frequency relation

$$c = \lambda \nu$$

Definition 3.2: Electromagnetic spectrum

From highest energy to lowest energy:

 γ rays, x-rays, ultraviolet, visible light, infrared, microwave, radiowave

Theorem 3.3: Photoeletric effect

$$E = \frac{hc}{\lambda} \qquad (KE)_{e^{-}} = E - w$$

Theorem 3.4: Line spectra

$$E_n = R_H \frac{1}{n^2}$$

Theorem 3.5: de Broglie Wavelength

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

Theorem 3.6: Heisenberg Uncertainty Principle

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

where Δx is uncertainty in position and Δp is uncertainty in momentum.

Definition 3.7: Quantum Numbers

n	ℓ	m_ℓ	m_s
Principal	Azimuthal/orbital angular momentum	Magnetic	Spin
$n \in \mathbb{N}$	$\ell \in \{0,\ldots,n-1\}$	$ m_{\ell} \le \ell$	$m_s = \pm \frac{1}{2}$

Proposition 3.8: Radial Functions

Definition 3.9: Radial Factor R(r)

- 1. n = 0 has an asymptote at x = 0
- 2. $n \ell 1$ radial nodes

Definition 3.10: Radial Electron Density $R(r^2)$

- 1. Probability of finding the electron as we move away from the nucleus in a fixed direction
- 2. Bumps decreases in magnitude
- 3. n = 0 has an asymptote at x = 0
- 4. $n \ell 1$ radial nodes
- 5. $n \ell$ maxima

Definition 3.11: Radial Distribution Function $r^2R(r^2)$

- 1. Bumps increase in magnitude
- 2. The maximum on the graph, r_{mp} , is the most probable distance between the electron and the nucleus
 - (a) r_{mp} increases as n increases
 - (b) For a fixed n, r_{mp} decreases as ℓ increases
- 3. All *n* values are 0 at x = 0
- 4. $n-\ell-1$ radial nodes
- 5. $n \ell$ maxima

4 Multielectron Atoms

Proposition 4.1: Ground State Electron Configurations

Definition 4.2: Pauli Exclusion Principle

No two electrons can have the same set of quantum numbers n, ℓ, m_{ℓ} , and m_s .

Definition 4.3: Aufbau Process

Orbitals are filled by the $n + \ell$ rule (diagonal chart meme).

Remark. The exceptions to this rule are $Cr = [Ar]3d^54s^1$ and $Cu = [Ar]3d^{10}4s^1$.

Definition 4.4: Hund's Rule

If there are not enough electrons to complete a set of energetically degenerate orbitals, the lowest energy arrangement is the one which has the maximum number of parallel spins.

Remark. For ions, negative ions are trivial. For positive ions, remove from the highest n value after obtaining the atomic ground state.

Definition 4.5: Paramagnetism and Diamagnetism

Paramagnetic atoms have one or more unpaired electron.

Diamagnetic atoms have all paired electrons.

Proposition 4.6: Periodic Trends

Increase down and left:

- 1. Atomic radii
- 2. Metallic character
- 3. Polarizability

Increase up and right:

- 1. Ionization energy
- 2. Electron affinity
- 3. Electronegativity
- 4. Non-metallic character

5 Bonding

Definition 5.1: Oxidation State and Formal Charge

Oxidation state: the charge an atom would have if all the bonding electrons were transferred to the most electronegative atoms in the bond.

Formal charge: the charge an atom would have if all bonding electrons were shared equally.

Theorem 5.2: Dipole Moments

Magnitude of dipole moment is given by

$$\mu = |\delta| r$$
.

If a bond is completely ionic, $\delta = e$. Percent ionic character is given by the extent to which observed dipole moments relate to theoretical ionic dipole moments.

6 VB and MO Theory

Proposition 6.1: Molecular Orbital Theory

Orbitals are filled from bottom to top as follows:

$\mathrm{Li},\ldots,\mathrm{N}$	O, F
σ_{2p}^*	σ_{2p}^*
π_{2p}^*	π_{2p}^*
$\sigma_{\mathbf{2p}}$	$\pi_{\mathbf{2p}}$
$\pi_{\mathbf{2p}}$	$\sigma_{\mathbf{2p}}$
σ_{2s}^*	σ_{2s}^*
σ_{2s}	σ_{2s}

The change from N to O is the result of **s-p mixing**, where the smaller atoms have smaller gaps between orbitals so σ_{2p} is pushed upwards in energy past π_{2p} and is filled afterwards.

Theorem 6.2: Bond Order

$$BO = \frac{1}{2}(n_b - n_a)$$

where n_b and n_a are the number of electrons in bonding and antibonding orbitals, respectively.

7 Real/Ideal Gases and IMFs

Proposition 7.1: Assumptions of Kinetic Molecular Theory

- 1. Molecules of gas are tiny and very far apart.
- 2. Molecules are in constant, random motion.
- 3. Molecules collide with each other and the walls of the container with perfect elasticity.
- 4. Molecules exert no attractive/repulsive forces on each other.
- 5. $KE_{avg} \propto T$.

Theorem 7.2: Ideal Gas Law

$$PV = nRT$$

Theorem 7.3: Partial Pressure

The sum of the partial pressures of each gas in a mixture is equal to the total pressure.

Remark. When collecting gas over water, remember to correct for the vapour pressure of water.

Theorem 7.4: Average and Root-mean-square Speed

$$v_{avg} = \sqrt{\frac{8RT}{\pi \mathcal{M}}}$$
 $v_{rms} = \sqrt{\frac{3RT}{\mathcal{M}}}$

A molecule moving with speed v_{rms} has a kinetic energy equal to the average kinetic energy.

Theorem 7.5: Graham's Law of Effusion

$$\frac{\text{rate}_x}{\text{rate}_y} = \sqrt{\frac{\mathcal{M}_y}{\mathcal{M}_x}}$$

Theorem 7.6: Van der Waals Equation

$$(P + a\frac{n^2}{V^2})(V - nb) = nRT$$

where a is a measure of the strength of intermolecular forces and b is a measure of molecule size.

Proposition 7.7: Stronger Intermolecular Forces

- 1. Lower vapour pressure
- 2. Higher boiling point
- 3. Greater surface tension
- 4. Greater viscosity