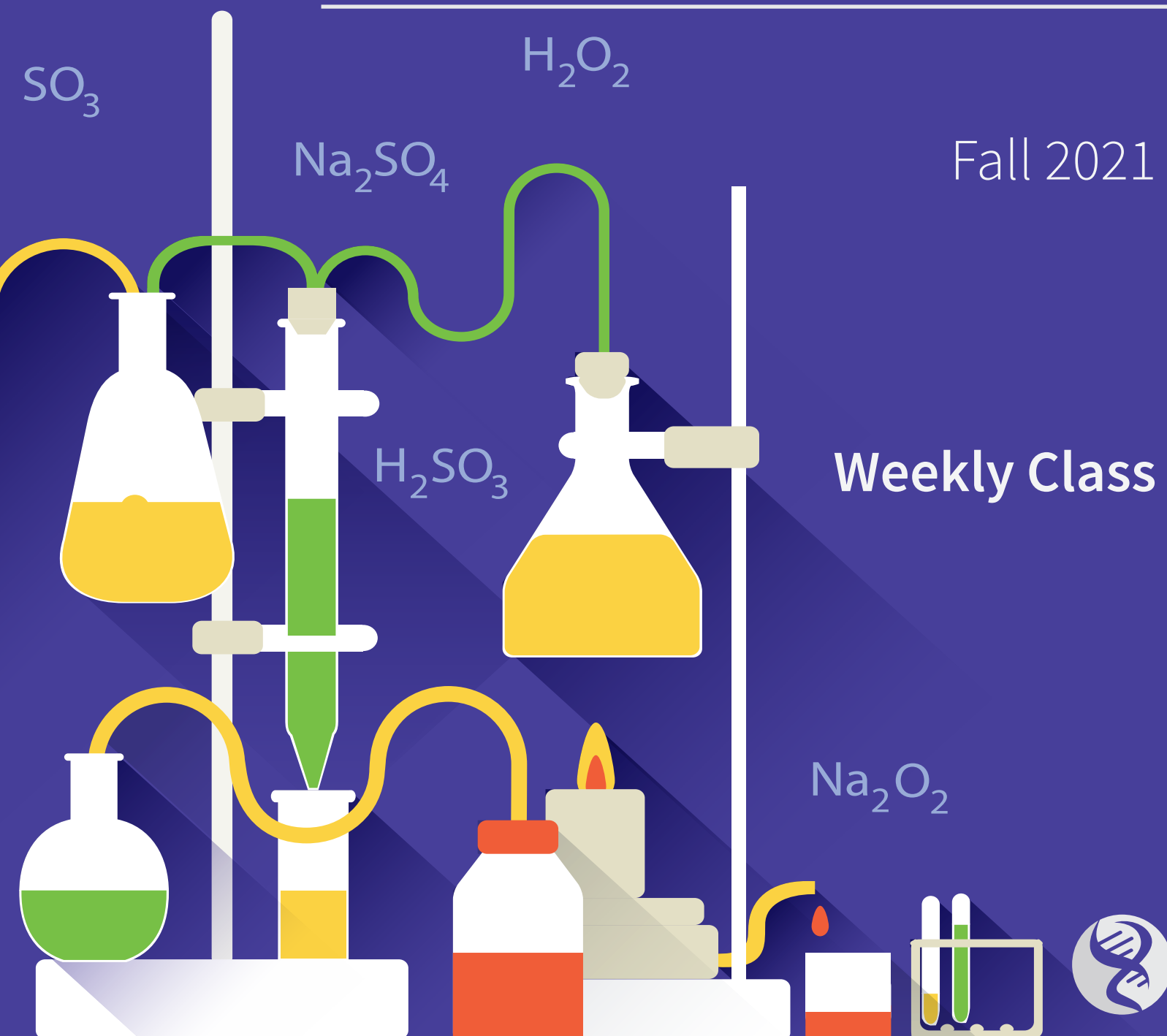




CHM135H:

Chemistry - Physical Principles





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Week 1-2

FUNDAMENTALS

- 1 Measurements
- 1 Model of Atom
- 2 Chemical Bonds
- 3 Chemical Formula

STIOCHIOMETRY

- 3 Mole
- 4 Dilution

QUANTUM MECHANICS

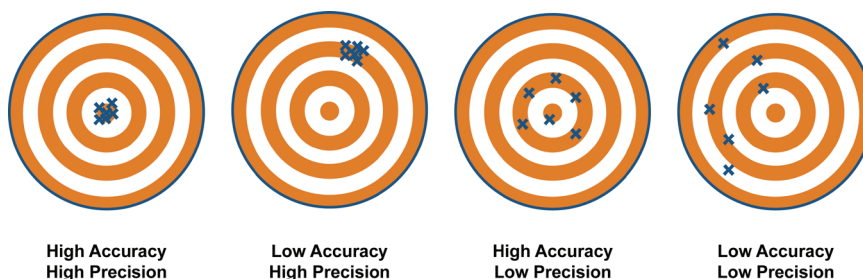
- 5 Electromagnetic Radiation
- 6 Energy of a Single Photon
- 6 Photoelectric Effect
- 7 Bohr Model of the Atom
- 8 Matter Wave
- 8 Uncertainty Principle
- 8 Wave Equation
- 9 Quantum Number and Orbitals
- 9 Electron Configuration
- 10 Shielding Effect of Electrons

PRACTICE

FUNDAMENTALS

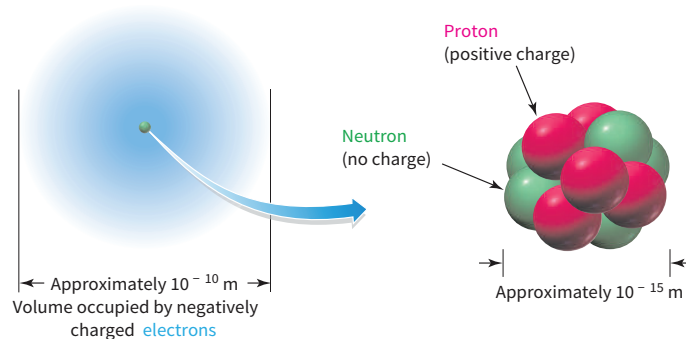
MEASUREMENTS

1. Measurement always comes with errors
 - a. Significant figure: use scientific notation.
 - b. When you are using a tool, estimate 1 significant figure followed by the max significant figure that the tool can report.
2. Precision & Accuracy
 - a. Precision: \uparrow Precision - \downarrow Standard deviation (Data points less spread)
 - b. Accuracy: \uparrow Accuracy - \downarrow Error to the true value (Measurement - True value)

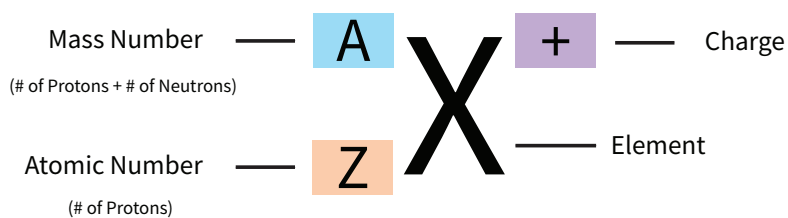


MODEL OF ATOM

1. Atomic Structure
 - a. Nucleus: +ve charge \rightarrow Responsible for Mass



- i. Proton: 1 +ve charge
- ii. Neutron: uncharged \rightarrow **Isotopes (Different number of neutrons)**
- b. Electron cloud: -ve charge \rightarrow Responsible for Volume
 - i. Electron: 1 -ve charge
- c. Atomic symbol



2. Mass of atom
 - a. Atomic mass unit (amu) = 1.66×10^{-24} g
 - b. Definition: $^{12}\text{C} = 12.0000$ amu
 - c. Proton and neutron have similar mass.
 - d. Mass of electron is negligible.
 - e. The atomic mass shown in the periodic table is averaged atomic mass according to the isotope abundance.

$$\text{Average Mass} = \sum_i (\text{Fractional Abundance} \times \text{Isotopic Mass})_i$$

3. Columns & Rows in periodic table
 - a. Elements in the same column will have similar properties because of the same number of valence electrons.
 - b. Rows are organized by filling the valence shell electrons.

TEST QUESTIONS

1. How many protons (p), neutrons (n), and electrons (e) are in one atom of $^{207}_{82}\text{Pb}^{2+}$?
 - a. 82 p, 125 n, 82 e
 - b. 84 p, 127 n, 82 e
 - c. 82 p, 125 n, 80 e
 - d. 84 p, 125 n, 84 e
 - e. 82 p, 123 n, 80 e

2. Lithium has two naturally occurring isotopes, ^6Li (isotopic mass = 6.015121 amu) and ^7Li (isotopic mass = 7.016003 amu). Lithium has an atomic mass of 6.9409 amu. What is the percent abundance of lithium-6?
 - a. 92.50%
 - b. 86.66%
 - c. 46.16%
 - d. 7.503%
 - e. 6.080%

CHEMICAL BONDS

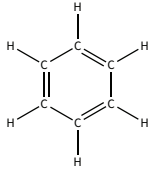
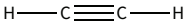
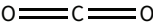
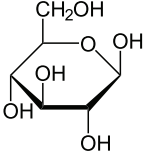
1. Collision is required to form a new chemical bond.
 - a. Model: Kinetic Energy vs. Repulsion
2. Types of chemical bonds:
 - a. **Ionic** – electron is drawn to one atom resulting in an attraction.
 - i. Example: NaCl, KCl
 - b. **Covalent** – electrons are shared between two atoms.
 - i. Example: H₂, H₂O, Methane.



CHEMICAL FORMULA

1. Empirical formula
 - a. Empirical formula indicates the **ratios** of the various elements present in a particular compound without regard to the actual numbers.
 - b. Different compounds may have the same empirical formula.
2. Molecular formula
 - a. Molecular formula indicates the **number of atoms of each element** present in a particular compound.
 - b. Isomers will have the same molecular formula.
3. Structural formula
 - a. Structural formula not only indicate the number of atoms of each element but also the **connection** between each atom.
 - b. Stereoisomers will have the same structural formula if the wedge and dash bonds are not used.

Summary: Comparison of different chemical formula

Name	Empirical	Molecular	Structural
Benzene	CH	C ₆ H ₆	
Ethyne	CH	C ₂ H ₂	
Carbon Dioxide	CO ₂	CO ₂	
Glucose	C ₆ H ₁₂ O ₆	CH ₂ O	

STOICHIOMETRY

MOLE

1. Notation of number of particle.
 - a. 1 mol = 6.02×10^{23} particle (Avogadro's number) with unit mol⁻¹.
 - b. Common units:
 - i. Number of particle: mol.
 - ii. Concentration: mol/L → M (Molarity).

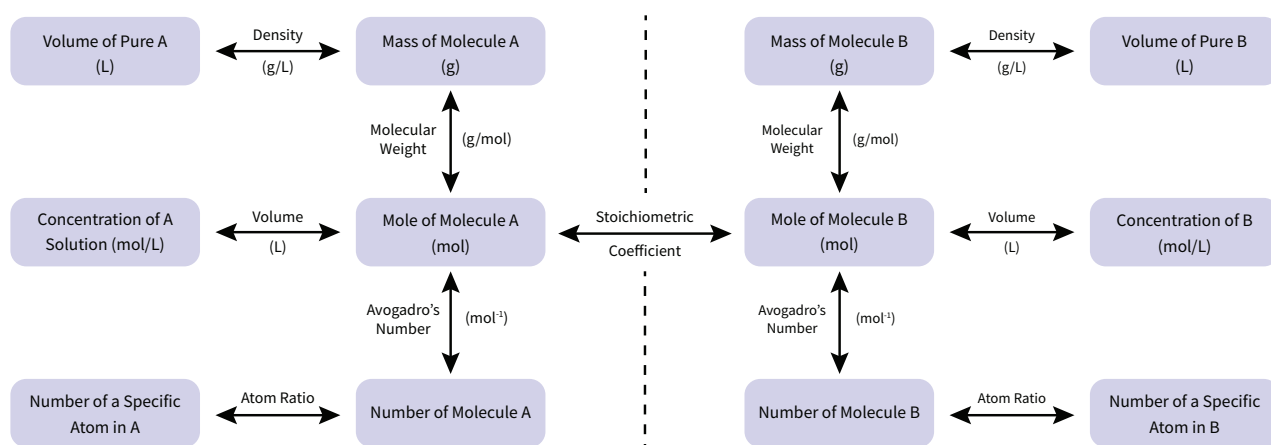
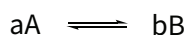
iii. Molecular weight: g/mol (can be obtained from periodic table).

2. Mole ratios

a. Balanced chemical equations.



b. Stoichiometry coefficients can be used to determine mole ratio.



c. **Limiting Reagent:** The first consumed reagent in a reaction is the limiting reagent.

DILUTION

1. More solvent is added to the solution to reduce concentration.

$$c_1 V_1 = c_2 V_2$$

a. Number of solute particles never change.

TEST QUESTIONS

- Potassium dichromate $\text{K}_2\text{Cr}_2\text{O}_7$ is used in tanning leather, decorating porcelain, and water proofing fabrics. Calculate the number of chromium atoms in 78.82 g of $\text{K}_2\text{Cr}_2\text{O}_7$.
 - 9.490×10^{25} Cr atoms
 - 2.248×10^{24} Cr atoms
 - 1.124×10^{24} Cr atoms
 - 3.277×10^{23} Cr atoms
 - 1.613×10^{23} Cr atoms
- If 5.97 mL of a solution of NaCl contains 2.54 mg of sodium ion, what is the molarity of the sodium chloride solution?
 - 0.425 M



- b. 1.85×10^{-2} M
- c. 1.85×10^{-5} M
- d. 7.28×10^{-3} M
- e. 102 mM

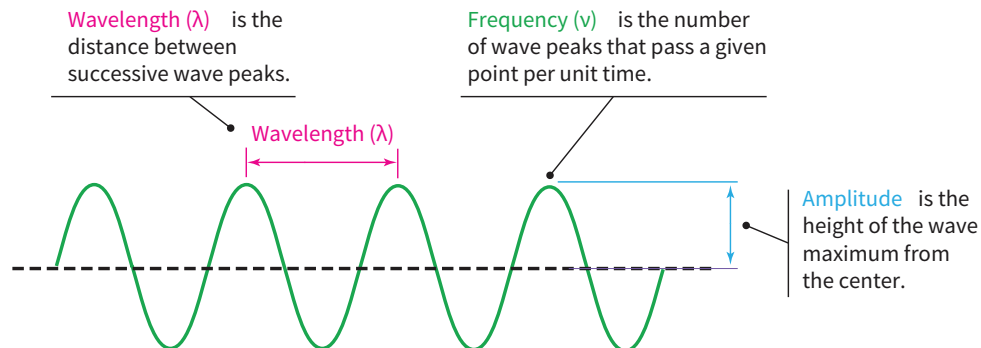
3. How many milliliters of a 6.0 M HNO_3 solution are needed to make 0.25 L of a 1.5 M HNO_3 solution?

- a. 0.25 L
- b. 150 mL
- c. 63 mL
- d. 75 mL
- e. 6.0 mL

QUANTUM MECHANICS

ELECTROMAGNETIC RADIATION

Consists of magnetic and electric fields that are perpendicular to each other.



1. Parameters:

- a. Wavelength: λ , distance between 2 peaks or troughs.
- b. Frequency: ν (Greek: nu), number of waves per second that pass through a given point.
- c. Amplitude: height of peak, related to **intensity** of light.

2. Link between λ and ν :

$$c = \lambda \nu$$

c: Speed of light (m/s) = 3.0×10^8 m/s

λ : Wavelength (m).

ν : Frequency (s^{-1} , Hz).

ENERGY OF A SINGLE PHOTON

Energy of a photon can be expressed by:

$$E = hv = \frac{hc}{\lambda}$$

E: Energy (J).

v: Frequency (s^{-1} , Hz).

λ : Wavelength(m).

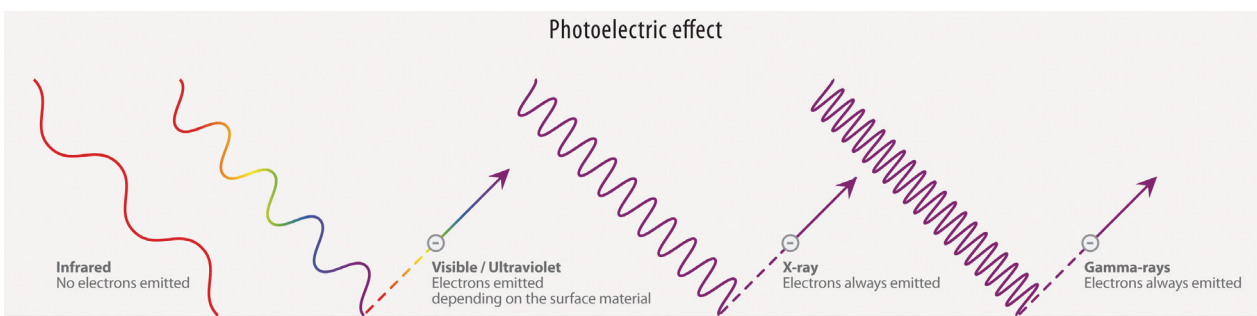
h: Planck's constant (Js) = 6.626×10^{-34} J·s

TEST QUESTIONS

- The amount of data that can be stored in an optical disc storage medium is related to the wavelength of the laser employed. Blu-ray discs are read by a laser emitting photons with a wavelength of 405 nm, while DVDs are read by a laser emitting photons with wavelength of 650 nm. If both video players emit 1.00×10^{17} photons per second, how much more light energy is released by the Blu-ray player as compared to the DVD player over the course of a 2.0-hour movie?
 - 130 kJ
 - 130 J
 - 67 kJ
 - 67 J
 - 25 J
- Strontium has an intense emission at 641 nm. What is the total energy (in kJ) emitted by 5.00 g of strontium chloride ($SrCl_2$)?
 - 0.453 kJ
 - 5.89 kJ
 - 36.7 kJ
 - 53.8 kJ
 - 58.9 kJ

PHOTOELECTRIC EFFECT

Photoelectric effect: Light hits metal surface and energy transfers from photons to electrons which frees electrons on metal.



1. Conservation of energy:

$$KE_{\text{electron}} = E_{\text{photon}} - E_{\text{binding}}$$

KE_{electron} : Kinetic energy of electron.

E_{photon} : Energy of photon (determined by either λ or ν)

E_{binding} (work function): Minimum or threshold energy for an electron to be ejected.

2. Intensity of light

- Intensity is an expression of **number of photons**.
- Frequency and wavelength remain unchanged → **Energy is unchanged**.

TEST QUESTIONS

- A photon with an energy of 5.3×10^{-19} J strikes an electron in metal. Of this energy, 3.6×10^{-19} J is the minimum energy required for the electron to escape from the metal. The remaining energy appears as kinetic energy of the photoelectron. What is the velocity of the photoelectron, assuming it was initially at rest?
 - 3.7×10^{14} m/s
 - 3.7×10^{11} m/s
 - 1.9×10^6 m/s
 - 6.1×10^5 m/s
 - 1.7×10^{-19} m/s
- The optic nerve needs a minimum energy of 2.0×10^{-17} J to trigger impulses that will reach the brain and detect light. What is the minimum number of photons of blue light (475 nm) that can be detected by the brain? Red light has a longer wavelength of light than blue light – would more or less photons of red light be needed to be detected?
 - 48 photons; more red photons
 - 48 photons; less red photons
 - 123 photons; more red photons
 - 123 photons; less red photons
 - The same number of photons of red and blue light would be needed to be detected by the brain.

BOHR MODEL OF THE ATOM

This model is only applied to the **single electron system** (H, He+...).

- Emission/ absorption wavelength can be calculated by:

$$\frac{1}{\lambda} = R_{\infty} \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

R_{∞} : Rydberg constant = $1.097 \times 10^{-2} \text{ nm}^{-1}$.

- m: Lower energy level (must be an integer).
 n: Higher energy level (must be an integer).
- Energy flow
 - Final energy level > Lower energy level → Energy is absorbed.
 - Lower energy level > Final energy level → Energy is released.
 - Energy for Bohr atom at each energy level can be calculated by:

$$E_n = -2.178 \times 10^{-18} \text{ J} \left(\frac{Z^2}{n^2} \right)$$

E_n : Energy of a specific energy level.

n: Energy level (must be an integer).

Z: Nuclear charge (for H, Z = 1).

MATTER WAVE

All matters can be considered as a wave.

- Wave property is only significant in tiny particles.
- Wave parameters can be obtained from:

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

λ : Wavelength (m).

m: Mass (kg).

v: Velocity (m/s).

p: Momentum (kg · m/s).

UNCERTAINTY PRINCIPLE

Two parameters cannot be measured at same time.

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

Δx : Uncertainty in position (m).

Δp : Uncertainty in momentum (kg · m/s).

h: Planck's Constant (J · s).

WAVE EQUATION

Wave function describes the distribution of the electron wave in the atom.

$$\hat{H}\Psi = E\Psi$$

\hat{H} : Hamiltonian operator.



E: Energy of the electron.

Ψ : Wave function (solution to wave equation).

QUANTUM NUMBER AND ORBITALS

Quantum number is used to describe certain wave function (orbital).

Week 1-2

1. Principal quantum number: n
 - a. Principal quantum number determines energy **level (or size)** of the orbital.
 - b. **Range: $n = 1, 2, 3, 4 \dots$**
2. Angular momentum quantum number: l
 - a. Angular momentum quantum number determines **shape** of the orbital.

l value	0	1	2	3	4	...
Subshell Notation	s	p	d	f	g	...

- b. **Range: $l = 0, 1, 2, 3, \dots, n-1$.**
3. Magnetic quantum number: m_l
 - a. Magnetic quantum number determines the **spacial orientation** of the orbital.
 - b. **$m_l = -l, \dots, 0, \dots, +l$.**
4. Spin quantum number: m_s
 - a. Spin quantum number determine the orientation of the electron.
 - b. **$m_s = +1/2$ or $-1/2$**

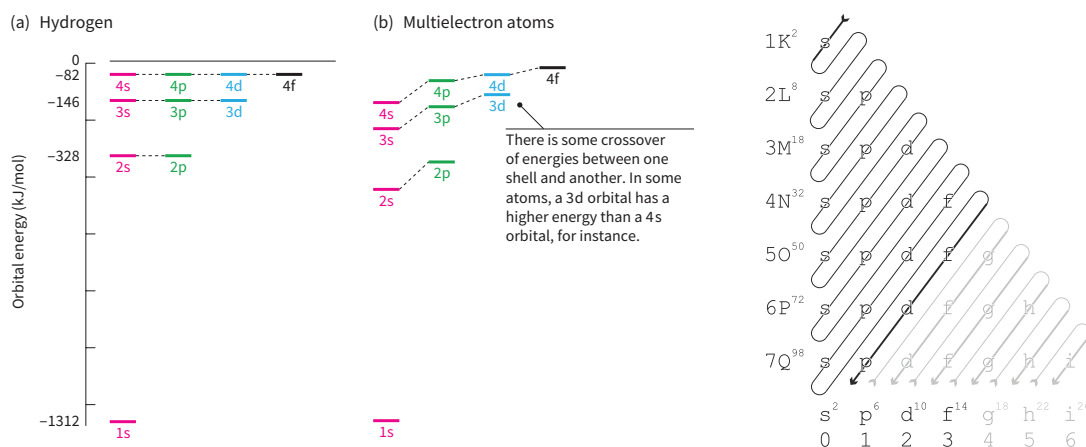
Allowed Quantum Number Combination						
n	l	m_l	Orbital Notation	Number of Orbitals in Subshell	Number of Orbitals in Shell	Number of Electrons in Shell
1	0	0	1s	1	1	2
2	0	0	2s	1	4	8
	1	-1, 0, +1	2p	3		
3	0	0	3s	1	9	18
	1	-1, 0, +1	3p	3		
	2	-2, -1, 0, +1, +2	3d	5		
...

Note: Number of magnetic quantum number (m_l) implies number of orbitals which contains max. 2 electrons.

ELECTRON CONFIGURATION

1. Pauli exclusion principle: Two electrons cannot have same quantum number.
2. Hund's rule: every orbital in a subshell is singly occupied with one electron before any one orbital is doubly occu-

paired, and all electrons in singly occupied orbitals have the same spin.



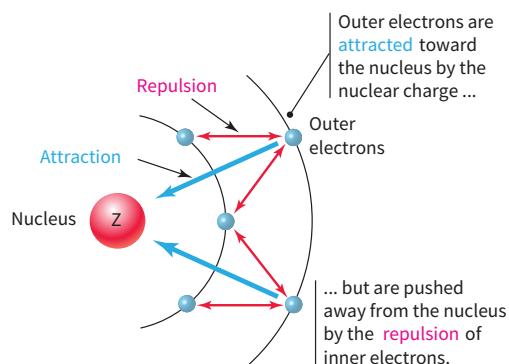
3. Special electron configuration

- Cr: $[\text{Ar}] 3d^5 4s^1$
- Mo: $[\text{Kr}] 4d^5 5s^1$
- Cu: $[\text{Ar}] 3d^{10} 4s^1$
- Ag: $[\text{Kr}] 4d^{10} 5s^1$

SHIELDING EFFECT OF ELECTRONS

Repulsions between electrons masks attraction between nuclear charge and electrons.

1. Effective nuclear charge



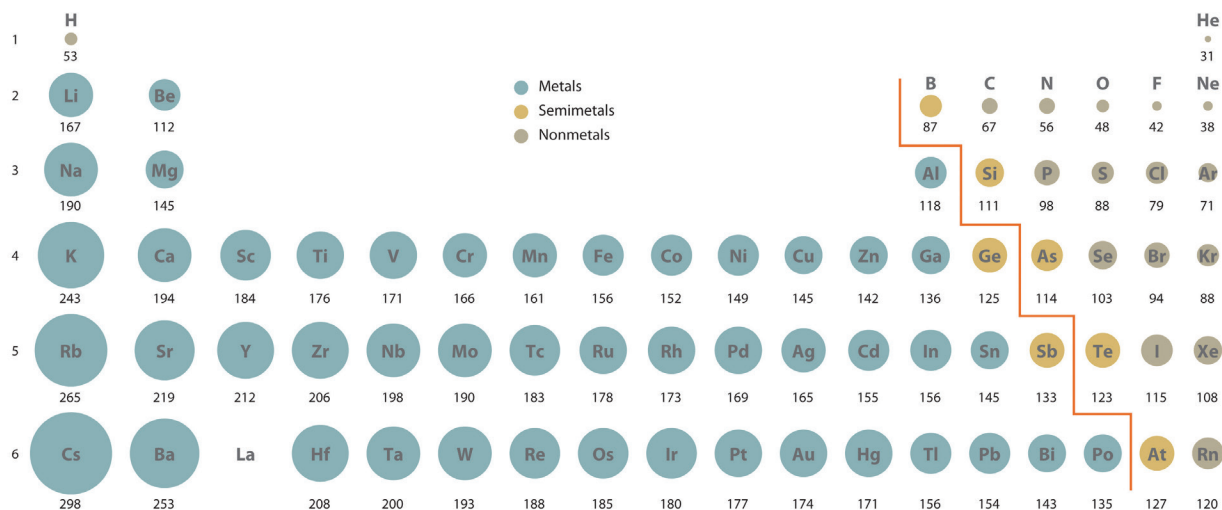
Effective nuclear charge:

$$Z_{\text{eff}} = Z_{\text{actual}} - S$$

Z_{actual} : Number of protons in the nucleus.

S : Number of inner-shell electrons.

2. Atomic size



PRACTICE

- Which one of the following is an empirical formula?
 - C_2F_6
 - H_2SO_2
 - $C_2H_4O_2$
 - P_4O_{10}
 - C_4H_8
- Which statement about diluted solutions is false? When the solution is diluted,
 - the concentration of the solution decreases.
 - the molarity of the the solution decreases.
 - the number of moles of solute remains unchanged.
 - the number of moles of solvent increases.
 - the number of moles of solvent remains unchanged.
- How many oxygen atoms are in 3.00 g of sodium dichromate, $Na_2Cr_2O_7$?
 - 0.0801 oxygen atoms
 - 9.85×10^{20} oxygen atoms
 - 6.90×10^{21} oxygen atoms
 - 4.83×10^{22} oxygen atoms
 - 9.83×10^{22} oxygen atoms
- Calculate the mass of 8.35×10^{22} molecules of CBr_4 .
 - 0.0217 g
 - 0.139 g
 - 7.21 g
 - 0.127 kg
 - 0.0460 kg
- If the percent yield of the following reaction is 65.0%, how many grams of $KClO_3$ are needed to produce 32.0 g of O_2 ?

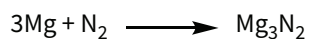


- 53.1 g
- 81.7 g
- 126 g
- 283 g
- 83.4 g

6. A sample containing CaCO_3 was reported as being 30.0% Ca by mass. Assuming the rest of the sample contains no calcium, what is the mass percent of CaCO_3 in the sample:
- 30%
 - 40%
 - 70%
 - 75%
 - 100%

7. How many milliliters of a 6.0 M HNO_3 solution are needed to make 0.25 L of a 1.5 M HNO_3 solution?
- 0.25 L
 - 150 mL
 - 63 mL
 - 75 mL
 - 6.0 mL

8. How many grams of N_2 are required to react with 2.30 moles of Mg in the following reaction?



- 21.5 g
 - 0.767 g
 - 64.4 g
 - 0.027 g
 - 193.2 g
9. Noscapine is an alkaloid that acts as a cough suppressant. It crystallizes from aqueous solution as a hydrate that contains 17.9% water by mass. This hydrate, Noscapine·n H_2O , has a molar mass of 503.56 g/mol.
- Determine n in Noscapine·n H_2O

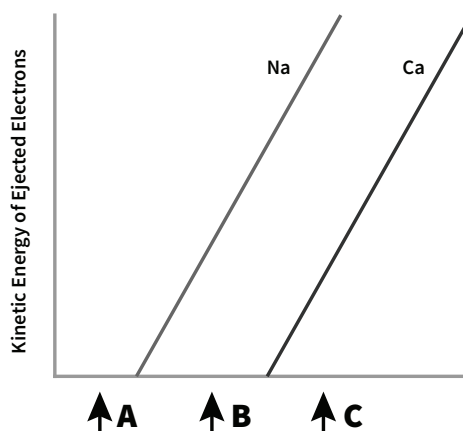
 - The molecular formula of Noscapine is $\text{C}_{22}\text{H}_{23}\text{A}_7\text{N}$. Determine the identity of element A.

10. Atomic orbitals developed using quantum mechanics:
- Describe regions of space in which one is most likely to find an electron
 - Describe exact paths for electron motions
 - Give a description of the atomic structure which is essentially the same as the Bohr model
 - Allow scientists to calculate the exact volume for the hydrogen atom
 - Are in conflict with the Heisenberg's Uncertainty Principle
11. Which of the following is not a valid set of quantum numbers?
- $n = 2, l = 1, m_l = 0$ and $m_s = -1/2$
 - $n = 2, l = 1, m_l = -1$ and $m_s = -1/2$
 - $n = 3, l = 0, m_l = 0$ and $m_s = +1/2$
 - $n = 3, l = 2, m_l = 3$ and $m_s = +1/2$
 - $n = 3, l = 1, m_l = 0$ and $m_s = +1/2$
12. For a particular orbital, as one goes away from the nucleus along the z-axis, the probability density decreases to zero, then increases, and finally decreases without increasing a second time. This is consistent with a
- 2s orbital
 - $2p_z$ orbital
 - 2s and a $2p_z$ orbital
 - 3s orbital
 - 2s and a 3s and a $2p_z$ orbital
13. An electron in a H atom has an energy of -2.42×10^{-19} J. What is the largest value of m_l (magnetic quantum number) possible for this energy level?
- 0
 - 1
 - 2
 - 3
 - 1
14. Of the electronic transitions in the hydrogen atom described below, which involves emission of a photon with the shortest wavelength?
- $n = 1 \rightarrow n = 2$
 - $n = 2 \rightarrow n = 3$
 - $n = 1 \rightarrow n = 4$
 - $n = 2 \rightarrow n = 1$
 - $n = 3 \rightarrow n = 1$

15. How many unpaired electrons are there in the ground state of element N?
- 1
 - 2
 - 3
 - 4
 - 5

16. An ion has 10 electrons, 9 protons and 10 neutrons. Which is the correct notation?
- ${}_{10}^{10}\text{Ne}^+$
 - ${}_{9}^{10}\text{F}^-$
 - ${}_{10}^{19}\text{Ne}^+$
 - ${}_{9}^{19}\text{F}^-$
 - ${}_{10}^{20}\text{Ne}^+$

17. The photoelectric effect is described by the graph below of the kinetic energy of the ejected electron vs. frequency of the light directed at the surface of sodium metal or calcium metal. Which of the following statements is true:



- When light with frequency A hits both metal surfaces, electrons are ejected from both metals.
- When light with a frequency B hits both metal surfaces, the electrons ejected from sodium are moving faster than the electrons ejected from calcium.
- When the intensity of the light with frequency A hitting the metal surfaces is increased, electrons are ejected from both metal surfaces.
- When the intensity of the light with frequency B is increased, more electrons will be ejected from sodium than before the intensity was increased.
- When light with frequency C hits both metal surfaces, the electrons ejected from calcium will be moving faster than the electrons ejected from sodium.

18. A ground state H atom absorbs a photon with a frequency of 3.16×10^{15} Hz, and its electron attains a higher energy state. The atom then emits two photons: one of wavelength 1281 nm to reach an intermediate level and a second to reach the ground state.

a. What is the highest energy level attained by the electron?

b. What was the wavelength of the second photon emitted to return the electron to the ground state?