AP Chemistry
A. Allan
Chapter 7 Notes - Atomic Structure and Periodicity

7.1 Electromagnetic Radiation
    A. Types of EM Radiation (wavelengths in meters)

| 10^{-12} | 10^{-10} | 10^{-8} | 4 to 7x10^{-7} | 10^{-4} | 10^{-2} | 1 | 10^{2} | 10^{4} |

gamma	xrays	UV	visible	IR	micro	Radio waves		
						FM	short	AM

Wavelength increases ⟶
Frequency decreases ⟶
Energy decreases ⟶
Speed is constant = 2.9979 x 10^8 m/sec

    B. Properties of EM Waves
        1. Wavelength (λ)
            a. Distance between two consecutive peaks or troughs in a wave
            b. Measured in meters (SI system)
        2. Frequency (ν)
            a. Number of waves that pass a given point per second
            b. Measured in hertz (sec^{-1})
        3. Speed (c)
            a. Measured in meters/sec

Electromagnetic Radiation
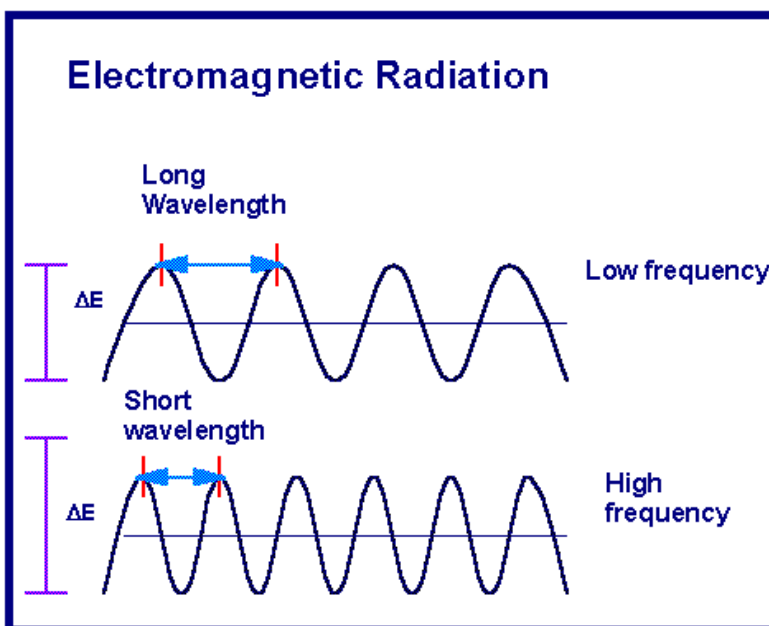
        4. Relationship of properties
            a. $\lambda\nu = c$

7.2 The Nature of Matter
  A. Max Planck and Quantum Theory
      1. Energy is gained or lost in whole number multiples of the quantity hv
          Frequency = v
          Planck's constant = h = 6.626 x 10^{-34} J•S

$$\Delta E = nh v$$

      2. Energy is transferred to matter in packets of energy, each called a
          quantum
  B. Einstein and the Particle Nature of Matter
      1. EM radiation is a stream of particles - "photons"

$$E_{photon} = h v = \frac{hc}{l}$$

      2. Energy and mass are inter-related

$$E = mc^2$$

  C. de Broglie and the Dual Nature of Light
      1. Light travels through space as a wave
      2. Light transmits energy as a particle
      3. Particle's have wavelength, exhibited by diffraction patterns
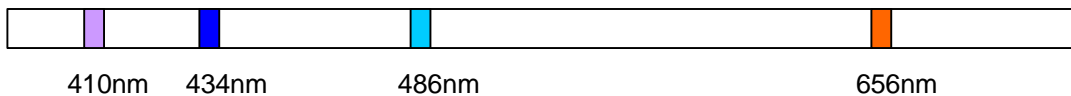
$$l = \frac{h}{mv}$$

          a. large particles have <u>very short</u> wavelengths
          b. <u>All matter</u> exhibits both particle and wave properties

7.3 The Atomic Spectrum of Hydrogen
  A. Continuous spectra
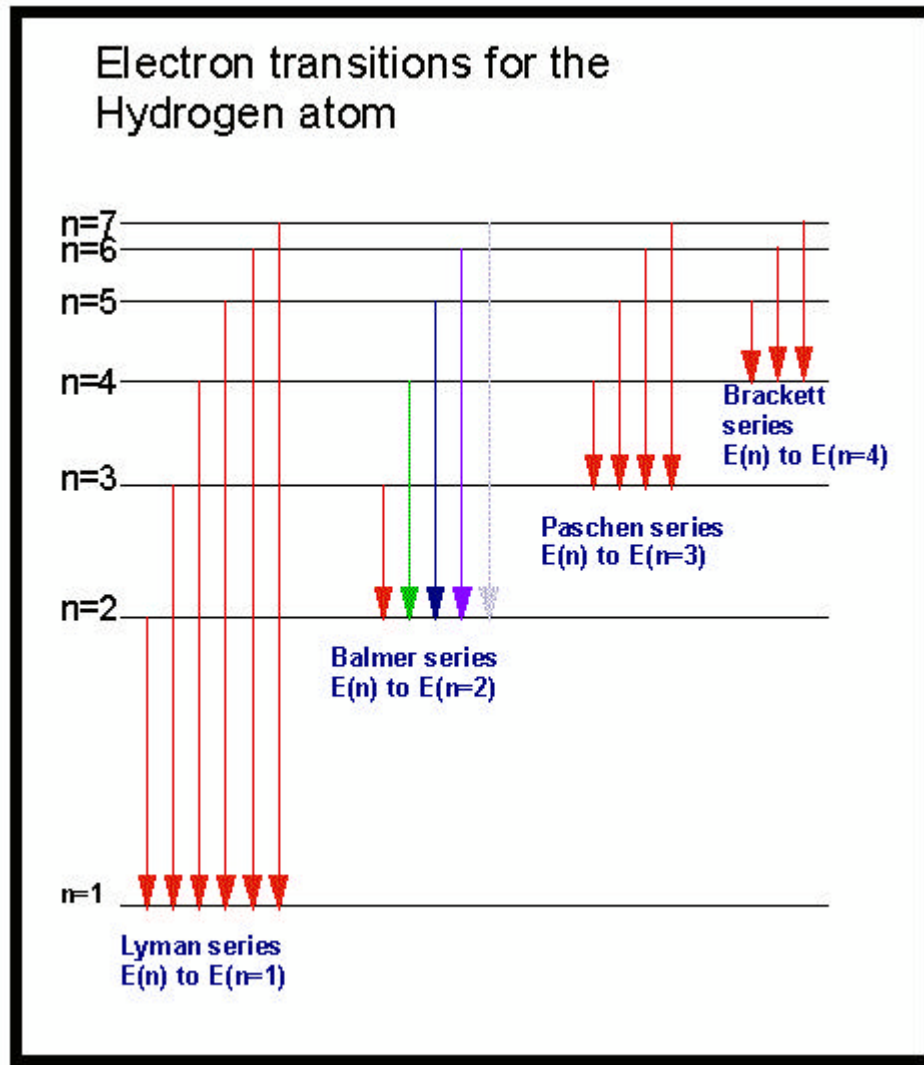   1. Contains all wavelengths of light
  B. Bright line spectra

410nm   434nm   486nm   656nm

      1. Excited electrons in an atom return to lower energy states
      2. Energy is emitted in the form of a photon of definite wavelength
      3. Definite change in energy corresponds to:
          a. Definite frequency
          b. Definite wavelength

$$\Delta E = h v = \frac{hc}{l}$$

      4. Only certain energies are possible within any atom

Electron transitions for the
Hydrogen atom

n=7
n=6

n=5

n=4
Brackett
series
E(n) to E(n=4)

n=3

Paschen series
E(n) to E(n=3)

n=2

Balmer series
E(n) to E(n=2)

n=1

Lyman series
E(n) to E(n=1)

7.4 Bohr Model (Neils Bohr, 1913)

A. Quantum Model

1. The electron moves around the nucleus only in certain allowed circular orbits

2. Bright line spectra confirms that only certain energies exist in the atom, and atom emits photons with definite wavelengths when the electron returns to a lower energy state

3. Energy levels available to the electron in the hydrogen atom

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

n = an integer   Z = nuclear charge   J = energy in joules

B. Calculating the energy of the emitted photon
    1. Calculate electron energy in outer level
    2. Calculate electron energy in inner level
    3. Calculate the change in energy (ΔE)
        ΔE = energy of final state - energy of initial state
    4. Use the equation:

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

        to calculate the wavelength of the emitted photon

C. Energy Change in Hydrogen atoms
    1. Calculate energy change between any two energy levels

$$\Delta E = -2.178 \times 10^{-18} J \left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2} \right)$$

D. Shortcomings of the Bohr Model
    1. Bohr's model does not work for atoms other than hydrogen
    2. Electron's do not move in circular orbits

7.5 The Quantum Mechanical Model of the Atom
  A. The Electron as a standing wave
    1. Standing waves do not propagate through space
    2. Standing waves are fixed at both ends
    3. Only certain size orbits can contain whole numbers of half wave lengths
        a. fits the observation of fixed energy quantities - "quanta"
  B. The Schrödinger Equation (Erwin Schrödinger)
    1. For the motion of one particle, in the along the x axis in space:

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

    2. Solution of the equation has demonstrated that E (energy) must occur in integer multiples
    3. Your book has done you the favor of greatly simplifying this and presents the general equation:

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

        $\hat{H}$ = a set of mathematical functions called an "operator"

        ψ = a wave function. Specific wave functions are called

        "orbitals"
    4. Orbitals
        1. Orbitals <u>are not</u> circular orbits for electron
        2. Orbitals <u>are</u> areas of probability for locating electrons

C. Heisenberg Uncertainty Principle (Werner Heisenberg)
   1. "There is a fundamental limitation on how precisely we can know both the position and momentum of a particle at a given time"

$$\Delta x \cdot \Delta(mv) \geq \frac{h}{4p}$$

Δx = uncertainty in the particle's position

$\Delta(mv)$ = uncertainty in the particle's momentum

   2. The more accurately we know the position of any particle, the less accurately we can know its momentum, and vice-versa
D. Physical Meaning of a Wave Function
   1. Square of the absolute value of the wave function gives a probability distribution.

$$\left| y \right|^2$$

   2. Electron density map indicates the most probable distance from the nucleus
   3. Wave functions and probability maps <u>do not</u> describe:
      a. How an electron arrived at its location
      b. Where the electron will go next
      c. When the electron will be in a particular location

7.6 Quantum Numbers
   A. Principal Quantum Number (n)
      1. Integral values: 1, 2, 3, ...
      2. Indicates probable distance from the nucleus
         a. Higher numbers = greater distance
         b. Greater distance = less tightly bound = higher energy
   B. Angular Momentum Quantum (l)
      (this was called the "orbital quantum number" in your general chem book)
      1. Integral values from 0 to n - 1 for each principal quantum number n
      2. Indicates the shape of the atomic orbitals

Table 7.1 Angular momentum quantum numbers and corresponding atomic orbital numbers					
Value of l	0	1	2	3	4
Letter used	s	p	d	f	g

   C. Magnetic Quantum Number (m_l)
      1. Integral values from l to $-l$, including zero
      2. Magnetic quantum number relates to the orientation of the orbital in space relative to the other orbitals
   D. Spin Quantum Number
      1. Covered in section 7.8

Table 7.2 Quantum numbers for the first four levels of orbitals in the hydrogen atom				
n	*l*	Orbital designation	*m$_l$*	# of orbitals
1	0	1s	0	1
2	0	2s	0	1
	1	2p	-1, 0, 1	3
3	0	3s	0	1
	1	3p	-1, 0, 1	3
	2	3d	-2, -1, 0, 1, 2	5
4	0	4s	0	1
	1	4p	-1, 0, 1	3
	2	4d	-2, -1, 0, 1, 2	5
	3	4f	-3, -2, -1, 0, 1, 2, 3	7

7.7 Orbital Shapes and Energies
   A. Size of orbitals
            1. Defined as the surface that contains 90% of the total electron probability
            2. Orbitals of the same shape (s, for instance) grow larger as n increases
    B. s Orbitals
            1. Spherical shape
            2. Nodes (s orbitals of n=2 or greater)
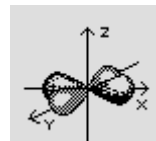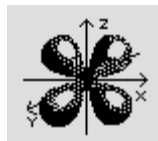   a. Internal regions of zero probability
    C. p Orbitals
            1. Two lobes each
            2. Occur in levels n=2 and greater
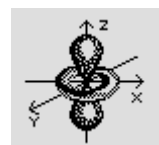   3. Each orbital lies along an axis (2p$_x$, 2p$_y$, 2p$_z$)
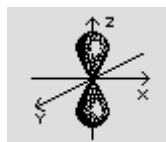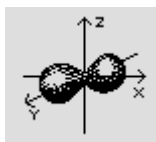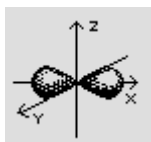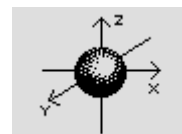
D. d Orbitals
1. Occur in levels n=3 and greater
2. Two fundamental shapes
   a. Four orbitals with four lobes each, centered in the plane indicated in the orbital label
   $$d_{xz} \quad d_{yz} \quad d_{xy} \quad d_{x^2-y^2}$$

   b. Fifth orbital is uniquely shaped - two lobes along the z axis and a belt centered in the xy plane
   $$d_{z^2}$$

E. f Orbitals
1. Occur in levels n=4 and greater
2. Highly complex shapes
3. Not involved in bonding in most compounds
F. Orbital Energies
1. All orbitals with the same value of n have the same energy
   a. "degenerate orbitals" (hydrogen only!)
2. The lowest energy state is called the "ground state"
3. When the atom absorbs energy, electrons may move to higher energy orbitals - "excited state"

7.8 Electron Spin and the Pauli Principle
A. Electronic Spin Quantum Number
1. An orbital can hold only two electrons, and they must have opposite spins
2. Spin can have two values, +1/2 and -1/2
B. Pauli Exclusion Principle (Wolfgang Pauli)
1. "In a given atom no two electrons can have the same set of four quantum numbers"

7.9 Polyelectronic Atoms
A. Internal Atomic energies
1. Kinetic energy of moving electrons
2. Potential energy of attraction between nucleus and electrons
3. Potential energy of repulsion between electrons
B. The Electron Correlation Problem
1. Electron pathways are not known, so electron replusive forces cannot be calculated exactly

2. We approximate the <u>average</u> repulsions of all other electrons

    C. Screening or Shielding
        1. Electrons are attracted to the nucleus
        2. Electrons are repulsed by other electrons
        3. Electrons would be bound more tightly if other electrons weren't present
    D. Variations in energy within the same quantum level
        1. Atoms other than hydrogen have variations in energy for orbitals having the same principal quantum number
        2. Electrons fill orbitals of the same n value in preferential order
$$E_{ns} < E_{np} < E_{nd} < E_{nf}$$
        3. Electron density profiles show that s electrons penetrate to the nucleus more than other orbital types
            a. Closer proximity to the nucleus = lower energy

7.10 The History of the Periodic Table
    No notes. Read this section. Notice especially Table 7.3 and 7.4. The periodic table is as useful for predicting properties of undiscovered elements today as it was in Mendeleev's time

7.11 The Aufbau Principle and the Periodic Table
    A. The Aufbau Principle
        1. "As protons are added one by one to the nucleus to build up elements, electrons are similarly added to these hydrogen-like orbitals
    B. Hund's Rule
        1. "The lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a particular set of degenerate orbitals

    ***Note: We will review configuration and orbital notation in class. This was covered extensively in General Chem, and will come back to you quickly

    C. Period Table Vocabulary
        1. Valence Electrons
            a. Electrons in the outermost principal quantum level of an atom
            b. Elements in the same group (vertical column) have the same valence electron configuration
        2. Transition metals
            a. What we have called the "d" block
        3. Lanthanide and Actinide Series
            a. The sets of 14 elements following lanthanum and actinium
            b. What we have called the "f" block
        4. Main-group, or Representative Elements
            a. Groups 1A through 8A
            b. Configurations are consistent
        5. Metalloids (semi-metals)

a. Found along the border between metals and nonmetals
b. Exhibit properties of metals and nonmetals

7.12 Periodic Trends in Atomic Properties
    A. Ionization Energy - the energy required to remove an electron from an atom
        1. Ionization energy increases for successive electrons
        2. Ionization energy tends to increase across a period
            a. electrons in the same quantum level do not shield as effectively as electrons in inner levels
            b. irregularities at half filled and filled sublevels due to extra repulsion of electrons paired in orbitals, making them easier to remove
        3. Ionization energy decreases with increasing atomic number within a group
            a. electrons farther from the nucleus are easier to remove
    B. Electron Affinity - the energy change associated with the addition of an electron
        1. Affinity tends to increase across a period
        2. Affinity tends to decrease as you go down in a period
            a. electrons farther from the nucleus experience less nuclear attraction
            b. Some irregularities due to repulsive forces in the relatively small p orbitals
    C. Atomic Radius
        1. Determination of radius
            a. half of the distance between radii in a covalently bonded diatomic molecule - "covalent atomic radii"
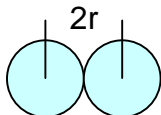
        2. Periodic Trends
            a. Radius decreases across a period
                (1) increased effective nuclear charge due to decreased shielding
            b. Radius increases down a group
                (1) addition of principal quantum levels

7.13 The Properties of a Group: the Alkali Metals
    A. Easily lose valence electron (Reducing agents)
        1. React with halogens to form salts
        2. React violently with water
            a. Lithium is not the most reactive because the heat of reaction is insufficient to melt lithium and expose all of its surface area
    B. Large hydration energy
        1. Positive ionic charge makes ions attractive to polar water molecules
    C. Radius and Ionization energy follow expected trends

See Table 7.8 for other properties of the Alkali metal group