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.

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

- Why are phase labels required? Because phase changes either absorb or release energy.

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

$1 \text{ mol } CH_3COCH_3 = -1800 \text{ kJ}$

$4 \text{ mol } O_2 = -1800 \text{ kJ}$

$3 \text{ mol } CO_2 = -1800 \text{ kJ}$

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

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

USING A THERMOCHEMICAL EQUATION

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

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

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

① H_2O – H: 2 x 1.008
O: 1 x 16.00
18.016 g H_2O = mol H_2O

② 3 mol H_2O = −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:
A) The reaction is EXOTHERMIC (negative sign for Q or delta H).
B) Provided the acetone is burned at constant pressure, Q = -830 kJ, meaning that this reaction will RELEASE 830 kJ from the system to the surroundings!

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.

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

heat of formation of carbon dioxide ΔH_f° or ΔH_f
or "enthalpy of formation"

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

$\Delta H^\circ_{f, O_2(g)} = 0$ kJ/mol

- 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:

$$2C_2H_2(g) + 5O_2(g) \longrightarrow 4CO_2(g) + 2H_2O(g);\ \Delta H = ?$$

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

C_2H_2: $2C(s) + H_2(g) \longrightarrow C_2H_2(g)$ $\Delta H = 227.4$

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

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

$C_2H_2(g) \longrightarrow 2C(s) + H_2(g)$ $\Delta H = -227.4$

$C_2H_2(g) \longrightarrow 2C(s) + H_2(g)$ $\Delta H = -227.4$

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

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$$2C_2H_2(g) + 5O_2(g) \longrightarrow 4CO_2(g) + 2H_2O(l)$$

$$\Delta H = 2(-227.4) + 4(-393.5) + 2(-241.8) = \boxed{-2512.4\ \text{kJ}}$$

* Enthalpy of formation data taken from Openstax Chemistry Appendix G

Hess' Law using enthalpy of formation:

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

$$\overset{227.4}{2C_2H_2(g)} + \overset{0}{5O_2(g)} \longrightarrow \overset{-393.5}{4CO_2(g)} + \overset{-241.8}{2H_2O(g)}\ ;\ \Delta H = ?$$

$$\Delta H = [4(-393.5) + 2(-241.8)] - [2(227.4) + 5(0)]$$

$$= -2512.4\ kJ$$

See Appendix G in the Openstax textbook for enthalpy of formation data!

* 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!

Example problems:

FORMULA WEIGHTS in g/mol in purple

$$\underset{2.016}{2H_2(g)} + \underset{32.00}{O_2(g)} \longrightarrow \underset{18.02}{2H_2O(g)}\ ;\ \Delta H = -484\ kJ$$

Calculate the enthalpy change for the combustion of 1000 g of hydrogen gas.

1) Convert 1000 grams of hydrogen gas to moles. Use FORMULA WEIGHT.
2) Convert moles hydrogen gas to enthalpy change. Use THERMOCHEMICAL EQUATION.

(1) $2.016\ g\ H_2 = mol\ H_2$ (2) $2\ mol\ H_2 = -484\ kJ$

$$1000.\ g\ H_2 \times \frac{mol\ H_2}{2.016\ g\ H_2} \times \frac{-484\ kJ}{2\ mol\ H_2} = \boxed{-120000\ kJ}\ \text{per kg}\ H_2$$

(1) (2)

34.086 g/mol

Heat of formation / enthalpy of formation!

$$\begin{matrix} -20.6 & 0 & -285.8 & -296.8 \end{matrix} \quad \Big] \Delta H_f^\circ, \text{kJ/mol}$$

$$2H_2S(g) + 3O_2(g) \rightarrow 2H_2O(l) + 2SO_2(g)$$

(Data from Appendix G!)

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

We need a THERMOCHEMICAL EQUATION to solve this! Use Hess' Law and formation enthalpies.

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

$$\Delta H = [2(-285.8) + 2(-296.8)] - [2(-20.6) + 3(0)] = -1124 \text{ kJ}$$

... so the thermochemical equaton is:

$$2H_2S(g) + 3O_2(g) \rightarrow 2H_2O(l) + 2SO_2(g) ; \Delta H = -1124 \text{ kJ}$$

1) Convert 25.0 grams of hydrogen sulfide to moles. Use FORMULA WEIGHT.
2) Convert moles hydrogen sulfide to enthalpy change. Use THERMOCHEMICAL EQUATION.

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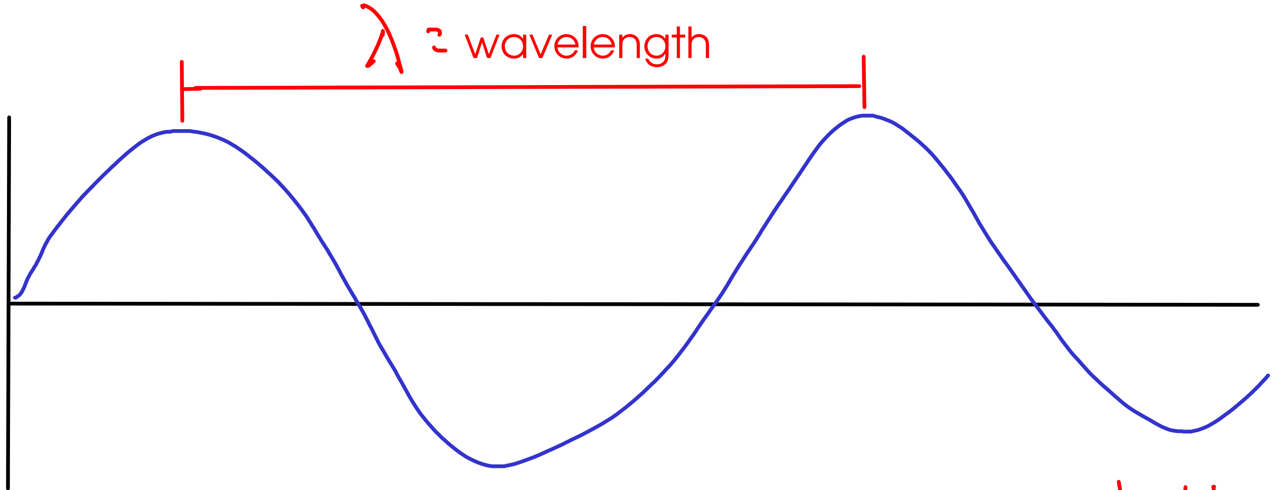
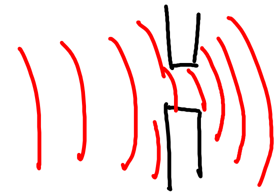
① $34.086\ g\ H_2S = \text{mol } H_2S$ ② $2 \text{ mol } H_2S = -1124 \text{ kJ}$

$$25.0\ g\ H_2S \times \frac{\text{mol } H_2S}{34.086\ g\ H_2S} \times \frac{-1124 \text{ kJ}}{2 \text{ mol } H_2S} = \boxed{-412 \text{ kJ}}$$

(①) (②)

LIGHT





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!

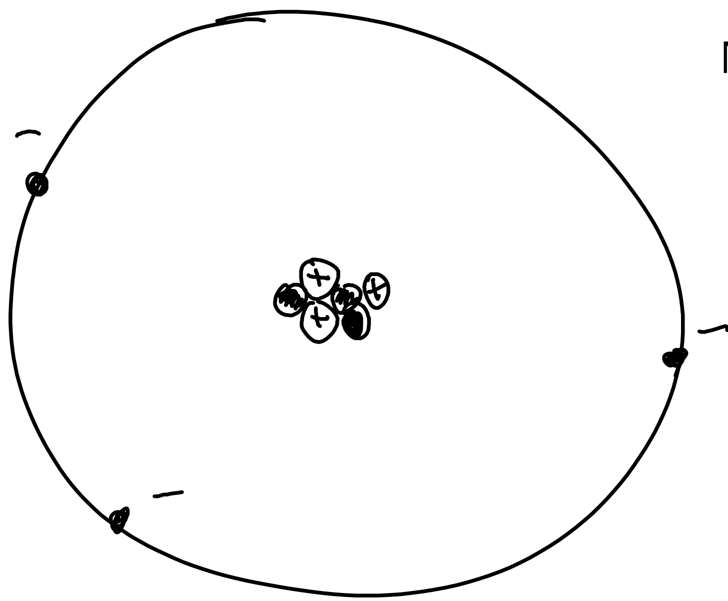
$$E_{photon} = h\nu$$

h — Planck's constant: 6.63×10^{-34} J·s

E_{photon} — 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:

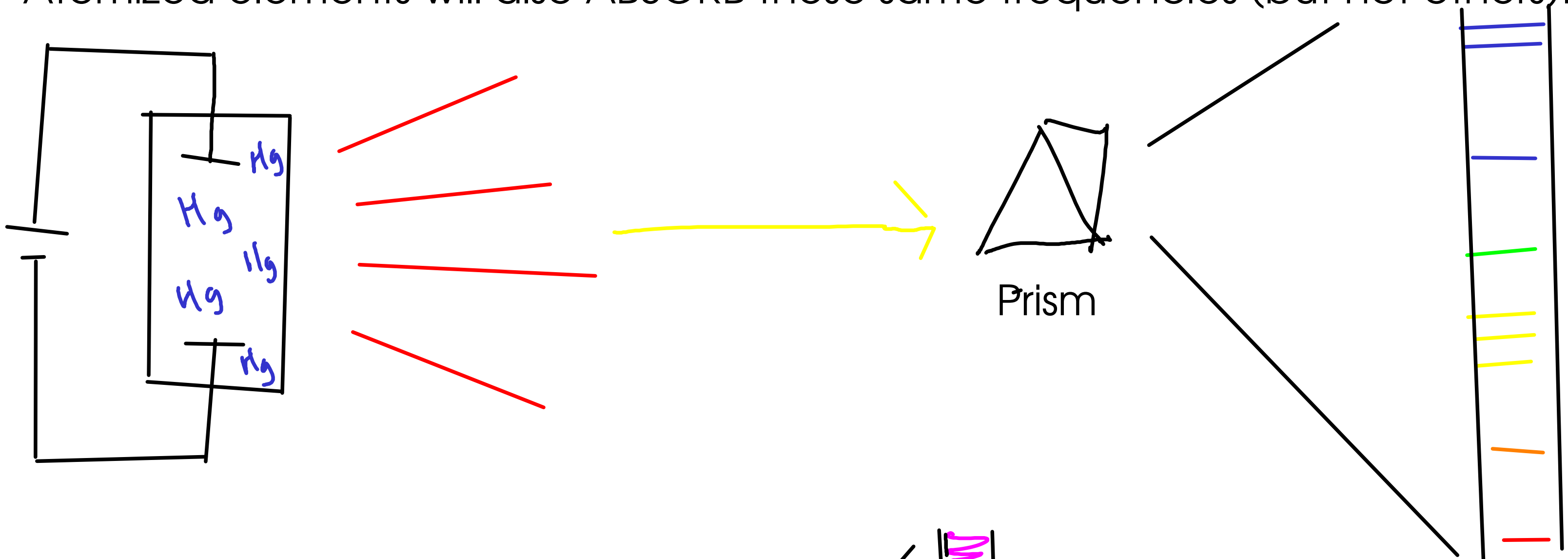
- Protons and neutrons in a dense NUCLEUS at center of atom
- Electrons in a diffuse (mostly empty) ELECTRON CLOUD surrounding NUCLEUS.

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

ATOMIC LINE SPECTRA

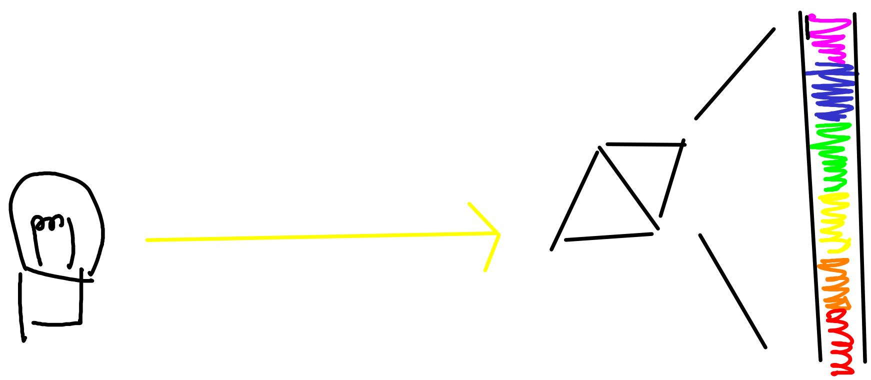
- if you take element and ATOMIZE it, if excited by energy it will emit light at unique frequencies. The set of emitted frequencies is called an ATOMIC LINE SPECTRUM.

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



(See page 291 in the Openstax book for some line spectrum examples)

Atomic line spectrum
Unique to each element.

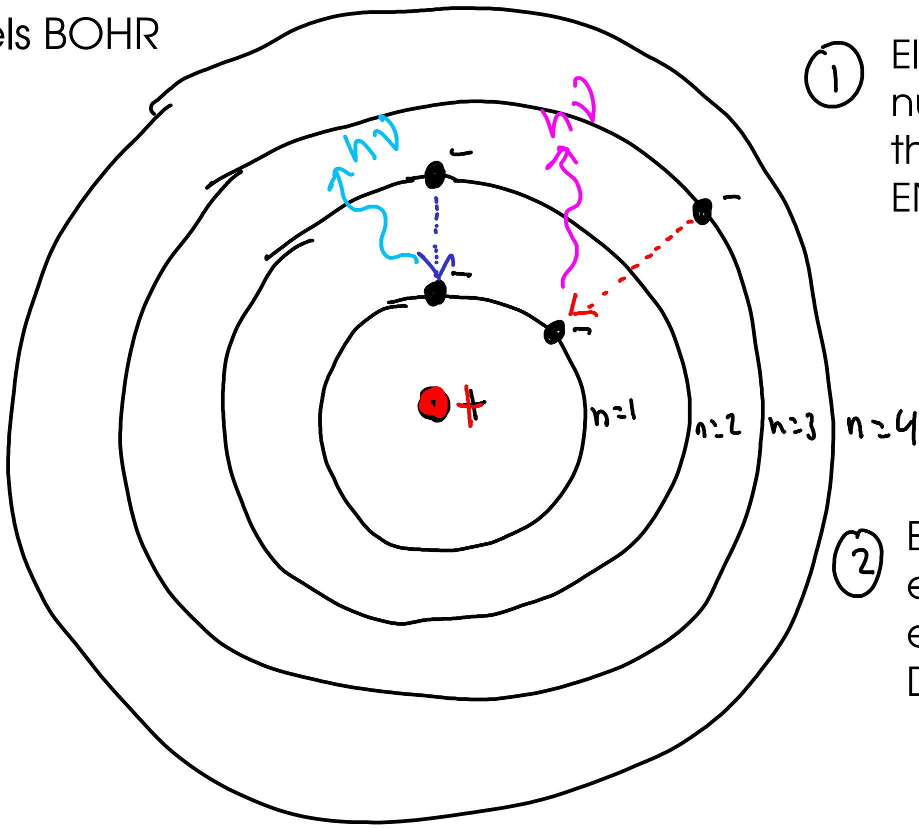


Continuous spectrum (from white light)

... 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

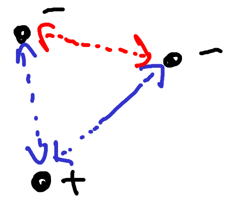


(1) Electrons can't be just ANYWHERE around a nucleus. They can exist only at certain distances from the nucleus. These distances correpsond to certain ENERGIES and are called ENERGY LEVELS!

(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

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

Planck's constant (h)

wavelength (λ)

mass (m)

velocity (m/s) (v)

Calculates the WAVELENGTH of ... matter?

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