$$HCl\,(aq) + NaOH\,(aq) \rightarrow NaCl\,(aq) + H_2O\,(\ell)$$

3 M HCl, 25°C

3 M NaOH, 25°C

3 M NaCl + H$_2$O, ~40°C

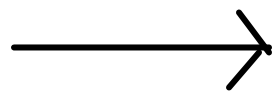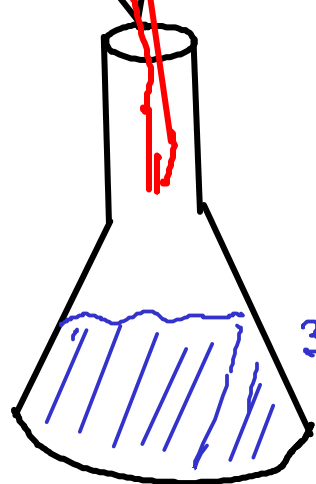This reaction is EXOTHERMIC. Energy is transferred from the reactants and products (the SYSTEM) to the water in the flask, the flask, etc. (the SURROUNDINGS)

$$Ba(OH)_2 \cdot 8H_2O\,(s) + 2\,NH_4NO_3\,(s) \longrightarrow 2\,NH_3\,(aq) + 10\,H_2O(\ell) + Ba(NO_3)_2\,(aq)$$

NH$_4$NO$_3$, 25°C

Ba(OH)$_2$·8H$_2$O, 25°C

NH$_3$, H$_2$O, Ba(NO$_3$)$_2$ (aq), <0°C
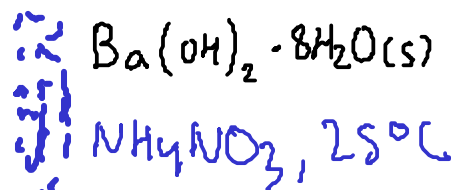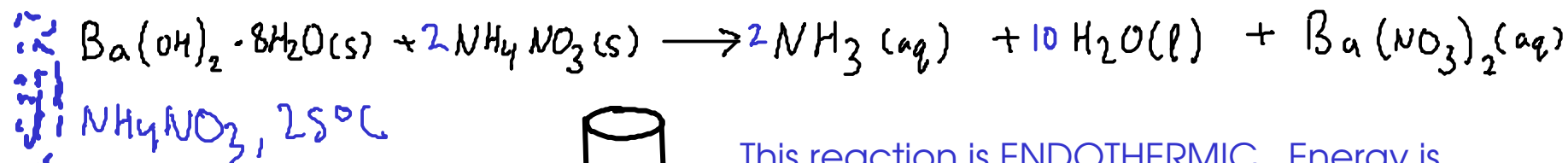
This reaction is ENDOTHERMIC. Energy is being transferred from the room/flask/etc. (the SURROUNDINGS) to the reaction itself (the SYSTEM).
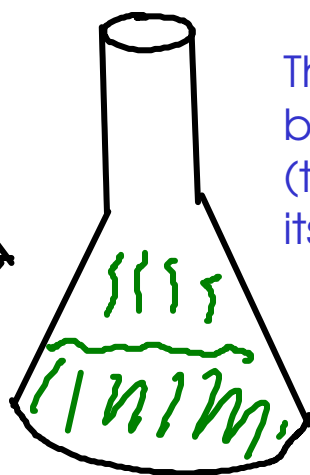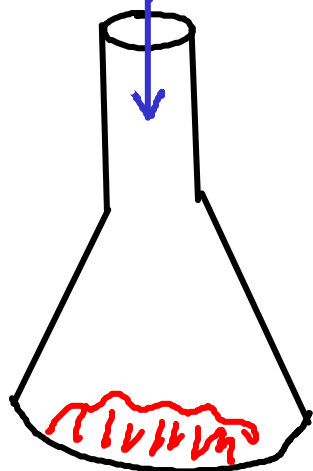
ENERGY UNITS

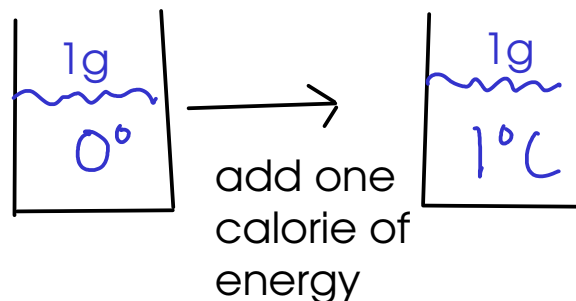- calorie (cal): the amount of energy required to change the temperature of one gram of water by one degree Celsius (or Kelvin)

1g

0°

add one
calorie of
energy

1g

1°C

$1g \approx 1mL$ for water

- Calories in food? The "Calorie" that is given on American food labels is actually the kilocalorie (kcal)

- Joule (J): SI unit for energy. It's defined based on the equation for kinetic energy.

$$1 J = 1 \frac{Kg \, m^2}{s^2}, \text{ from}$$
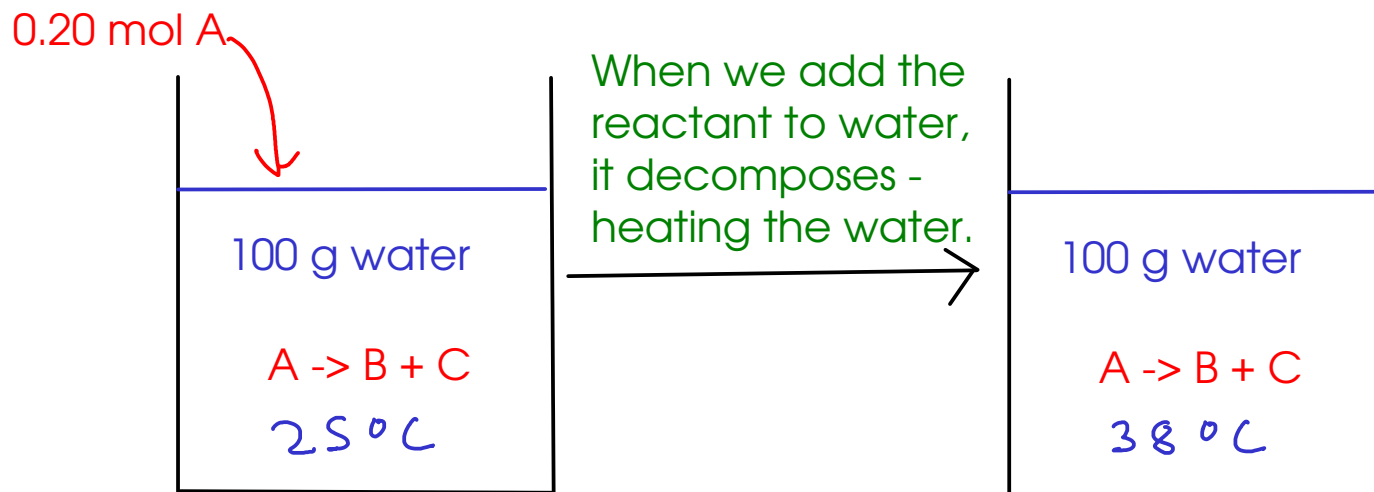
$$E_K = \frac{1}{2} m v^2$$

kinetic
energy

mass

velocity

4.184 J = 1 cal

- the Joule is a small unit. For most reactions at lab scale, we'll use kilojoules (kJ).

CALORIMETRY

- the measurement of heat. But how do we measure heat?

0.20 mol A

100 g water

A -> B + C

25°C

When we add the
reactant to water,
it decomposes -
heating the water.

100 g water

A -> B + C

38°C

... what is Q for this reaction?

Assuming that no heat is lost from the water to the surrounding air,

$$Q_r + Q_w = 0$$

reaction   water

Conservation of energy. The terms add to
zero because they have opposite signs.

... if we knew something about the WATER, we could use that to find the heat of
the REACTION!

SPECIFIC HEAT

- a measured quantity. The amount of energy required to change the temperature of one gram of a particular substance by one degree Celsius.

- Specific heat information for common substances is readily available. For water,

$$4.184 \frac{J}{g°C} = 1.000 \frac{cal}{g°C}$$

$$Q = m \times S \times \Delta T$$

m = mass
s = specific heat
$\Delta T = T_{final} - T_{initial}$

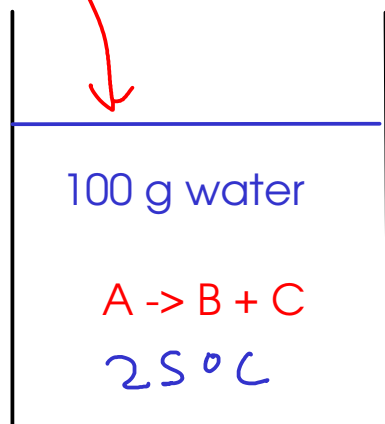This is ALWAYS final temp minus initial temp!

- For objects, like reaction vessels, you might know the HEAT CAPACITY, which is the amount of energy required to change the temperature of an object by one degree Celsius

Units: $\frac{J}{°C}$ or $\frac{cal}{°C}$

$$Q = C \times \Delta T$$

c = heat capacity

0.20 mol A

100 g water

A -> B + C

$25 °C$

When we add the reactant to water, it decomposes - heating the water.

100 g water

A -> B + C

$38 °C$
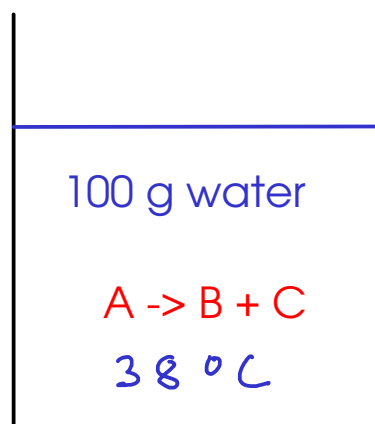
Specific heat of water:

$4.184 \frac{J}{g°C}$

$$Q_r + Q_w = 0$$

$$Q_w = m_w \times S_w \times \Delta T_w = (100g)(4.184 \, J/g°C)(38°C - 25°C)$$
$$= 5439.2 \, J$$

$$Q_r + Q_w = 0; \quad Q_r + 5439.2J = 0; \quad Q_r = -5439.2 \, J$$

To report the energy change in this reaction to others, we should express it in terms of heat transfer per mole of something. A different amount of reactant would have a different Q

$$Q_{rxn} = \frac{Q_r}{moles \ A} = \frac{-5439.2 \, J}{0.20 \, mol \, A} = -27000 \frac{J}{mol \, A} = \boxed{-27 \frac{kJ}{mol \, A}}$$

This number is usually called the "HEAT OF REACTION" ...

One problem ...

PATH. The amount of energy required for a process depends on how the process is carried out.

Example: Driving from Florence to Columbia. How much energy is required? (gas)

2000 Jeep Cherokee vs 2008 Toyota Prius. The Jeep will use much more fuel than the Prius even though they start and end from exactly the same place. So the fuel usage is what we call a PATH FUNCTION, while the location is a STATE FUNCTION.

- so the heat of reaction depends on how the reaction is done.

- we need (for reporting) some kind of standard condition. At constant pressure, we can define a state function called ENTHALPY (H)

H = U + PV

$$\Delta H = Q_{constant\ pressure}$$

... we record the "enthalpy change of reaction" in our data books.

$$\Delta H_r$$

SINCE the enthalpy change does NOT depend on path, this means that we can use standard values for enthalpy to predict the heat change in reactions that we have not tested in a calorimeter.

THERMOCHEMICAL EQUATIONS

- is like a regular chemical equation, except that phase labels are REQUIRED and the enthalpy for the reaction is given along with the equation.

$$CH_3COCH_3(l) + 4O_2(g) \longrightarrow 3CO_2(g) + 3H_2O(l) \; ; \Delta H = -1800 \, kJ$$
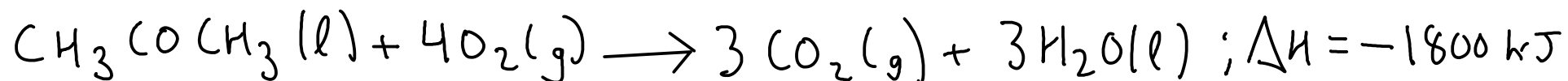
- Why are phase labels required? Because phase changes either absorb or release energy.

$\Delta H = -1800 \, kJ$ ... what does this mean?

$$1 \, mol \; CH_3COCH_3 = -1800 \, kJ$$

$$4 \, mol \; O_2 = -1800 \, kJ$$

$$3 \, mol \; CO_2 = -1800 \, kJ$$

$$3 \, mol \; H_2O = -1800 \, kJ$$

We treat the enthalpy change as if it's another product of the reaction!

$$CH_3COCH_3(l) + 4O_2(g) \longrightarrow 3CO_2(g) + 3H_2O(l) ; \Delta H = -1800 \, kJ$$

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

1 - Convert 25 grams of water to moles. Use FORMULA WEIGHT.
2 - Convert moles water to enthalpy change. Use THERMOCHEMICAL EQUATION.

① $H_2O - H: 2 \times 1.008$
    $O: 1 \times 16.00$
    $\overline{18.016 \, g \; H_2O = mol \; H_2O}$

② $3 \, mol \; H_2O = \sim 1800 \, KJ$

$$25 \, g \; H_2O \times \frac{mol \; H_2O}{18.016 \, g \; H_2O} \times \frac{-1800 \, KJ}{3 \, mol \; H_2O} = \boxed{-830 \, KJ}$$
  ①   ②

Notes: This is an EXOTHERMIC reaction!

This value (-830 kJ) is also equal to the HEAT (Q), provided pressure is constant.

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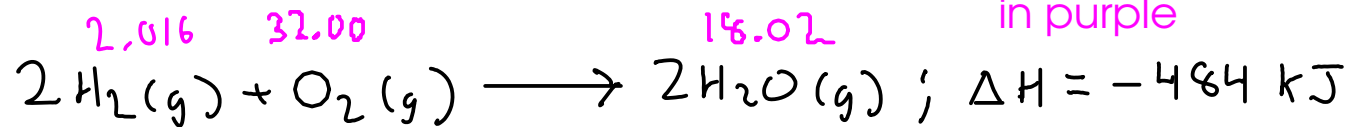
- Enthalpy of fusion / heat of fusion: The enthalpy change when a mole of liquid changes to the solid state.

Phase changes require energy, too!

Example problems:

FORMULA WEIGHTS in g/mol
in purple

$$2.016 \quad 32.00 \qquad 18.02$$

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

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

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1 - Convert 1.00 kg of hydrogen gas to moles. Use FORMULA WEIGHT.
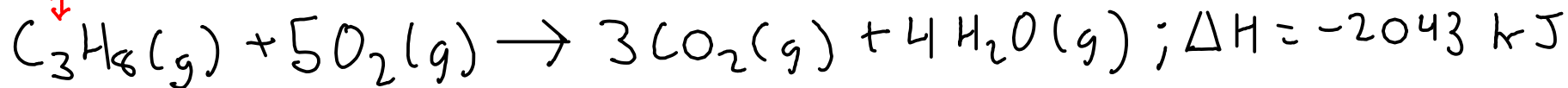2 - Convert moles hydrogen gas to enthalpy change. Use THERMOCHEMICAL EQUATION.

① $2.016 g \, H_2 = mol \, H_2 \qquad kg = 10^3 g$ ② $2 \, mol \, H_2 = -484 \, kJ$

$$1.00 \, kg \, H_2 \times \frac{10^3 g}{kg} \times \frac{mol \, H_2}{2.016 g \, H_2} \times \frac{-484 \, kJ}{2 \, mol \, H_2} = \boxed{-120000 \, kJ} \; \text{per kg} \, H_2$$

$$\underset{①}{} \qquad \underset{②}{}$$

propane
↓

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

Calculate the volume of propane gas at 25.0 C and 1.08 atm required to provide 565 kJ of heat using the reaction above.

1 - Convert heat requirement (565 kJ) to moles propane. Use THERMOCHEMICAL EQUATION.
2 - Convert moles propane to volume. Use IDEAL GAS EQUATION.

① $mol \; C_3H_8 = -2043 \, kJ$

Keep in mind that the 565 kJ of heat required is from the point of view of the surroundings, but the CALCULATION is about the SYSTEM. So, from the system's point of view, it's -565 kJ

$$-565 \, kJ \times \frac{mol \; C_3H_8}{-2043 \, kJ} = 0.276554087l \; mol \; C_3H_8$$

② $PV = nRT$ $n = 0.276554087l \; mol \; C_3H_8$ $P = 1.08 \, atm$

$V = \frac{nRT}{P}$ $R = 0.08206 \frac{L \cdot atm}{mol \cdot K}$

$T = 25.0°C = 298.2 \, K$

$$V = \frac{(0.276554087l \; mol \; C_3H_8)(0.08206 \frac{L \cdot atm}{mol \cdot K})(298.2 \, K)}{(1.08 \, atm)} = \boxed{6.27 \, L \; propane}$$

(at 25.0 C and 1.08 atm)

END OF CHAPTER 6

LIGHT
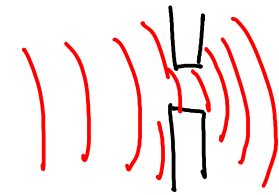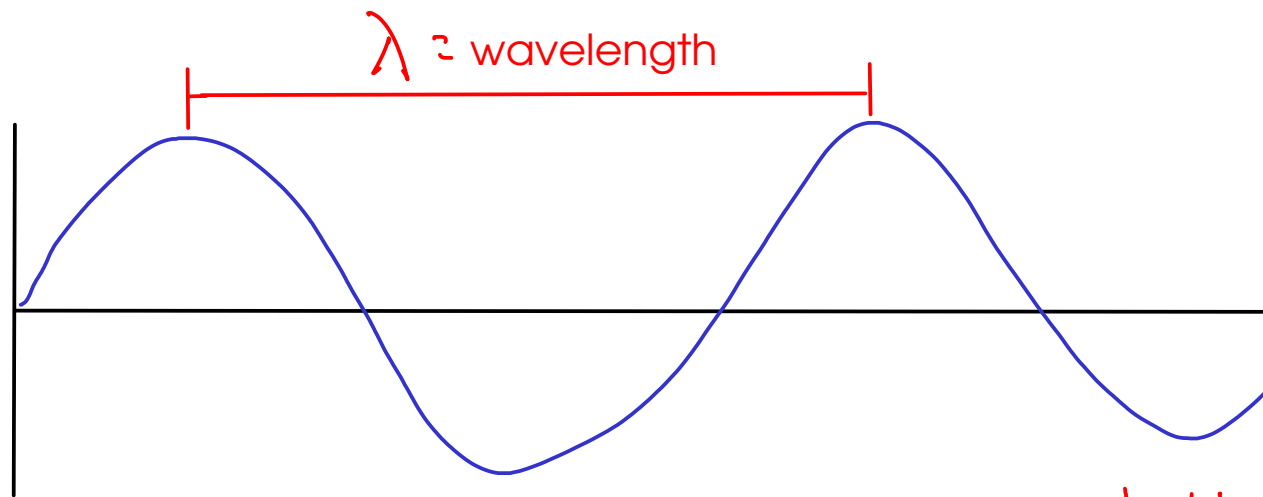
λ = wavelength

Diffraction

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:
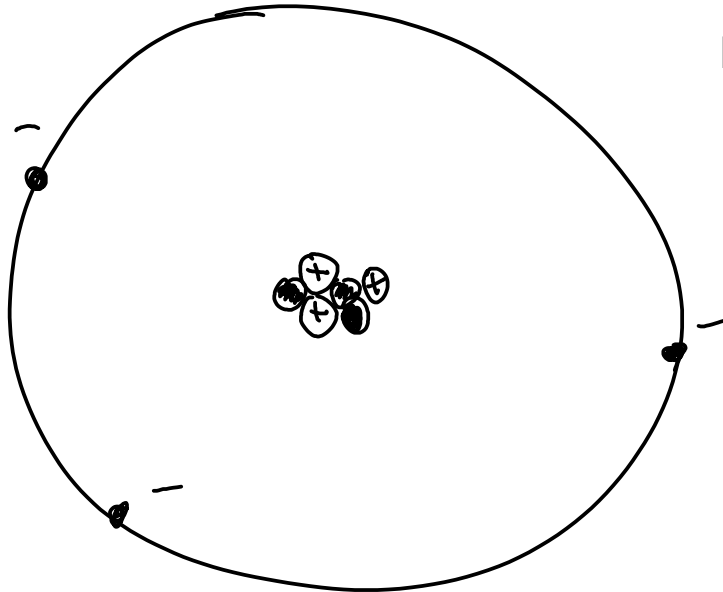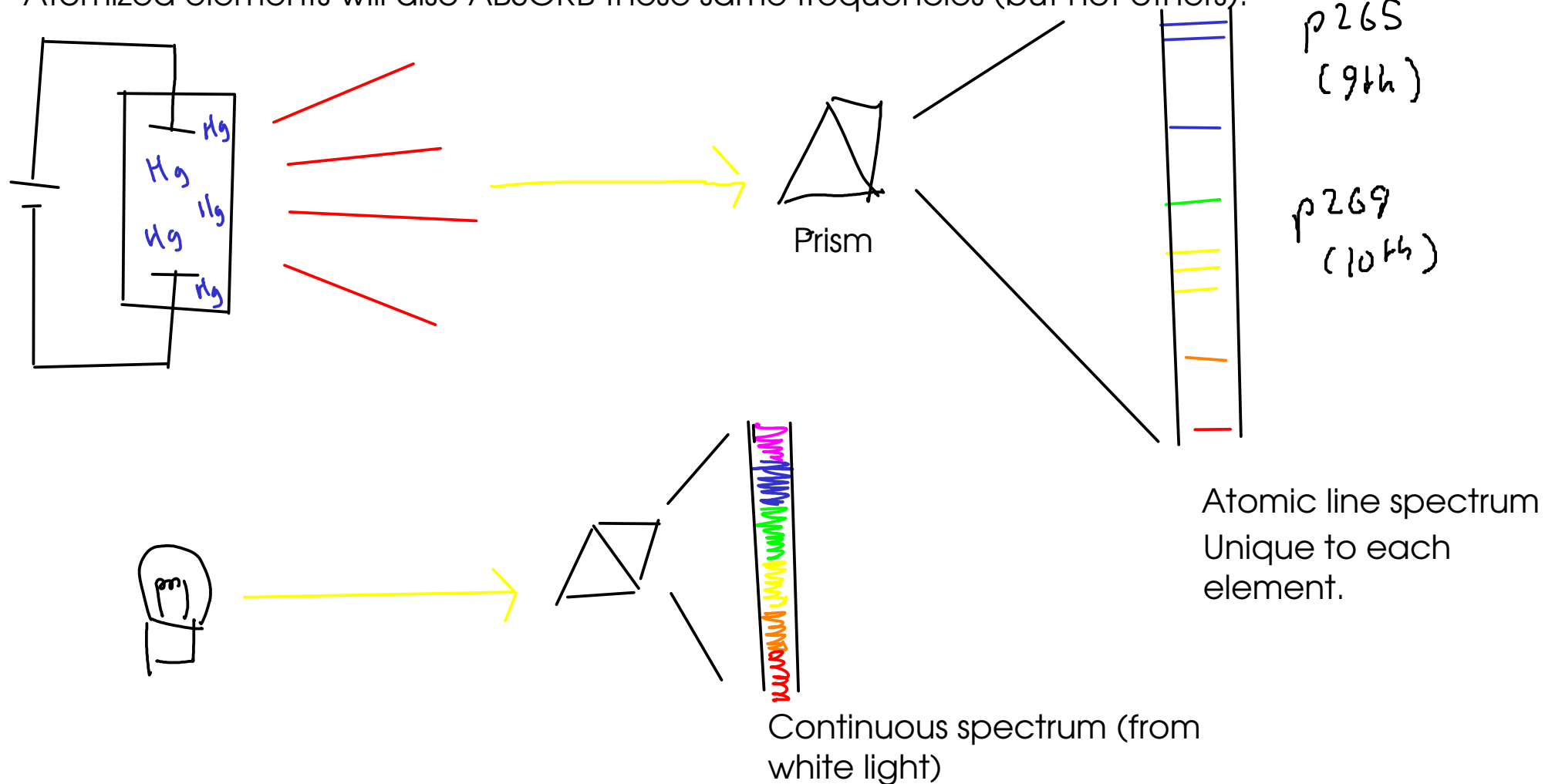

Nuclear model:

- 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)!

Hg
Hg
Hg
Hg
Hg

Prism

p265
(9th)

p269
(10th)

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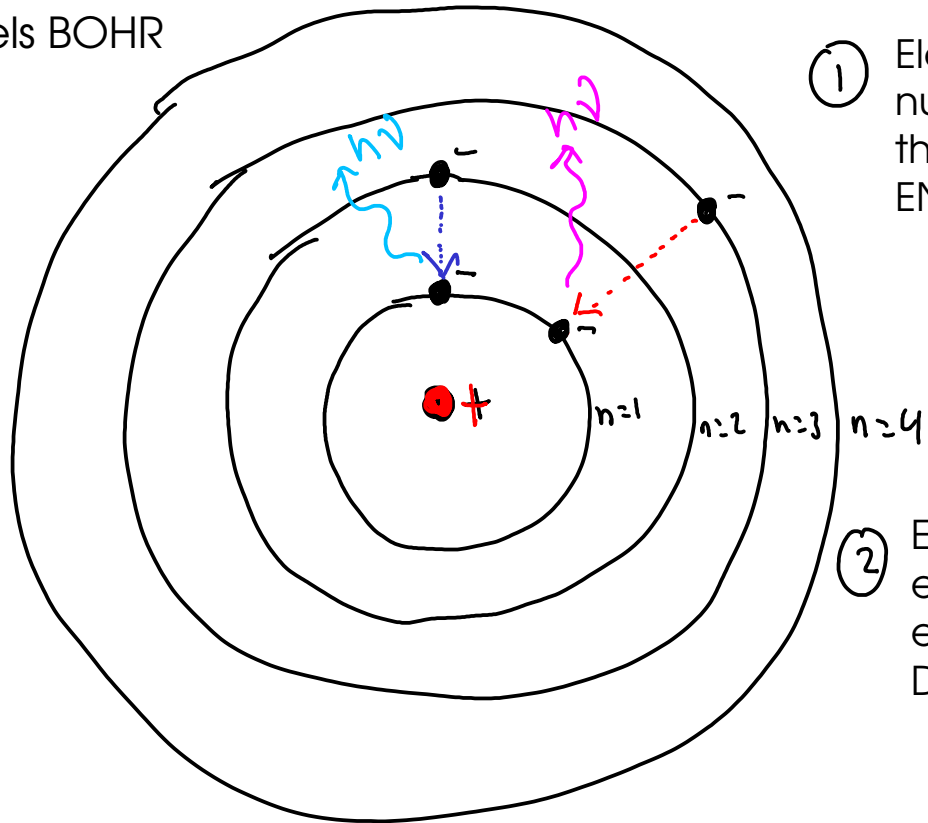
① Electrons can't be just ANYWHERE around a nucleus. They can exist only at certain distances from the nucleus. These distances correpsond to certain ENERGIES and are called ENERGY LEVELS!

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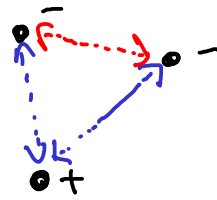
Multi-electron atoms have interactions between electrons, not just interactions between electrons and nucleus!

- 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 WAVELENGTH 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 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"

① Principal quantum number

② Angular momentum quantum number

③ Magnetic quantum number

④ Spin quantum number