FORMATION REACTIONS

- A reaction that forms exactly one mole of the specified substance from its elements at their STANDARD STATE at 25C and 1 atm pressure.

(O2(g):
$$(s,graphite) + O2(g) \rightarrow (O2(g);\Delta H=-393.5 kJ)$$

heat of formation of carbon dioxide $\Delta H_{\epsilon}^{\circ}$ or ΔH_{ϵ}
"enthal py of formation"
 $(s,graphite) + \frac{1}{2}O2(g) \rightarrow (O(g);\Delta H=-110.5 kJ)$

you may see fractional coefficients in these formation reactions, because you MUST form exactly one mole of the product!

- The heat of formation for an element in its standard state at 25C and 1 atm is ZERO.

- What are formation reactions good for?

... finding enthalpies for more interesting reactions!

Let's say we would like to find the enthalpy of reaction for this equation:

 $2(2H_2(g) + 5O_2(g) \longrightarrow 4(O_1(g) + 2H_2O(g); \Delta H = 1)$

Hess' Law: If you add two reactions to get a new reaction, their enthalpies also add.

$$Co_{2}$$
 $Co_{2}(g) \rightarrow Co_{2}(g) \Delta H = -393.5$

$$H_{20}$$
, $H_{2}(q) + \frac{1}{2}O_{2}(q) \longrightarrow H_{2}O(q) \Delta H_{2}^{-2}(q)$

$$(2H_2l_g)$$
 $\rightarrow 2(s) + H_2(g)$
 $(2H_2l_g)$ $\rightarrow 2(s) + H_2(g)$

$$\begin{array}{cccc} C(s) & + & O_2(s) & \longrightarrow & CO_2(s) \\ C(s) & + & O_2(s) & \longrightarrow & CO_2(s) \end{array}$$

$$\longrightarrow (O_2(g)$$

$$\begin{array}{cccc} (\zeta(s) + O_2(g) & \longrightarrow & (O_2(g) \\ (s) + O_2(g) & \longrightarrow & (O_2(g) \end{array}$$

$$\rightarrow (0_2(g))$$
 $\Delta H = -393.5$
 $\rightarrow (0_2(g))$ $\Delta H = -393.5$

$$|H_2(q)| + \frac{1}{2}O_2(q) \longrightarrow$$

 $|H_2(q)| + \frac{1}{2}O_2(q) \longrightarrow$

DH = -226.7

DH = -226.7

DH = -393.5

2(2H2(g) + SOz(g) -> 4CO2(4) + 2H20(l)

Hess' Law using enthalpy of formation:

$$\Delta H = \sum_{0} \Delta H_{f,pNJNLt_{S}} - \sum_{0} \Delta M_{f,mnchnt_{S}}$$

$$\frac{226.7}{2(2H_{2}(g) + 5O_{2}(g))} \rightarrow \frac{393.5}{4(O_{2}(g) + 2H_{2}O(g); \Delta H_{2}}$$

$$\Delta H = \left[4(-393.5) + 2(-241.8)\right] - \left[2(226.7) + 5(0)\right]$$

$$= -2511 \text{ kJ}$$

See Appendix C in the textbook for enthalpy of formation data: p A-8 to A-11

* Remember:

- Multiply each enthalpy by its stoichiometric coefficient from the reaction
- Enthalpy of formation of an element at its standard state is zero
- Watch phase labels. You will usually find SEVERAL enthalpies of formation for a given substance in different phases!
- For ionic substances in solution, remember that they exist as free ions, so look up the aqueous IONS!

Heat of formation / enthalpy of formation!
$$-20.50$$

$$0$$

$$-285.8$$

$$-296.8$$

$$2 H_2 S(g) + 3 O_2(g) \longrightarrow 2 H_2 O(l) + 2 SO_2(g)$$

$$(Anpendix ())$$

What is the enthalpy change at standard conditions when 25.0 grams of hydrogen sulfide gas is reacted?

- 1 Calculate the enthalpy change for the reaction AS WRITTEN using Hess's Law
- 2 Convert 25.0 g hydrogen sulfide to moles. Use FORMULA WEIGHT.
- 3 Convert moles hydrogen sulfide to enthalpy change. Use THERMOCHEMICAL EQUATION.

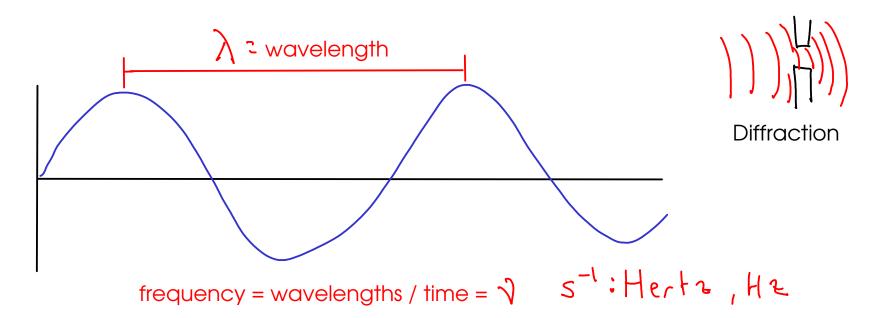
$$\Delta H = \sum \Delta H_{f,prod} - \sum \Delta H_{f,reach}$$

$$= \sum (-285.8) + 2(-296.8) - [2(-20.50) + 3(0)] = -1124.2 \text{ kJ}$$
So the THERMOCHEMICAL EQUATION is ...
$$2 H_2S(g) + 3 O_2(g) \longrightarrow 2 H_2O(l) + 2 SO_2(g) + \Delta H_2 = -1124.2 \text{ kJ}$$

$$= \sum 34.086 \text{ g} \text{ H}_2S = \text{mol H}_2S = -1124.2 \text{ kJ}$$

$$= \sum 34.086 \text{ g} \text{ H}_2S \times \frac{\text{mol H}_2S}{34.086 \text{ g} \text{ H}_2S} \times \frac{-1124.2 \text{ kJ}}{2 \text{ mol H}_2S} = -412 \text{ kJ}$$

LIGHT



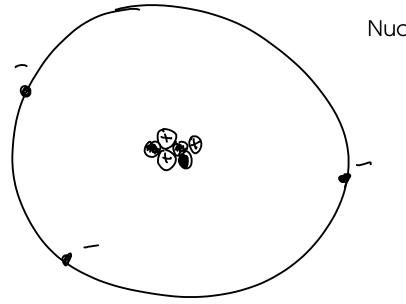
- Light has properties of WAVES such as DIFFRACTION (it bends around small obstructions).
- Einstein noted that viewing light as a particle that carried an energy proportional to the FREQUENCY could explain the PHOTOELECTRIC EFFECT!

Ephoton =
$$\frac{1}{2}$$
 Planck's constant: 6-63×10⁻³⁴ J-s

photon = particle or packet of light

(The photoelectric effect is the emission of electrons from a metal caused by exposure to light. Einstein discovered that if the light were not of the correct FREQUENCY, increasing the INTENSITY of the light would not cause electron emission. He concluded that individual photons must have enough energy to excite an electron - i.e. they must have the appropriate frequency.)

The photoelectric effect and Einstein's ideas about the energy content of light led us to discover a new model for the atom! How? Let's start with the nuclear model:



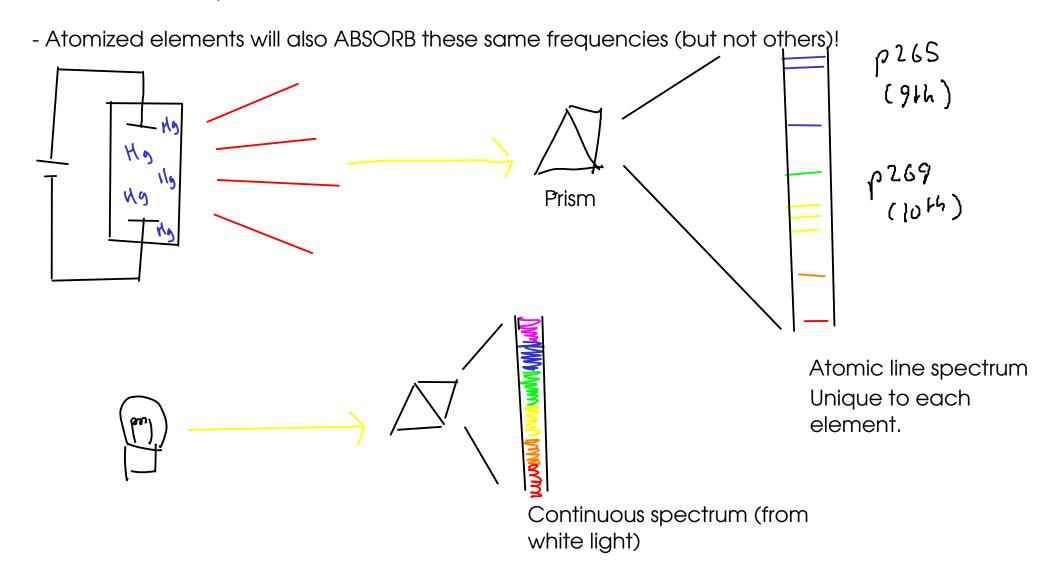
Nuclear model:

- Protons and neutrons in a dense NUCLEUS at center of atom
- Electrons in a diffuse (mostly empty)
 ELECTRON CLOUD surrounding
 NUCLEUS.

... so what's wrong with the nuclear model? Among other things, it doesn't explain ...

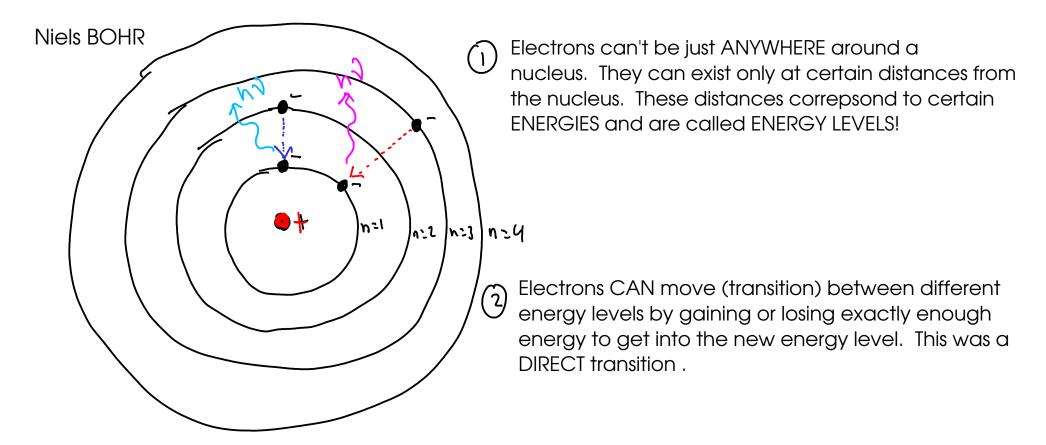
ATOMIC LINE SPECTRA

- if you take element and ATOMIZE it, if excited by energy it will emit light at unique frequencies. The set of emitted frequencies is called an ATOMIC LINE SPECTRUM.



... so, why don't atoms by themselves emit continuous spectra like a flashlight would?

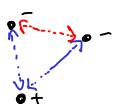
- The regular patterns of emission and absorption of light by atoms suggest that the electron cloud has some sort of regular structure. The specific frequencies of light emitted and abosrbed relate to specific values of ENERGY in the electron cloud.



Bohr's model was the first proposal that predicted the existence of atomic line spectra, and it exactly predicted the spectra of hydrogen and "hydrogen-like" (i.e. one-electron) species.

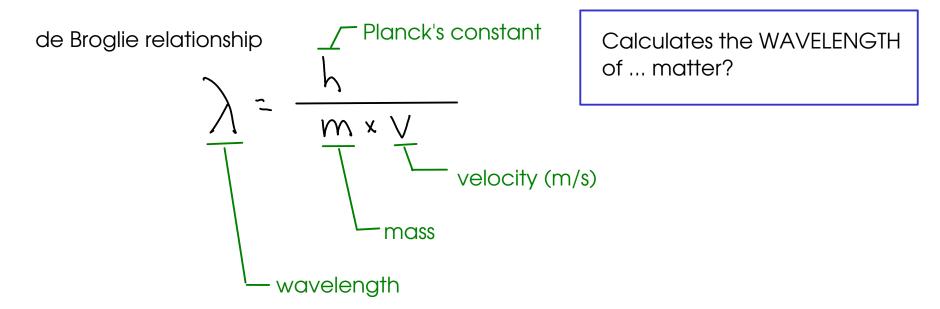
The spectra were "off" for multi-electron atoms.





Multi-electron atoms have interactions between electrons, not just interactions between electrons and nucleus!

- The additional interactions in multi-electron atoms introduced added complexity to the model of the atom! Bohr's model was too simple.
- Improvements in Bohr's model came from treating electrons as WAVES.



... for very large particles, the wavelength is very small.

- To describe the electrons, we use WAVEFUNCTIONs which are mathematical descriptions of the behavior or electrons.
- The wavefunction describes the probability of finding an electron in a given space
- For larger objects, the wave behavior isn't very important and quantum mechanics becomes traditional Newtonian physics.

When we talk about describing electrons ... we will talk about the PARAMETERS that go into this WAVEFUNCTION ... without doing the actual math.

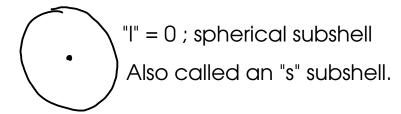
- There are FOUR of these parameters. (the Bohr model had only one!)
- The parameters are called "quantum numbers"
 - Principal quantum number
 - (1) Angular momentum quantum number
 - 3 Magnetic quantum number
 - (4)Spin quantum number

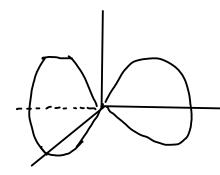
- Giving the four parameters will uniquely identify an electron around an atom. No two electrons in the same atom can share all four. These parameters are called QUANTUM NUMBERS.

- PRINCIPAL QUANTUM NUMBER (n):
 - "energy level", "shell"
 - Represents two things:
 - * The distance of the electron from the nucleus.
 - * Energy. "n" is one factor that contributes to the energy of the electron.

- ANGULAR MOMENTUM QUANTUM NUMBER: χ
 - "subshell"
 - Represents the SHAPE of the region of space where the electron is found.
 - (Bohr assumed CIRCULAR orbits for electrons ... but there are more possibilities.)
 - -"I" also contributes ENERGY. Higher values for "I" mean the electron has higher energy.

$$l = 0$$
 to $n-1$, integers $n=1$; $l=0$



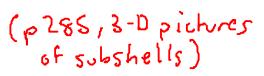


"I"=1; dumbbell shaped
Also called a "p" subshell

"I"=2; flower-shaped

Also called a "d" subshell

Higher values for "I" translate to higher energies for the electron!



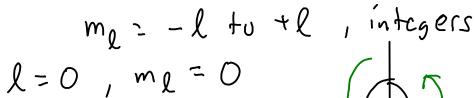
For convenience, and partially for historical reasons, we use letters to $(\rho 290, 0)$ designate the different subshells.

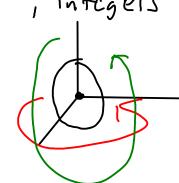
The rest follow the alphabet

(3) MAGNETIC QUANTUM NUMBER \mathfrak{M}_{\emptyset}

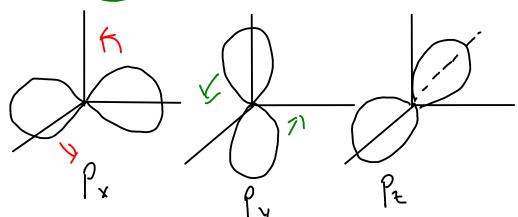
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- Represents the ORIENTATION of a subshell in 3D space.





There is only one possible orientation for an "s" subshell!



There are THREE possible orientations for a "p"

subshell!

$$l=2$$
, $m_e=-2$, -1 , 0 , 1 , 2 (five orentations)

 $picture$
 $p285$,

 $p290$ (fenth)

$$l=3$$
, $m_e=-3$, -2 , -1 , 0 , 1 , 2 , 3 (seven orentations)

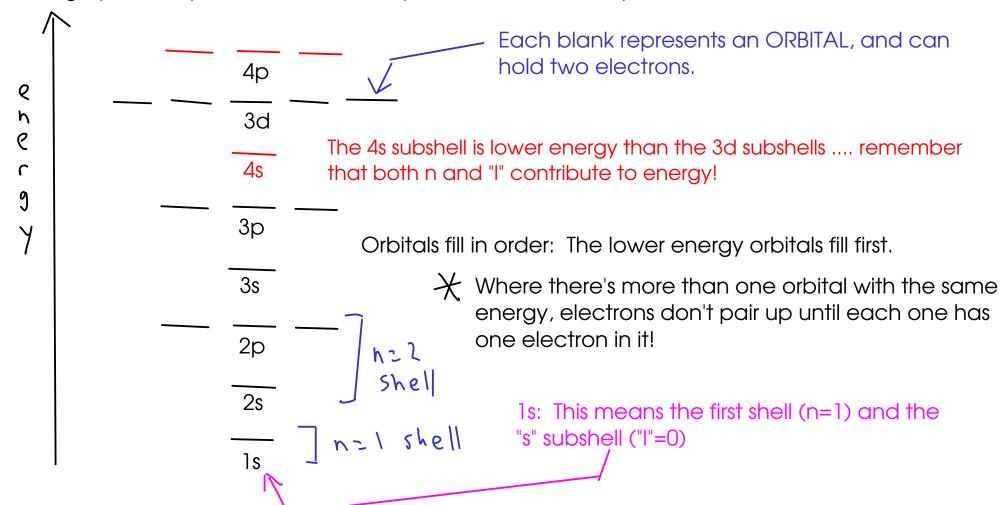
... all the arrangements of a single subshell have the same energy. The magnetic quantum number DOESN'T contribute to the energy of an electron.

(MAGNETIC) SPIN QUANTUM NUMBER: MS MS = -1/2 of 1/2 "spin down" or "spin up"

- An ORBITAL (region with fixed "n", "I" and "mI" values) can hold TWO electrons.

ORBITAL DIAGRAM

- A graphical representation of the quantum number "map" of electrons around an atom.



4p

3р

3s

2р

1s

How would an orbital diagram for the element POTASSIUM look?

$$K$$
, $\frac{2}{2} = 19$

Electrons in the outermost shell of an atom are called VALENCE electrons. THESE electrons are normally involved in chemical bonding.

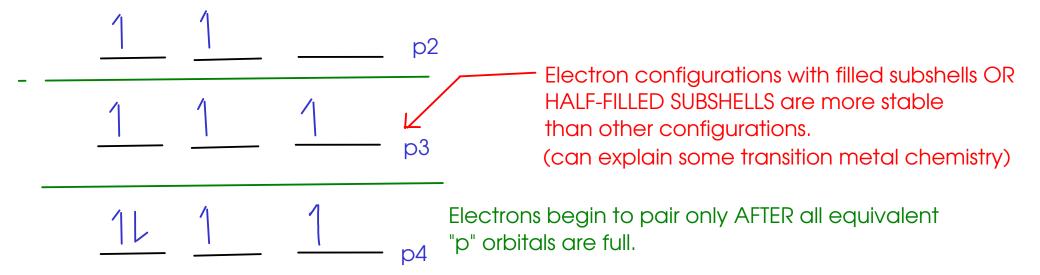
Remember: Potassium tends to lose a single electron (forming a cation) in chemical reactions.

A note on chemical bonding and electron arrangement:

- Filled and half-filled subshells seem to be preferred by atoms.

Hund's Rule

- When you have two or more orbitals with equivalent energy, electrons will go into each equivalent orbital BEFORE pairing. Pairing costs a bit of energy - less than going to a higher-energy orbital, but more than going to another equivalent orbital.

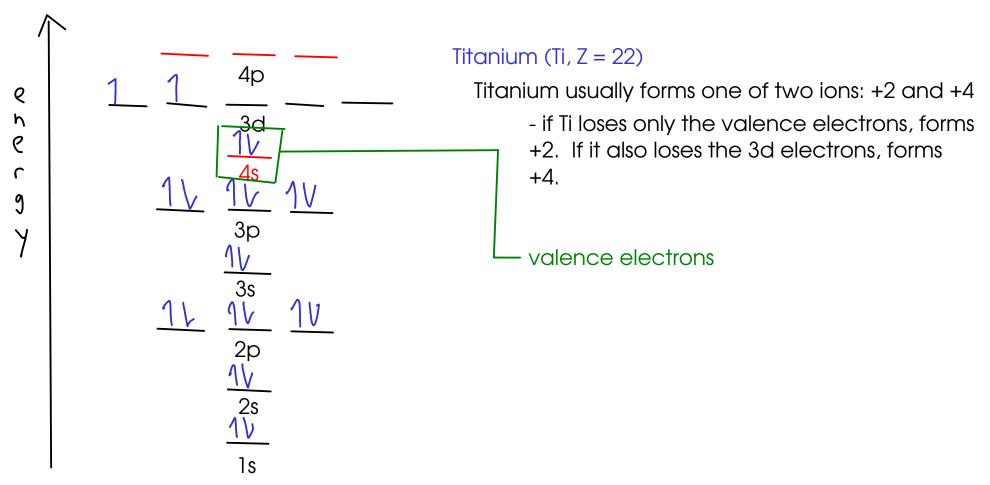


Experimental evidence for Hund's rule:

"Paramagnetism" - attraction of an atom to a magnetic field

- Spinning electrons are magnetic, but OPPOSITE spins cancel each other out.
- Atoms with unpaired electrons are paramagnetic, while atoms containing only paired electrons are not.

A little bit about transition metals...



- Most transition metals have TWO valence electrons (in an "s" subshell), and the other ions they form come from electron loss in "d" subshells.