$$CH_3COCH_3(l) + 4O_2(g) \rightarrow 3CO_2(g) + \underline{\underline{3}}H_2O(l) \; ; \Delta H = \underline{\underline{-1800 \text{ kJ}}}$$

What would be the enthapy change when 25 g of water are produced by the reaction?

$18.02 \text{ g } H_2O = \text{mol } H_2O \qquad -1800 \text{ kJ} = 3 \text{ mol } H_2O$

$$25 \text{ g } H_2O \times \frac{\text{mol}}{18.02 \text{ g}} \times \frac{-1800 \text{ kJ}}{3 \text{ mol } H_2O} = \boxed{-830 \text{ kJ} = \Delta H}$$

This is the heat at constant pressure, too!

A few more terms related to enthalpy:

- Enthalpy of vaporization / heat of vaporization: The enthalpy change on vaporizing one mole of a substance. (from liquid to vapor)

- Enthalpy of fusion / heat of fusion: The enthalpy change when a mole of liquid changes to the solid state.

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.

$$CO_2(g): C(s, \text{graphite}) + O_2(g) \longrightarrow CO_2(g) \; ; \Delta H = \underline{-393.5 \text{ kJ}}$$

heat of formation of carbon dioxide ΔH_f° or ΔH_f

$$CO(g): C(s, \text{graphite}) + \underline{\underline{\tfrac{1}{2}}} O_2(g) \rightarrow CO(g) \; ; \Delta H = -110.5 \text{ kJ}$$

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?

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

$$2C_2H_2(g) + 5O_2(g) \longrightarrow 4CO_2(g) + 2H_2O(g) \; ; \; \Delta H = ? \; -2511 \text{ kJ}$$

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

C_2H_2: $2C(s) + H_2(g) \longrightarrow C_2H_2(g) \quad \Delta H = 226.7$

CO_2: $C(s) + O_2(g) \longrightarrow CO_2(g) \quad \Delta H = -393.5$

H_2O: $H_2(g) + \frac{1}{2}O_2(g) \longrightarrow H_2O(g) \quad \Delta H = -241.8$

$$2C_2H_2(g) \longrightarrow \boxed{4C(s)} + \boxed{2H_2(g)} \; ; \; \Delta H = -2(226.7)$$

$$\boxed{4C(s)} + 4O_2(g) \longrightarrow 4CO_2(g) \; ; \; \Delta H = 4(-393.5)$$

$$\boxed{2H_2(g)} + O_2(g) \longrightarrow 2H_2O(g) \; ; \; \Delta H = 2(-241.8)$$

$$2C_2H_2(g) + 5O_2(g) \rightarrow 4CO_2(g) + 2H_2O \; ; \; \Delta H = -2(226.7) + 4(-393.5) + 2(-241.8) = -2511 \text{ kJ}$$

Hess' Law using enthalpy of formation:

$$\Delta H = \sum \Delta H_{f,\,products} - \sum \Delta H_{f,\,reactants}$$

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

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

* Remember:

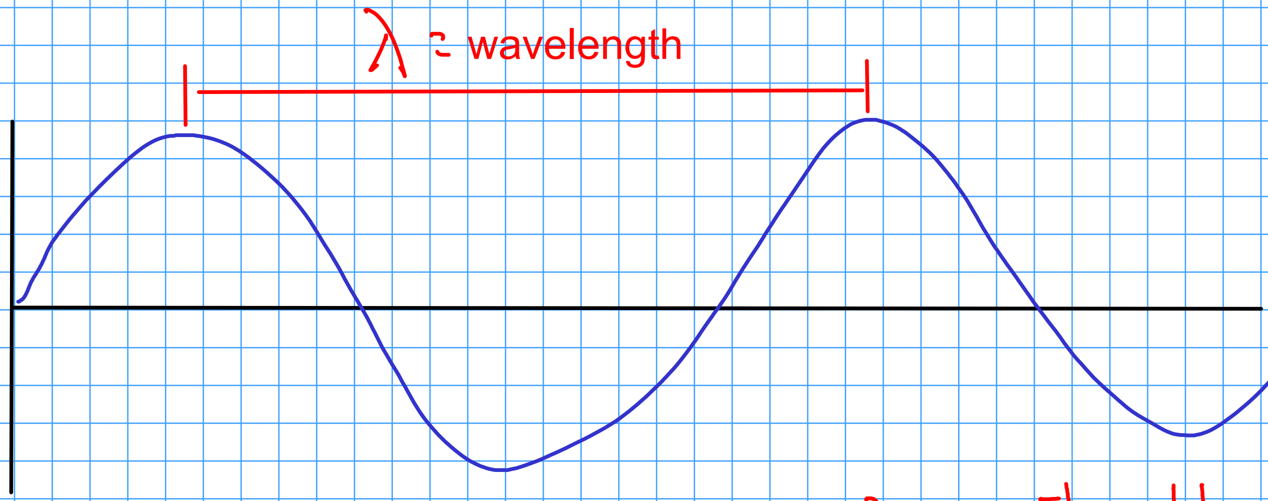
- Multiply each enthalpy by its stoichiometric coefficient from the reaction

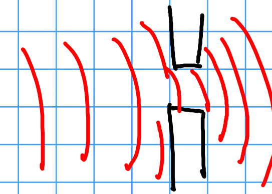
- Enthalpy of formation of an element at its standard state is zero

- 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!

LIGHT





frequency = wavelengths / time = ν s^{-1} Hertz, Hz

- 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!

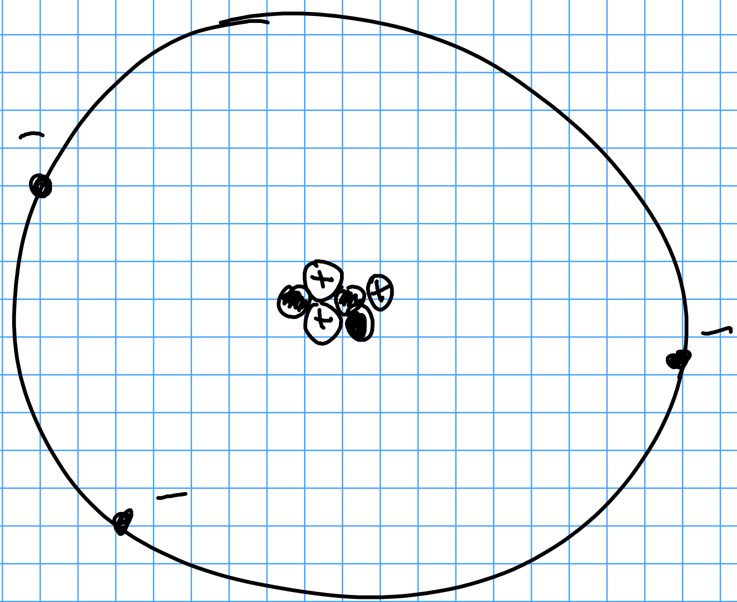
$$E_{photon} = h\nu$$

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.

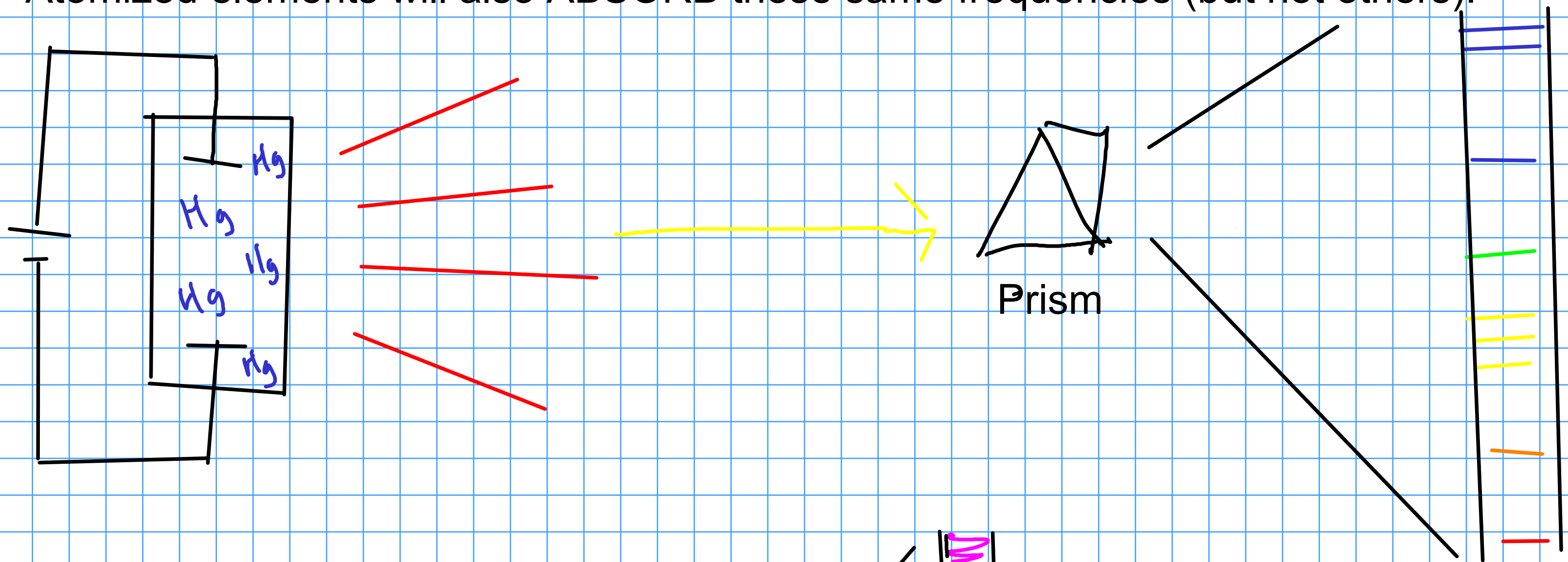
... so what's wrong with the nuclear model? Among other things, it doesn't explain ...

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.

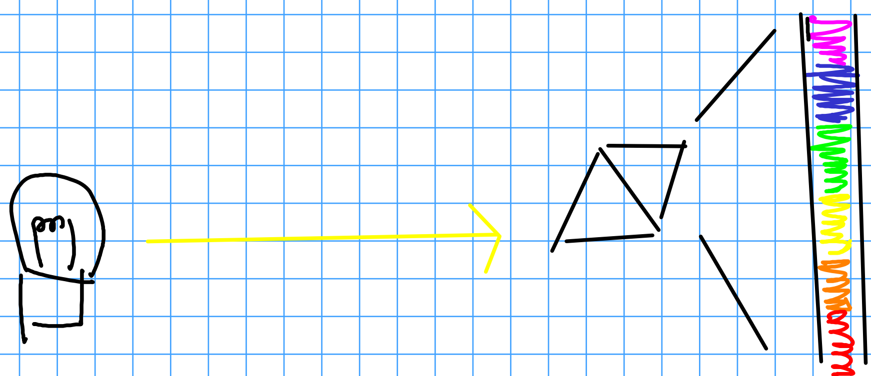
- Atomized elements will also ABSORB these same frequencies (but not others)!

p266



Atomic line spectrum

Unique to each element.

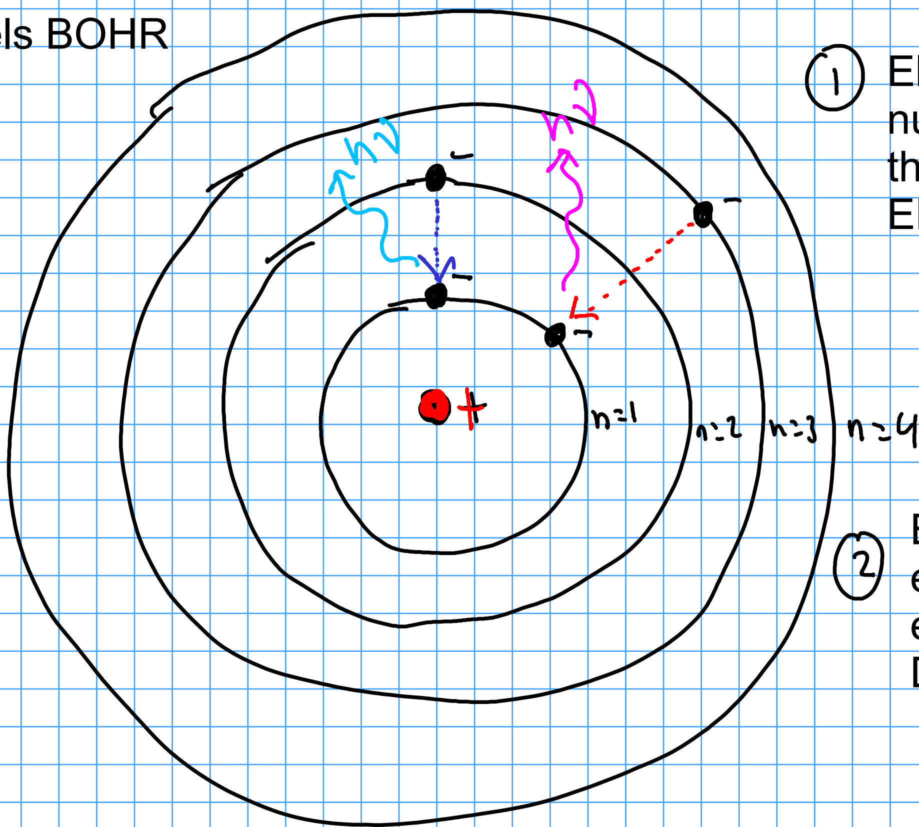


Continuous spectrum (from white light)

... 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.

Niels BOHR

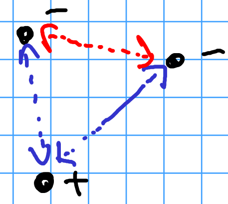


1. Electrons can't be just ANYWHERE around a nucleus. They can exist only at certain distances from the nucleus. These distances correpsond to certain ENERGIES and are called ENERGY LEVELS!

2. Electrons CAN move (transition) between different energy levels by gaining or losing exactly enough energy to get into the new energy level. This was a DIRECT transition .

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.

de Broglie relationship

Planck's constant

$$\lambda = \frac{h}{m \times v}$$

Calculates the WAVLENGTH of ... matter?

velocity (m/s)

mass

wavelength

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

Quantum mechanics treats the electrons as waves and models THAT behavior

- To describe the electrons, we use WAVEFUNCTION - which is a mathematical description of the behavior or electrons.

- The wavefucntion 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.

$$y = 14 + x + \frac{3}{x}$$

$$\Big\downarrow \text{ for large } x$$

$$y = 14 + x$$

When we talk about describing electrons ... we will talk about the PARAMETERS that go into this WAVEFUNCTION ... essentually, the SOLUTIONS to the wavefunction!

- There are FOUR of these parameters. (the Bohr model had only one!)

- 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.

1. 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.

$n = 1, 2, 3, 4, \ldots$ (integers)

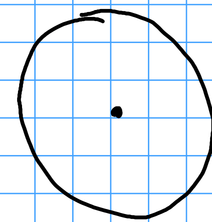
2. ANGULAR MOMENTUM QUANTUM NUMBER: ℓ

- "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.)

-"l" also contributes ENERGY. Higher values for "l" mean the electron has higher energy.

$\ell = 0$ to $n-1$, integers.

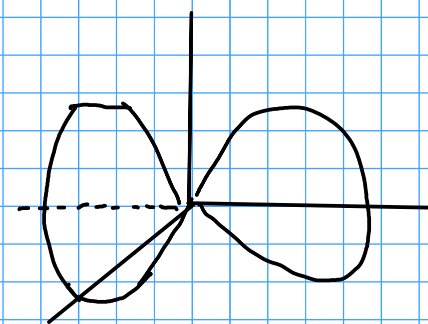
$n=1$; $\ell = 0$



"l" = 0 ; speherical subshell

Also called an "s" subshell.

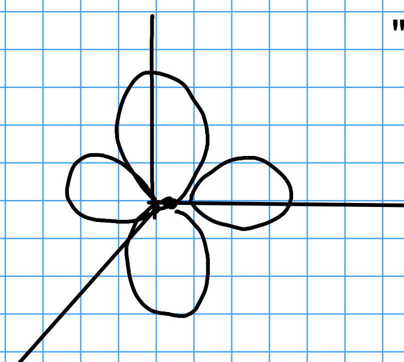
$n=2$; $\ell = 0, 1$



"l"=1 ; dumbbell shaped

Also called a "p" subshell

$n=3$, $\ell = 0, 1, 2$



"l"=2; flower-shaped

Also called a "d" subshell

letter designations for subshells:

$\ell = 0$ "s"

$\ell = 1$ "p"

$\ell = 2$ "d"

$\ell = 3$ "f"

$\ell = 4$ "g"

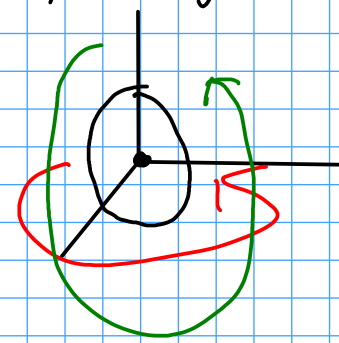
↓ follow alphabet.

3 MAGNETIC QUANTUM NUMBER m_ℓ

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

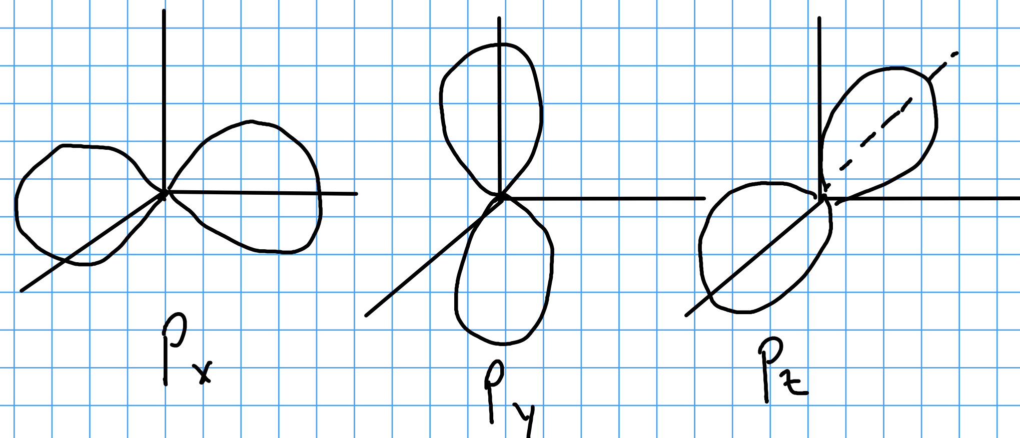
$m_\ell = -\ell$ to $+\ell$, integers

$\ell = 0$, $m_\ell = 0$



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

$\ell = 1$; $m_\ell = -1, 0, 1$



There are THREE possible orientations for a "p" subshell!

$\ell = 2$, $m_\ell = -2, -1, 0, 1, 2$ (five orentations)

$\ell = 3$, $m_\ell = -3, -2, -1, 0, 1, 2, 3$ (seven orentations)

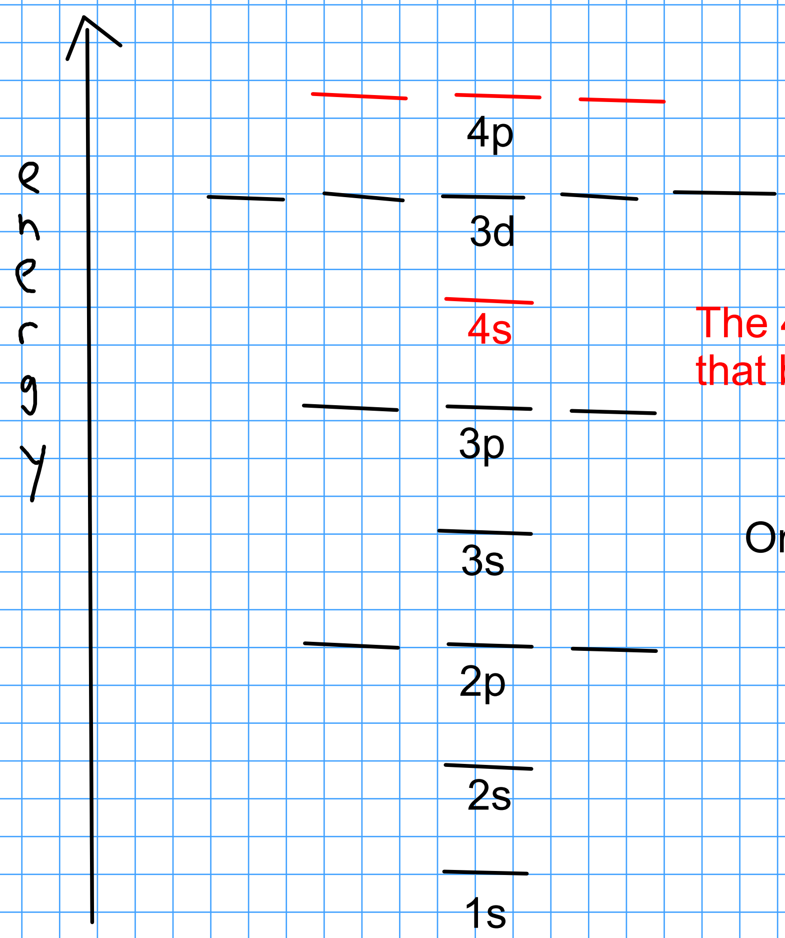
4 (MAGNETIC) SPIN QUANTUM NUMBER: m_s

$m_s = -\frac{1}{2}$ OR $+\frac{1}{2}$ "spin down" or "spin up"

- Each "orbital" (region with fixed "n", "l" and "ml") can hold TWO electrons.

ORBITAL DIAGRAM

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

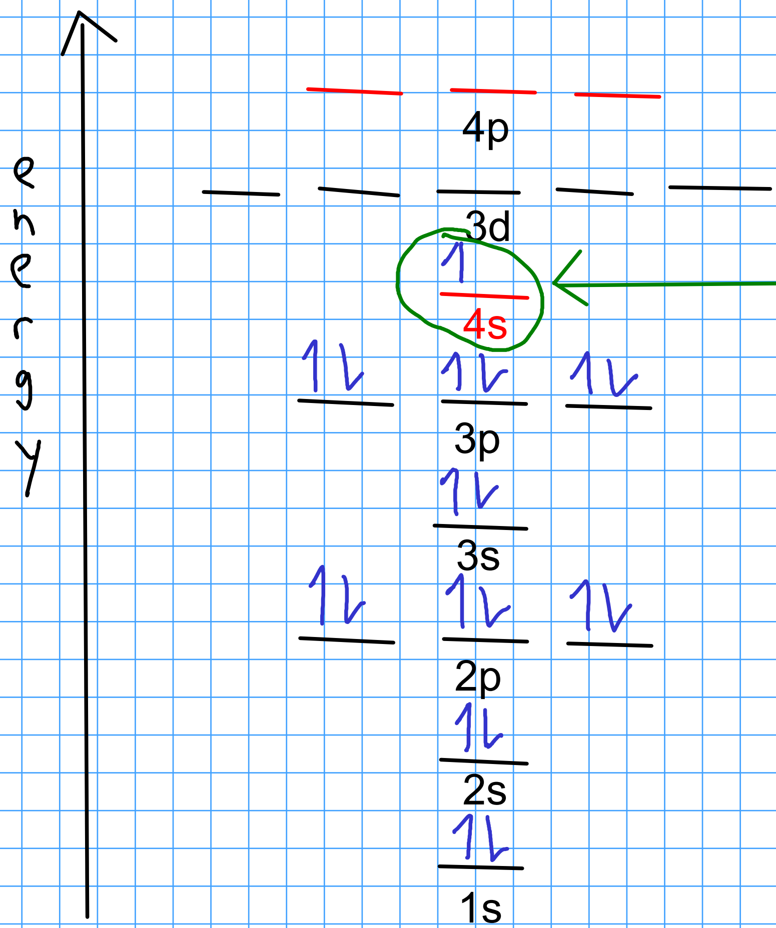


The 4s subshell is lower energy than the 3d subshells .... remember that both n and "l" contribute to energy!

Orbitals fill in order: The lower energy orbitals fill first.

Where there's more than one orbital with the same energy, electrons don't pair up until each one has one electron in it!

How would an orbital diagram for the element POTASSIUM look?

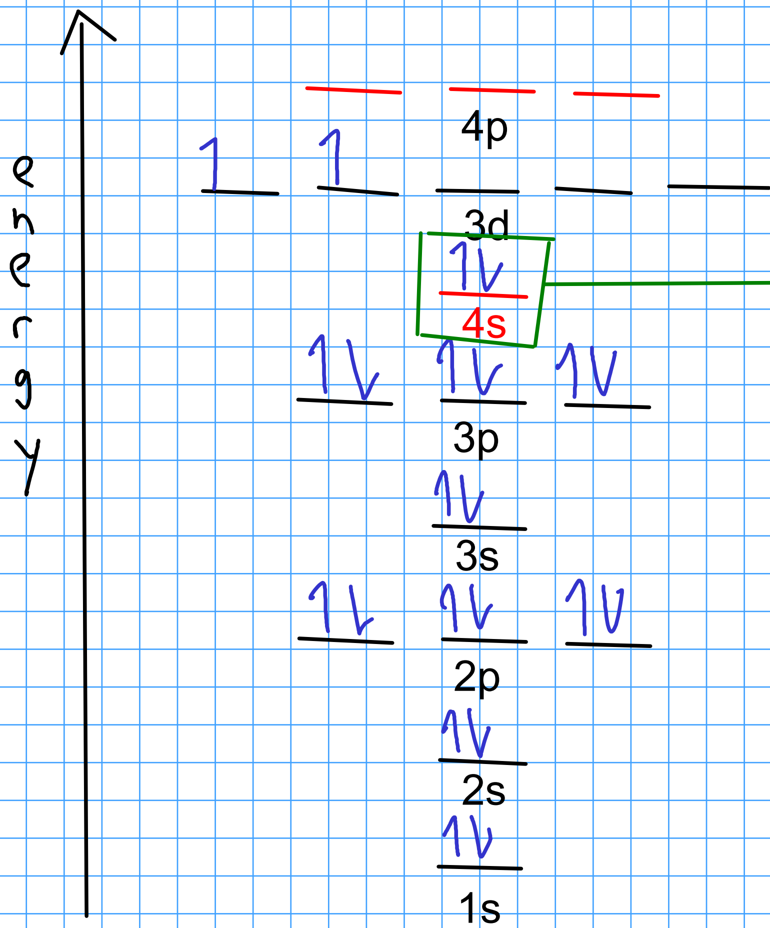


K , $\underline{Z}$ = 19

atomic number

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

A little bit about transition metals...



Titanium (Ti, Z = 22)

Titanium usually forms one of two ions: +2 and +4

- if Ti loses only the valence electrons, forms +2. If it also loses the 3d electrons, forms +4.

valence electrons

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

BONDING AND ELECTRON CONFIGURATION

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

ELECTRON CONFIGURATION (SHORT FORM)

- We can represent the electron configuration without drawing a diagram or writing down pages of quantum numbers every time. We write the "electron configuration".

# of electrons in the subshell

$$\mathrm{Ti}: 1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 \underline{4s^2}$$

ℓ

n

valence electrons

$$\mathrm{Ti}: \underline{[Ar]}\, 3d^2 \underline{4s^2}$$

valence electrons

"noble gas core". We're saying that titanium has the same electron configuration as argon does, with the addition of the electrons that follow. This is a useful shorthand, since the "core" electrons generally don't get involved in bonding.

ELECTRON CONFIGURATION AND THE PERIODIC TABLE

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	*Ac	Rf	Db	Sg	Bh	Hs	Mt									

*"inner" transition metals go here

"s" block: last electron in these atoms is in an "s" orbital!

"p" block: last electron in these atoms is in a "p" orbital!

"d" block: last electron is these atoms is in a "d" orbital

- To write an electron configuration using the periodic table, start at hydrogen, and count up the electrons until you reach your element!

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
	Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt									

*"inner" transition metals go here

Example: Phosphorus (P): $\underbrace{1s^2 2s^2 2p^6}\underbrace{3s^2 3p^3}$

$[Ne]3s^2 3p^3$

Phosphorus has five valence electrons!