Atom Spectroscopy Intro!

- If we have knowledge about electrons, we can understand the bonding and properties of matter.
- Masses are the average mass of all of it's isotopes
  - Isotopes – different # of neutrons, same # p^+ and same # e
  - – different atomic mass, same atomic #
- Relative atomic mass (relative abundance) is ratio between average mass and 1/12 mass of carbon

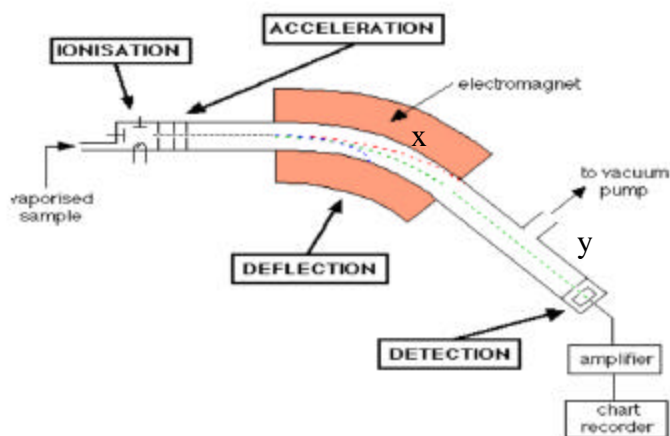Relative Atomic Mass (A_r)

Calculate the relative atomic mass (Ar) of Chlorine.

$$\frac{(75 \times 35) + (25 \times 37)}{100} = 35.5 \text{ amu}$$

| $^{37}_{17}$ Cl | $^{35}_{17}$ Cl |
| 25 % | 75 % |

Mass Spectrometer

- Determine the relative abundance of the isotopes of the element, and their isotopic masses; the weighted mean of these is then the atomic mass.
- The amount of deflection is a result of two factors:
  - 1. Mass – the lighter particle will deflect more
  - 2. Charge – the greater the charge, the greater the deflection
- The process is separated into 5 steps: VIADD
  - V – Vapourize, with heat
  - I – Ionization, shoot a high energy electron or heat even more, make singly charged cation
  - A – Accelerate them with a negative electric field so you can move them and deflect them.
  - D – Deflect with a very strong magnetic field. Deflection depends on:
    - 1. Deflection $\propto$ mass^{-1}
    - 2. Deflection $\propto$ |charge|
  - D – Detection, use analog detector which converts signal to a charge

- y is lighter
- y has a greater charge

- the relative atomic mass, A_T of an element is defined as the mass of one atom of that element relative to 1/12th the mass of one carbon atom (since ^{12}C = exactly 12)

Periodic Table Trends

Effective Nuclear Charge

- Attraction felt by the valence electrons from the nucleus
- ? across a period, more protons but # of energy levels do not change
- ? down a group, more protons being added, also the core electrons shield the valence electrons from the nucleus, hence decreasing effective nuclear charge.

Atomic Radius

- The distance from the centre to the outermost energy level.
- ? across a period because effective nuclear charge increases, pulling it in closer
- ? down a group because more energy levels are being added

Ionic Radii: Size of Cations and Anions

- A cation has a smaller ionic radius than the neutral atom, effective nuclear charge is greater and an energy level may have been removed.
- An anion has a greater ionic radius than a neutral atom, more repulsion when another electron is added in an orbital where there is already an existing electron resulting in an increase in the ionic radius.
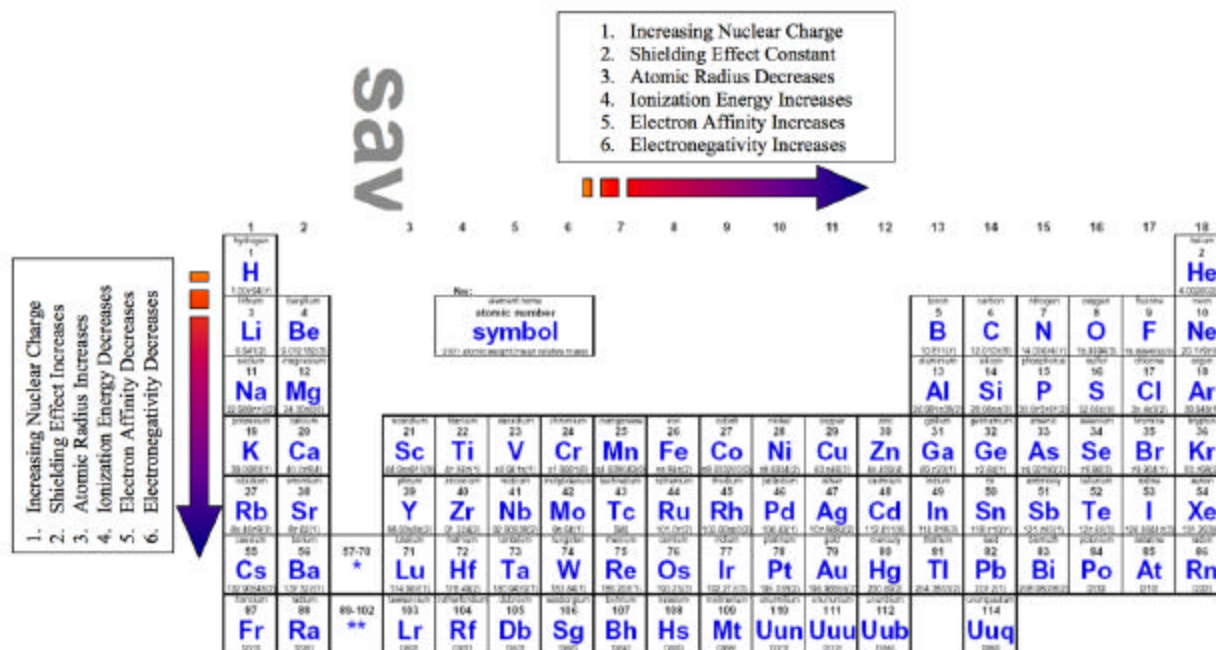
Ionization Energy

- The energy required to remove and electron from a gaseous atom in its ground state to form a gaseous cation.
- $X_{(g)} + IE \rightarrow X^{+1}_{(g)} + e^-$ where IE_1 = first ionization energy $IE_2 > IE_1$
- The first ionization energy depends on:
    - 1. Effective nuclear charge
    - 2. Atomic radius
    - 3. Shielding effect by lower energy levels
- ? across a period due to increasing nuclear charge and decreasing atomic radius
- ? down a group due to decreasing nuclear charge and increasing atomic radius
- Low IE indicates that electrons are easily lost, i.e. ALKALI earth metals (group I)
- High IE indicates that electrons aren't easily lost, i.e. Inert gasses (group VIII)

Electron Affinity

- The energy released when an electron is added to a gaseous atom in it's ground state to form a gaseous anion (gas because we don't want to measure change of state)
- $X_{(g)} + e^- \rightarrow X^-_{(g)} + EA_1$
- More stable, minimum energy = max stability (what atoms want)
- ? across a period, atoms get closer to wanting full shell across period, to be stable
- ? down a group due to the fact that adding an electron will destabilize the metallic atom
- 1st EA is exothermic, successive addition is endothermic (has to overcome repulsion more)

<u>Electronegativity</u>
- The measure of attraction an atom has for electrons in a covalent bond between it and another atom. (covalent bond = metal + non metal)
- If the difference between electronegativity values are:
    less that 0.4 = purely covalent bond (shares electrons)
      0.4 – 1.6 = polar covalent bond
  greater than 1.6 = ionic bond (one takes the electron)
- ? across a period, ? down a group

1. Increasing Nuclear Charge
2. Shielding Effect Constant
3. Atomic Radius Decreases
4. Ionization Energy Increases
5. Electron Affinity Increases
6. Electronegativity Increases

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1. Increasing Nuclear Charge
2. Shielding Effect Increases
3. Atomic Radius Increases
4. Ionization Energy Decreases
5. Electron Affinity Decreases
6. Electronegativity Decreases

Atomic Spectroscopy

<u>Electromagnetic Spectrum</u>
- Exciting an atom causes it to jump to a higher shell, then back down to become stable. The energy released is release in waves, in a spectrum – the spectrum of atoms.
- The wavelength (?) is the distance between similar points in a set of waves.
- The frequency (f or v) is the number of waves that pass through a point per unit of time.
- ? Energy
  = ? Frequency,
  ? Wavelength
- c = f ?
  where c is the speed of light in a vacuum $(3\times10^8 \text{ ms}^{-1})$
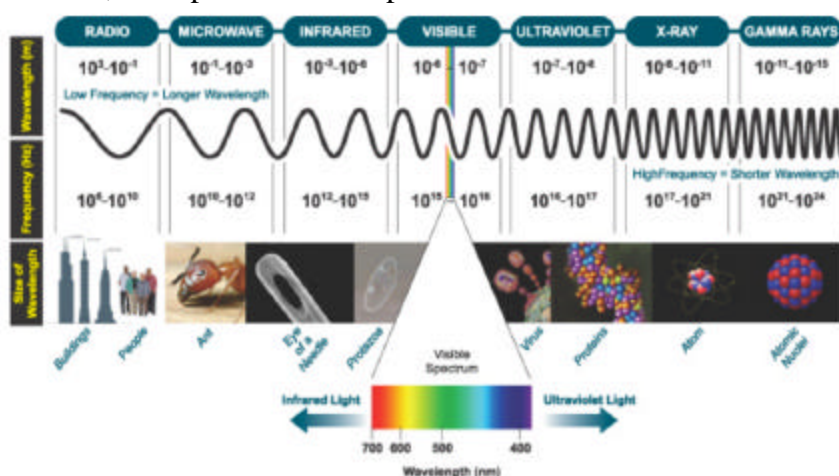
The Bohr Model of the Atom

- Bohr said that electrons have specific quantities of energy called quanta (1: quantum)
- Each specific quantity corresponds to the principal quantum number(n), the integer distance from the nucleus in representing energy level.
- When an electron is in it's lowest energy level, it is in it's ground state. If enough energy is added, it can jump to a higher level and is said to be in an excited state. When it falls back down, it emits energy in the form of light. This is why each element has a characteristic line spectrum.

Atomic Emission Line Spectra: Line Spectrum

- The frequency of radiation depends on the size of the jump and level it lands.
- The principal energy levels get closer as n reaches 8
- Bohr proposed two rules as well as electron configurations similar hydrogen:
  - 1. Additional electrons always occupy the lowest available energy level.
  - 2. The max number of electrons that can be placed in an energy level is given by
    max # of electrons $= 2n^2$ where n = principal quantum number
- Planck suggested the energy values of the atoms varied by small whole numbers, "packets" (called photons) of energy; and that the energy was proportional to the frequency of the light wave. The following equations resulted:
  $E = hf$ $E = hc/?$ $c = f?$ (h = Planck's constant $= 6.626 \times 10^{-34}$)
- More equations resulting from quantum discoveries:
 — where $R_H = 2.18 \times 10^{-18}$ J

  The change of energy where electrons jump to and from can also be calculated:
 —— —— the wavelength of this is given as —

The Atomic Emission Line Spectrum of Hydrogen

- The lines observed in the line spectrum of hydrogen arise from transition of upper energy levels to n=2 principal quantum level.

These transitions to the n = 2 level are referred to as the *Balmer Series* of lines in the spectrum, as shown in the diagram below:
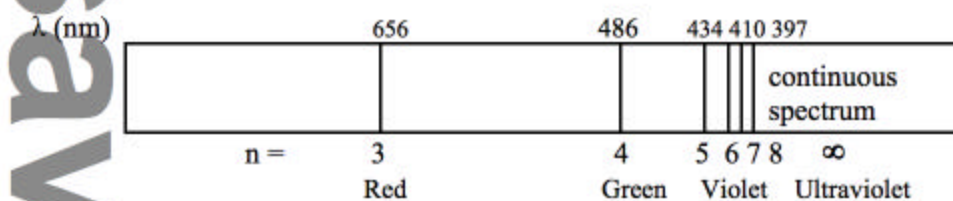
- Only certain ? (or frequencies) are observed for the spectral lines, thus discrete lines.
- The intervals between lines converge to form a continuum of light.
- In addition to the visible light spectrum where the electrons bounce back to n=2, ultraviolet wavelengths can be observed when the electron bounces to n=1. The hydrogen spectrum consists of five series of lines, named for the men who discovered them. The first interpretation of the hydrogen spectrum was an empirical one based on the observed spectrum, Lyman (n = 1), Balmer (n = 2), Paschen (n = 3), Brackett (n = 4), Pfund (n = 5).
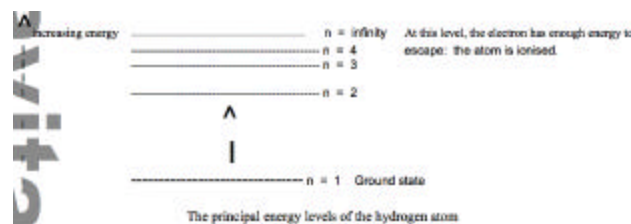
The Wave Mechanical Model of the Atom

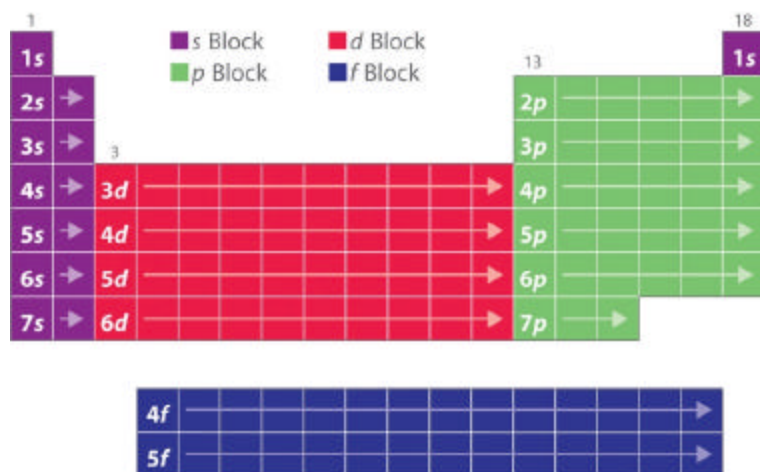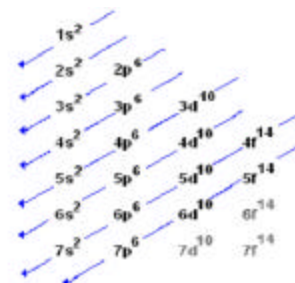| Value of l	0 1 2 3 4 5...
Letter description	s p d f g h...

The Birth of the Quantum Theory

- Heisenberg's uncertainty principal explains that we can never know for sure where exactly an electron is, and the best we can do is calculate the probability of where it is. Orbitals are the volumes of space where electrons are likely to be, each containing a maximum of 2 electrons.

Sommerfield's Addition to the Bohr Model

- Each principal energy level has sublevels of slightly varying energies. They are identified using the secondary quantum number: l.
1. The number of sublevels in a given energy level correspond to the value of n.

$1s^2$
$2s^2$ $2p^6$
$3s^2$ $3p^6$ $3d^{10}$
$4s^2$ $4p^6$ $4d^{10}$ $4f^{14}$
$5s^2$ $5p^6$ $5d^{10}$ $5f^{14}$
$6s^2$ $6p^6$ $6d^{10}$ $6f^{14}$
$7s^2$ $7p^6$ $7d^{10}$ $7f^{14}$

e.g. when n = 2 there are two sublevels: 2s and 2p

2. An s sublevel can hold 2 electrons, a p electron can hold 6, a d sublevel can hold a maximum of 10 and an f sublevel can hold up to 14 electrons (each successive level holds 4 more electrons than its predecessor).

3. Because the energy levels are closer together as the value of n increases, the energy of sublevel 4s is less than that of 3d, so 4s fills before 3d. This can get a bit confusing at higher levels of n. A pattern for orbital filling is shown below.

- With this we can write the electron configurations of the periodic table.

- However, there are some exceptions (see your electron configuration chart).

| Electron as a wave :	photon	$E = hf$
Electron as a particle:	mass	$E = mc^2$
de Broglie Equation		$\lambda = \dfrac{h}{mv}$

The Third Quantum Number — Magnetic Quantum number, m_l

- This quantum number is concerned with how an orbital is oriented in space
- The possible values of m_l range from $-l$ to $+l$
- m_l has a value of 0 when l=0, so an s sublevel has only one orbital

  $n = 1$ $l = 0$ $m_l = 0$
- a p sublevel has $l = 1$, meaning that m_l can have a value of $+1,0,-1$
- a d sublevel has $l = 2$, meaning that m_l can have a value of $+2,+1,0,-1,-2$

Shapes of Orbitals

- $\rightarrow$
- The orbitals that are the same but in different direction are called degenerate orbitals
- We say $2p_x$, $2p_y$, or $2p_z$ for the orientation (in m_l)

Shapes of Orbitals
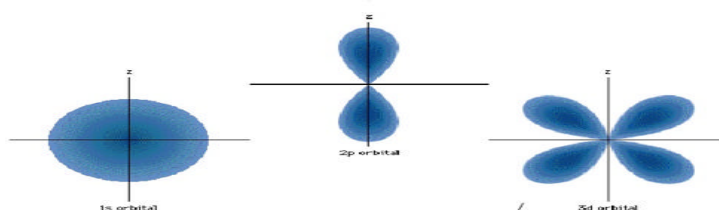
The Fourth Quantum Number, $m_s = \pm \frac{1}{2}$

- The Paulson Exclusion Principal states that no two electrons in the same atom may have identical values for all four quantum numbers.
- Because electrons act as tiny magnets, each will spin in a different direction
- This means that in the 1s shell, one electron will be $m_s = + \frac{1}{2}$, and the other $m_s = - \frac{1}{2}$

|		
n	The principal quantum number	Tells you the main energy level the electron is in
l	The secondary quantum number	Tells you what type of orbital the electron is in, the shape, (s, p, d, f, etc)
m_l	The magnetic quantum number	Tell you the orientation of the electron
m_s	The spin quantum number	Tells you the spin on the electron

Electron Configuration: Order of Filling Electrons in Atoms

- The order of filling electrons in represented to the right, following the arrows (note: you fill 4s before 3d, 5s before 4d, etc.)

n = 1   1s

n = 2   2s   2p

n = 3   3s   3p   3d

n = 4   4s   4p   4d   4f

n = 5   5s   5p   5d   5f   5g
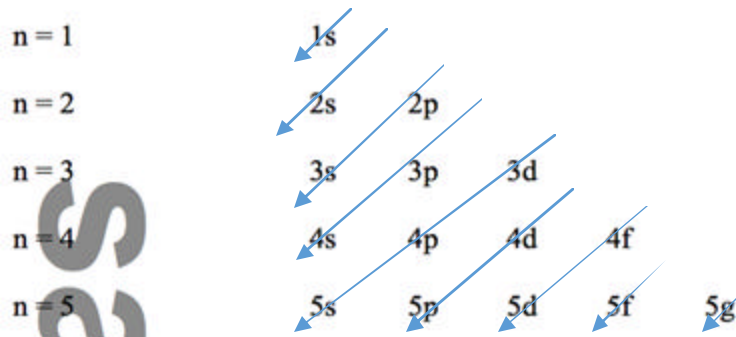
- The electrons fill according to the following set of rules:

1. The Aufbau Principal
   Each electron to an electron configuration will occupy the lowest available energy level.

2. The Pauli Exclusion Principle
   No two electrons within an atom can have the same set of quantum numbers.

3. Hund's Rule
   Electrons must be distributed among orbitals of equal energy in such a way that as many electrons remain unpaired as possible.

- The order of filling is not standard because of overlapping and intertwining between the levels, since they get so close. They are still written in a normal order because once the electrons go in, they go back to their regular position.
- There are exceptions for Cr and Cu, and the elements underneath them.
- Abbreviations can be written, starting with the Noble Gas and the electrons following that ie. K can be written as $[Ar]4s^1$

- Isoelectronic ions are those which have the same number of electrons
  ie. N^{3-} $[He]2s2p^6$ and O^{2-} $[He]2s^22p^6$ are isoelectronic
- Can also tell us which has the most unpaired electrons, can tell you if electrons in degenerate orbitals are paired or not with the strength of them, since paired ones cancel each other's effects.

- IE exceptions can be explained with electron configurations:
- Be $1s^22s^2$ and B $1s^22s^22p^1$
  Be has a much higher IE than B, despite B being further across the period. This is because 2p is farther from the nucleus and requires less energy to take. The same applies for Mg and Al.
- N $1s^22s^22p^3$ and O $1s^22s^22p^4$
  N has a higher IE, despite O being further across the period. This is because O has a pair of electrons, and N has an unpaired electron, thus the repulsion makes it easier to take an electron away from O.

- Orbital diagrams for P look like this

Orbital Diagram for Phosphorus

1s   2s   2p   3s   3p
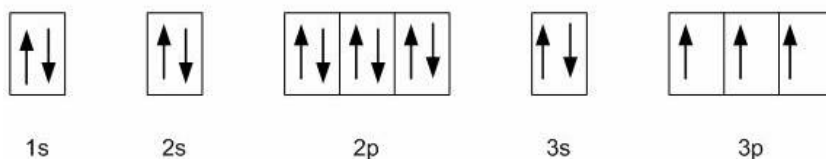
Alpha Radiation:
Alpha particles are the heaviest forms of radiation, and thus they are the relatively lowest speed. Also due to this, they can be stopped by a 3-cm layer of air, or a sheet of paper. Alpha radiation is composed of a single helium atom, with 2 protons and 2 neutrons. The Alpha particles are positively charged. Alpha particles also do not travel in waves. 1/10 of c

Beta Radiation:
Beta particles are much lighter energy particles, and thus they are faster than alpha particles but not as fast as gamma rays. Also due to this, they can be stopped by an aluminium sheet a few millimetres thick or by 3 metres of air. The beta particle is an energetic electron given off by the nucleus of unstable isotopes, and thus they are negatively charged. They also do not travel in waves. 9/10 of c

Gamma Radiation:
The gamma ray is a high-energy "X-ray". It is an energetic photon or light wave in the same electromagnetic family as light and x-rays, and are relatively quick compared to beta and alpha particles. They can be stopped by concrete, lead, or steel. They have neutral charges, and can easily damage living cells with their high energy. 10/10 of c