Example problems:

$$2 H_2(g) + O_2(g) \longrightarrow 2 H_2O(g) \; ; \; \Delta H = -484 \; kJ$$

(2.016 above H_2)

Calculate the enthalpy change for the combustion of 1.00 kg of hydrogen gas.

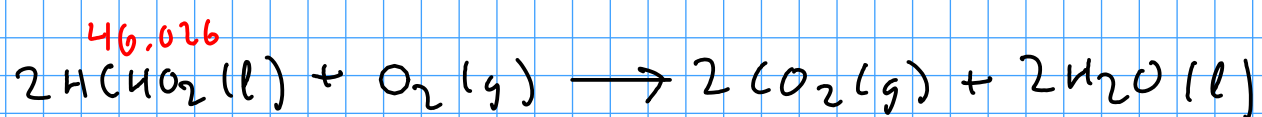$$2 \; mol \; H_2 = -484 \; kJ \qquad\qquad kg = 10^3 \; g$$

$$2.016 \; g \; H_2 = 1 \; mol \; H_2$$

$$1.00 \; kg \; H_2 \times \frac{10^3 \; g}{kg} \times \frac{1 \; mol \; H_2}{2.016 \; g \; H_2} \times \frac{-484 \; kJ}{2 \; mol \; H_2} =$$

$$-120000 \; kJ / kg$$

46.026

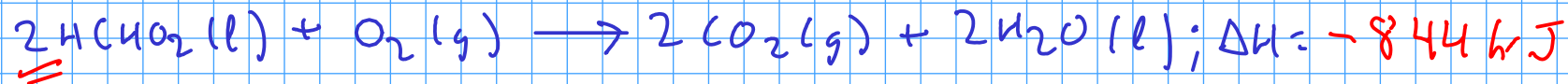$$2 \, HCHO_2 \, (l) + O_2 \, (g) \longrightarrow 2 \, CO_2 \, (g) + 2 \, H_2O \, (l)$$

If 50.3 kJ of heat was released when 5.48 g of formic acid are burned at constant pressure, then what is the enthalpy change of this reaction per mole of formic acid?
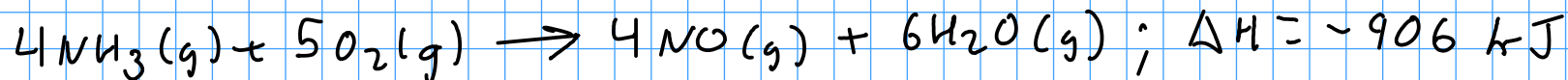
$$\Delta H = ? \quad \text{same as } Q \text{ here } = \quad \Delta H = \frac{Q}{moles}$$

$$5.48 \, g \, HCHO_2 \times \frac{mol \, HCHO_2}{46.026 \, g \, HCHO_2} = .119 \, mol$$

$$\Delta H = \frac{-50.3 \, kJ}{.119 \, mol} = -422 \, kJ/mol \, HCHO_2$$

The thermochemical equation is written in terms of TWO moles of formic acid, so the enthalpy change of this reaction as written is -844 kJ

$$2 \, HCHO_2 \, (l) + O_2 \, (g) \longrightarrow 2 \, CO_2 \, (g) + 2 \, H_2O \, (l); \; \Delta H = -844 \, kJ$$

$$4NH_3(g) + 5O_2(g) \longrightarrow 4NO(g) + 6H_2O(g) ; \Delta H = -906 \, kJ$$

What is the enthalpy change when 150. L of nitrogen monoxide are formed by this reaction at 25.0 C and 1.50 atm pressure?   4 mol NO = -906 kJ
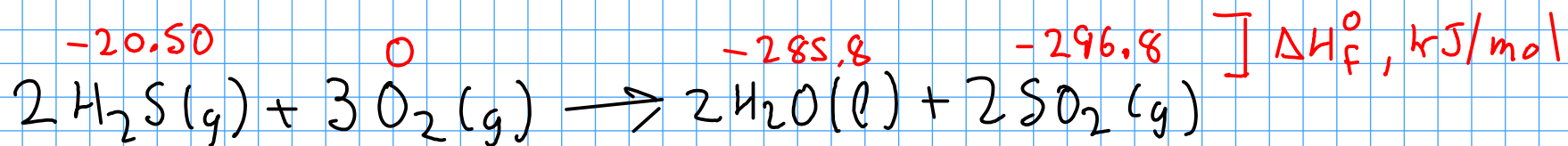
First, calculate the moles of NO formed by using the ideal gas equation. Then, use the enthalpy of reaction and the coefficient of NO in the equation to find the enthalpy change for the formation of 150. L of NO.

$$PV = nRT$$

$$n = \frac{PV}{RT} = \frac{(1.50 \, atm)(150.L)}{\left(0.08206 \frac{L \cdot atm}{mol \cdot K}\right)(298.2 K)}$$

$$= 9.19 \, mol \, NO$$

$$9.19 \, mol \, NO \times \frac{-906 \, kJ}{4 \, mol \, NO} = \boxed{-2080 \, kJ}$$

$$-20.50 \qquad 0 \qquad\qquad -285.8 \qquad -296.8 \quad] \Delta H_f^o, \, kJ/mol$$

$$2H_2S(g) + 3O_2(g) \longrightarrow 2H_2O(\ell) + 2SO_2(g)$$

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

To solve this problem, first calculate the enthalpy of reaction from standard enthalpies of formation. Use Hess's Law:
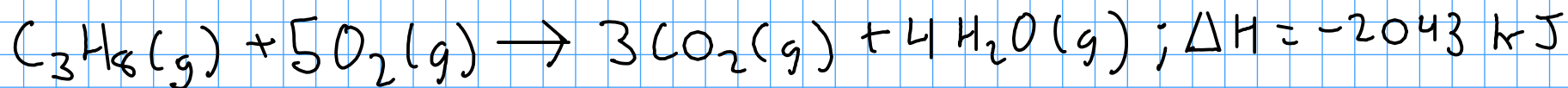
$$\Delta H = \sum \Delta H_f^o \text{ products} - \sum \Delta H_f^o \text{ reactants.}$$

$$\Delta H = 2(-285.8) + 2(-296.8) - \left[2(-20.50) + 3(0) \right]$$

$$= -1124.2 \, kJ, \text{ for rxn as written}$$

Next, we use the enthalpy or reaction to find the enthaply change for 25.0 grams of hydrogen sulfide.

$$34.08 \, g \, H_2S = 1 \, mol \, H_2S \qquad 2 \, mol \, H_2S = -1124.2 \, kJ$$

$$25.0 \, g \, H_2S \times \frac{1 \, mol \, H_2S}{34.08 \, g \, H_2S} \times \frac{-1124.2 \, kJ}{2 \, mol \, H_2S} = \boxed{-412 \, kJ}$$

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g) \; ; \Delta H = -2043 \text{ kJ}$$

Calculate the volume of propane gas at 25 C and 1.08 atm required to provide 565 kJ of heat using the reaction above.

298.2 K

To solve this problem, you need to start with the heat: 565 kJ. From the point of view of the propane, this is negative. The reaction releases energy, and is exothermic.

$$1 \text{ mol } C_3H_8 = -2043 \text{ kJ}$$

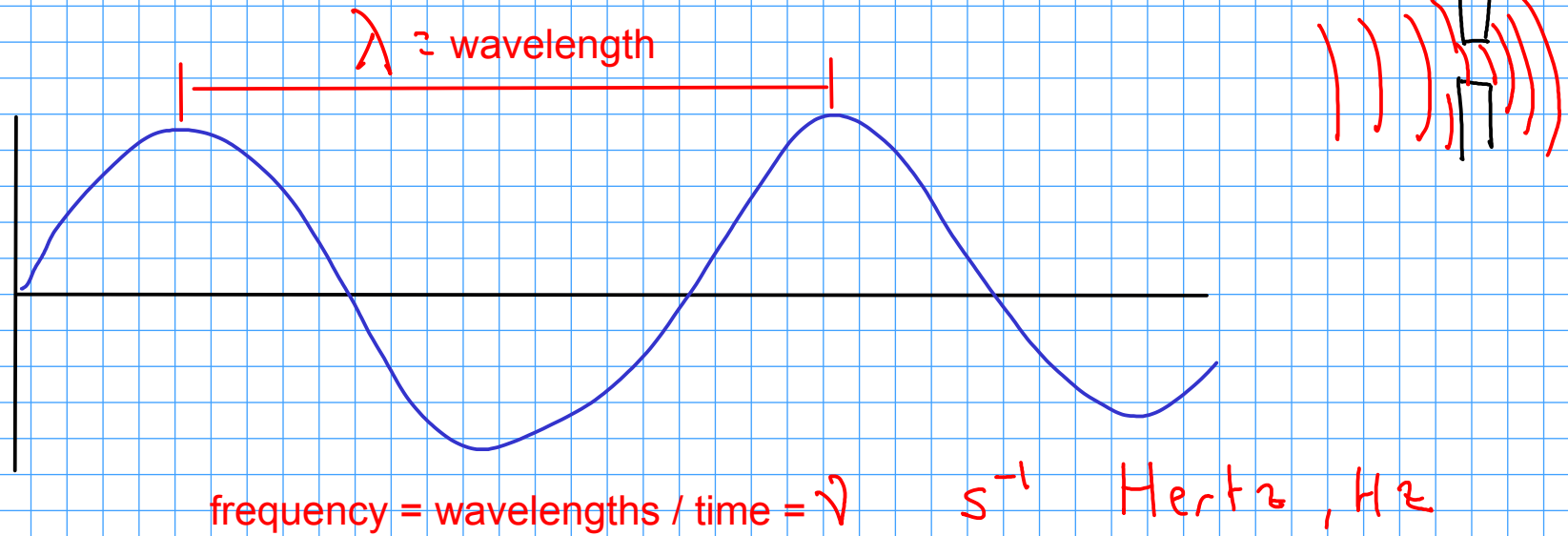$$-565 \text{ kJ} \times \frac{1 \text{ mol } C_3H_8}{-2043 \text{ kJ}} = 0.27655 \text{ mol } C_3H_8 = n$$

Now, find the volume of propane gas required using the ideal gas equation.

$$V = \frac{nRT}{P} = \frac{(0.27655 \text{ mol } C_3H_8)(0.08206 \frac{L \cdot atm}{mol \cdot k})(298.2 k)}{(1.08 \text{ atm})}$$

$$= \boxed{6.27 \text{ L}}$$

LIGHT

λ = wavelength

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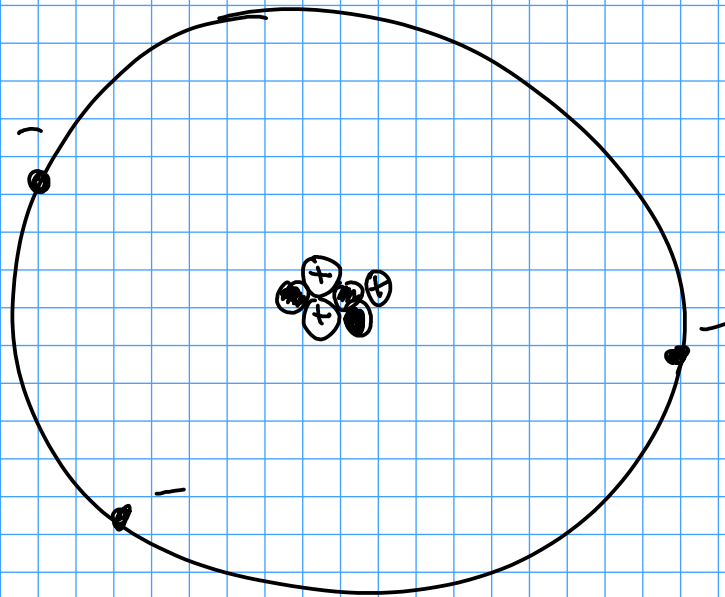
$$E_{photon} = h\nu$$

Planck's constant: 6.63×10^{-34} J·s

photon = particle or packet of light

The photoelectric effect 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:
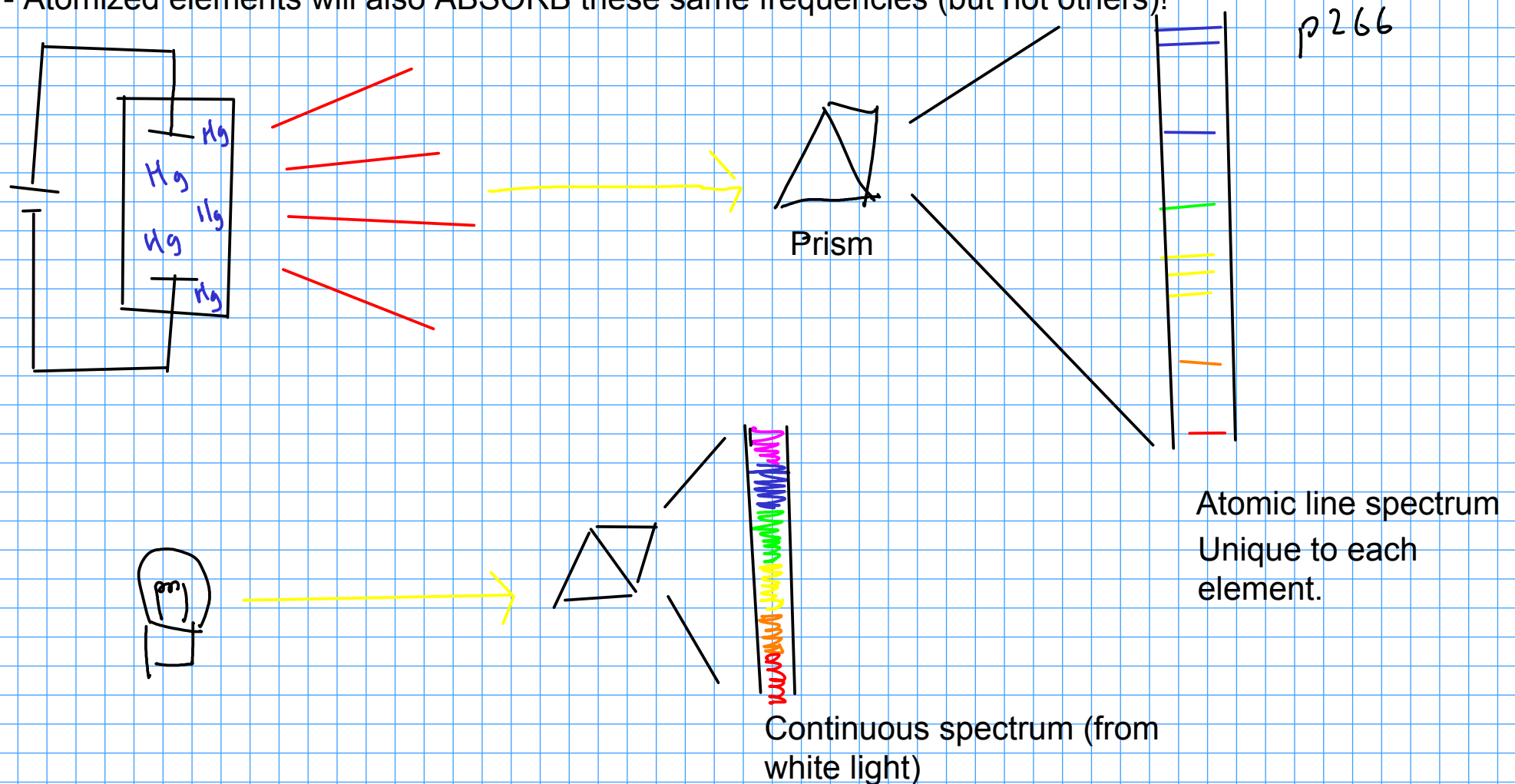

Nuclear model:

- 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

Hg   Hg   Hg   Hg   Hg

Prism

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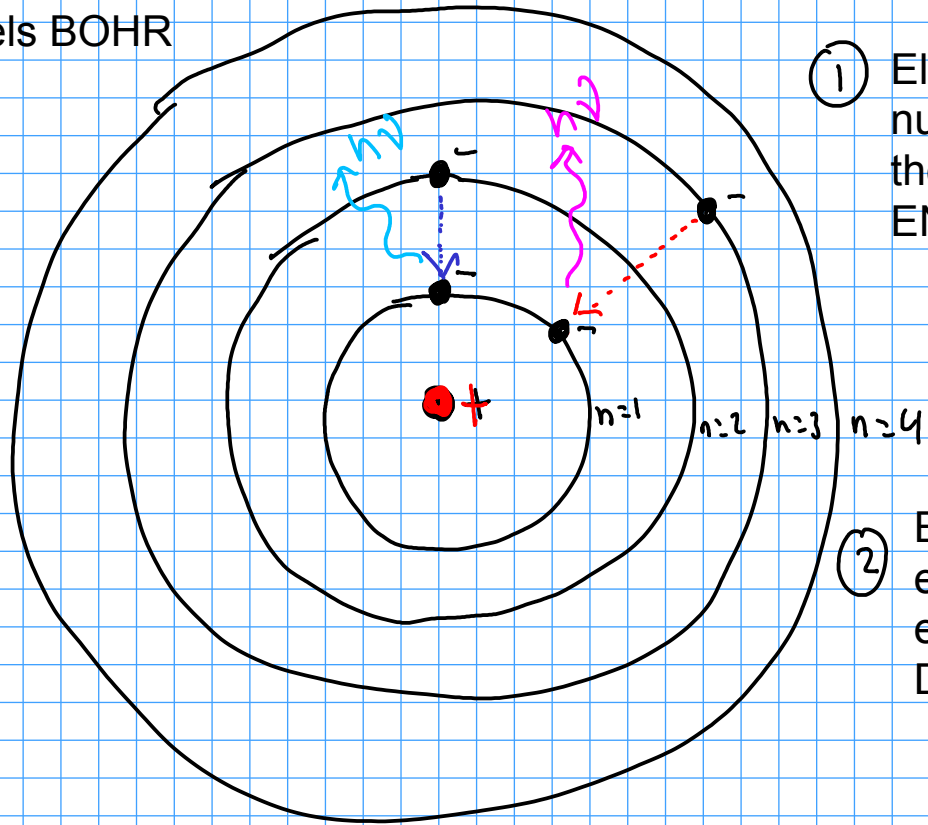
(1) Electrons can't be just ANYWHERE around a nucleus. They can exist only at certain distances from the nucleus. These distances correpsond to certain ENERGIES and are called ENERGY LEVELS!

$n=1$ $n=2$ $n=3$ $n=4$

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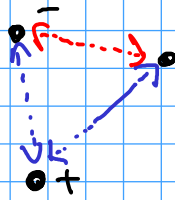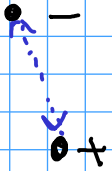
Multi-electron atoms have interactions between electrons, not just interactions between electrons and nucleus!

- 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 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"

① Principal quantum number

② 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.

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.

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

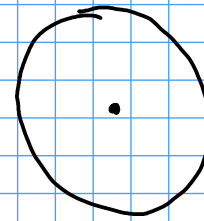② ANGULAR MOMENTUM QUANTUM NUMBER: ℓ

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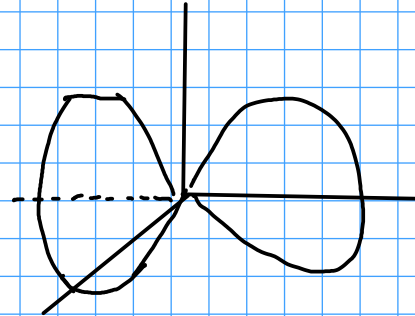
$\ell = 0$ to $n-1$, integers

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

"l" = 0 ; speherical subshell
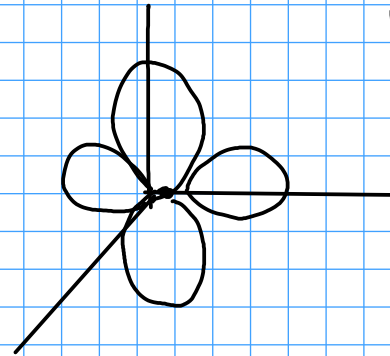
Also called an "s" subshell.

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

"l"=1 ; dumbbell shaped

Also called a "p" subshell

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

"l"=2; flower-shaped

Also called a "d" subshell

For convenience, and partially for historical reasons, we use letters to designate the different subshells.

$\ell = 0$ "s" $\ell = 2$ "d" $\ell = 4$ "g"
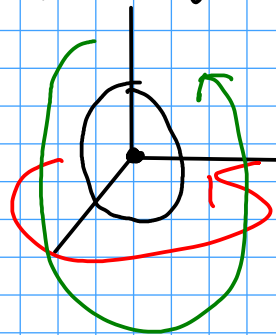
$\ell = 1$ "p" $\ell = 3$ "f"   The rest follow the alphabet

③ MAGNETIC QUANTUM NUMBER m_ℓ
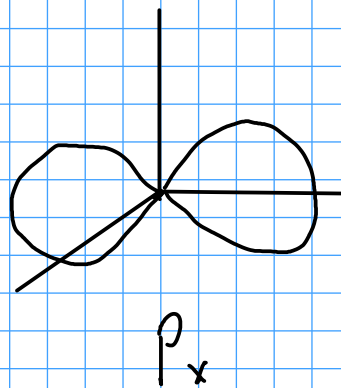
- Represents the ORIENTATION of a subshell in 3D space.

$$m_\ell = -\ell \text{ to } +\ell \text{ , integers}$$

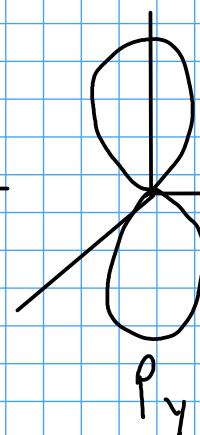$$\ell = 0 \text{ , } m_\ell = 0$$

There is only one possible orientation for an "s" subshell!
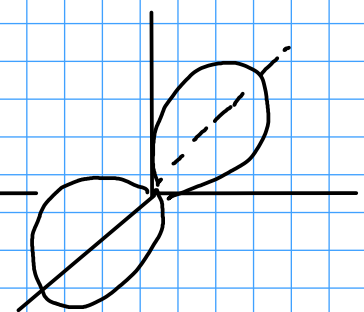
$$\ell = 1 \text{ ; } m_\ell = -1, 0, 1$$

p_x p_y p_z

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

$$\ell = 2 \text{ , } m_\ell = -2, -1, 0, 1, 2 \quad \text{(five orentations)}$$

$$\ell = 3 \text{ , } m_\ell = -3, -2, -1, 0, 1, 2, 3 \quad \text{(seven orentations)}$$

④ (MAGNETIC) SPIN QUANTUM NUMBER: m_S

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

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

ORBITAL DIAGRAM

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

energy

Each blank represents an ORBITAL, and can hold two electrons.

4p

3d

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

3p

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

3s   ✗ Where there's more than one orbital with the same energy, electrons don't pair up until each one has one electron in it!

2p ⎤
   ⎥ n=2
2s ⎦ shell

1s ⎤ n=1 shell   1s: This means the first shell (n=1) and the "s" subshell ("l"=0)