

- What sort of energy concerns chemists? Energy that is absorbed or released during chemical reactions.

- Energy can be stored in chemicals ... molecules and atoms.

INTERNAL ENERGY: "U"



related to the kinetic and potential energy of atoms, molecules, and their component parts.

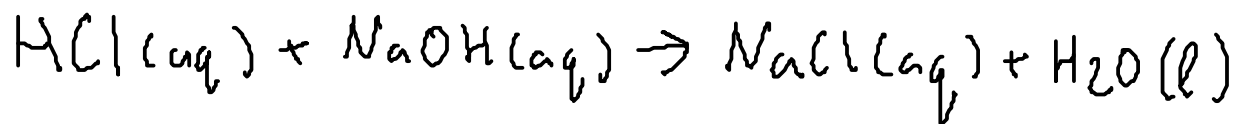
- We measure energy transfer ... which is called HEAT. (HEAT is the flow of energy from an area of higher temperature to an area of lower temperature)

Q: heat

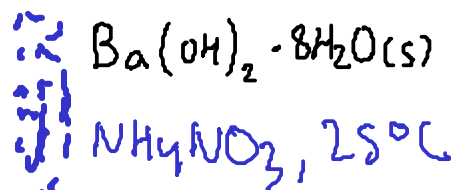
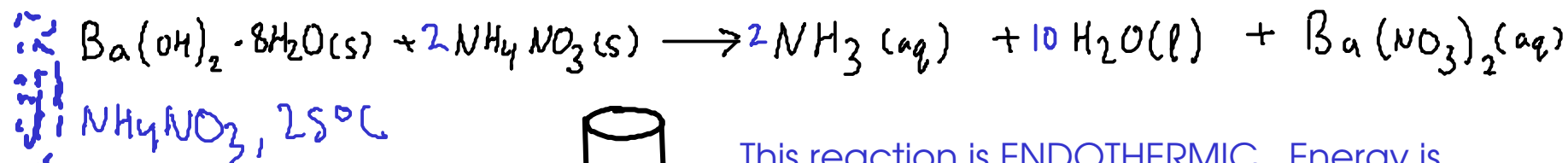
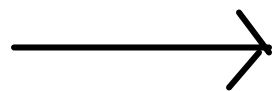
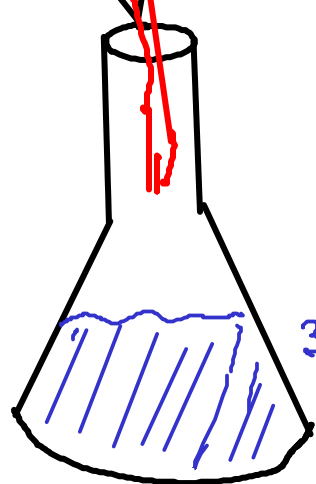
SYSTEM: the object or material under study

SURROUNDINGS: everything else

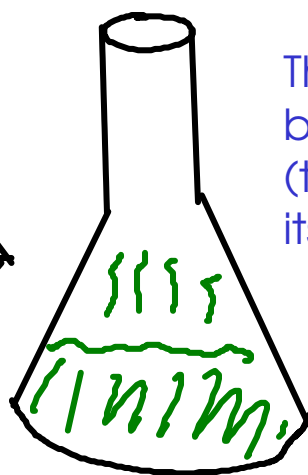
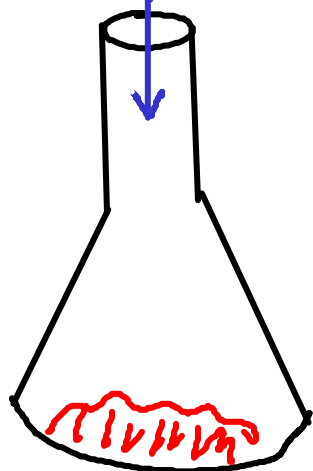
| Type of process | Energy is ... | Sign of Q | Temp of SURROUNDINGS ... |
|-----------------|---|-----------|--------------------------|
| ENDOTHERMIC | transferred from SURROUNDINGS to SYSTEM | + | decreases |
| EXOTHERMIC | transferred from SYSTEM to SURROUNDINGS | - | increases |



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)

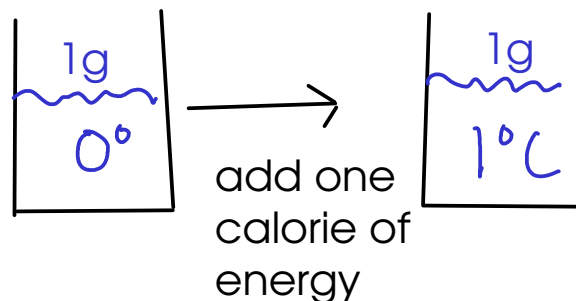


This reaction is ENDOTHERMIC. Energy is being transferred from the room/flask/etc. (the SURROUNDINGS) to the reaction itself (the SYSTEM).



ENERGY UNITS

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



$1\text{g} \approx 1\text{mL}$ 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.

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

$$E_K = \frac{1}{2} m v^2$$

kinetic
energy

mass

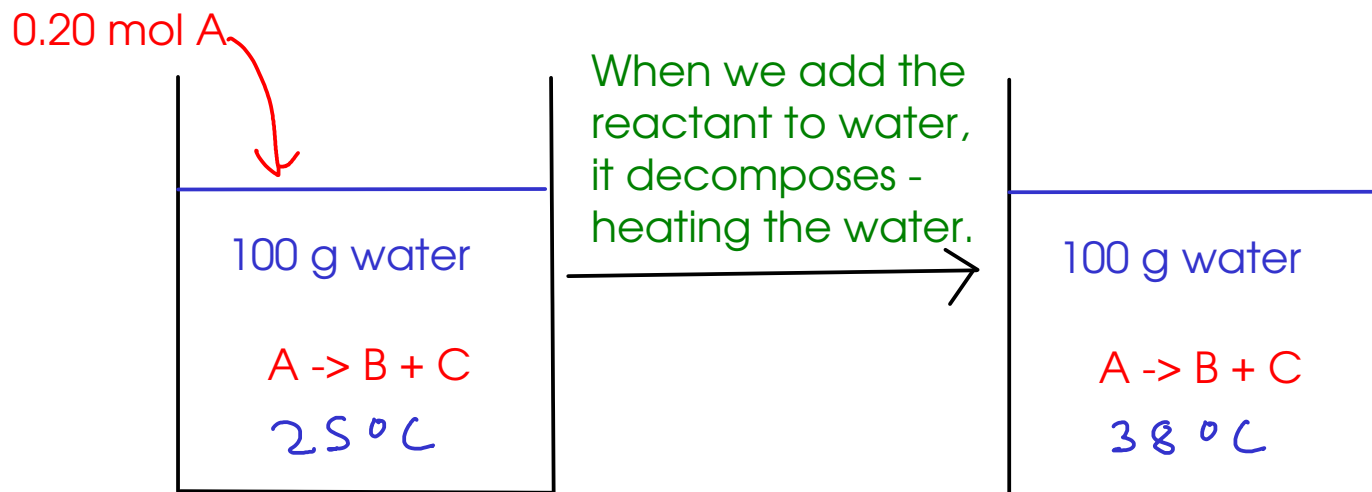
velocity

$$4.184\text{ J} = 1\text{ cal}$$

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

CALORIMETRY

- the measurement of heat. How do we measure heat?



... what is Q for this reaction?

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

$$\underbrace{Q_r}_{\text{reaction}} + \underbrace{Q_w}_{\text{water}} = 0$$

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,

$$4.184 \frac{\text{J}}{\text{g}^\circ\text{C}} \quad \underline{\underline{=}} \quad 1.000 \frac{\text{cal}}{\text{g}^\circ\text{C}}$$

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

m = mass
 s = specific heat
 ΔT = $T_{\text{final}} - T_{\text{initial}}$

This is ALWAYS final temp minus initial temp!

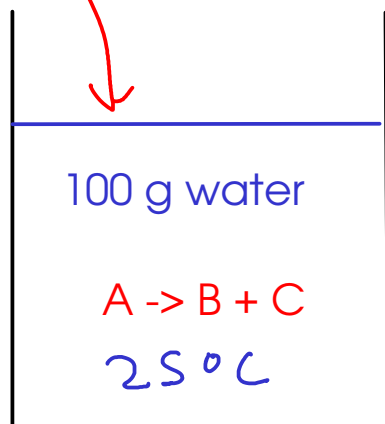
- For objects, like reaction vessels, you might know the HEAT CAPACITY, which is the amount of energy required to change the temperature of an object by one degree Celsius

$$\text{units: } \text{J}/^\circ\text{C} \quad \text{or} \quad \text{cal}/^\circ\text{C}$$

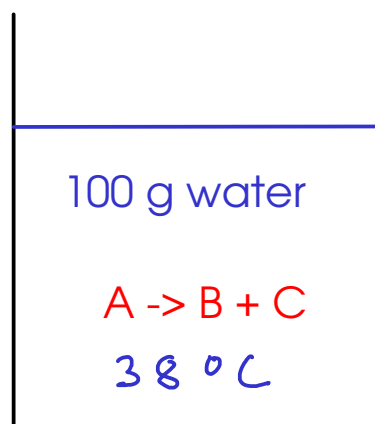
$$Q = C \times \Delta T$$

c = heat capacity

0.20 mol A



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



Specific heat of water:

$$4.184 \frac{\text{J}}{\text{g}^\circ\text{C}}$$

$$Q_r + Q_w = 0$$

$$Q_w = m_w \times S_w \times \Delta T_w = (100 \text{ g}) (4.184 \frac{\text{J}}{\text{g}^\circ\text{C}}) (38^\circ\text{C} - 25^\circ\text{C}) = 5439.2 \text{ J}$$

$$Q_r + Q_w = 0; \quad Q_r + 5439.2 \text{ J} = 0 \quad Q_r = -5439.2 \text{ J}$$

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

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

We usually call this kind of number 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)

$$H = U + PV$$

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

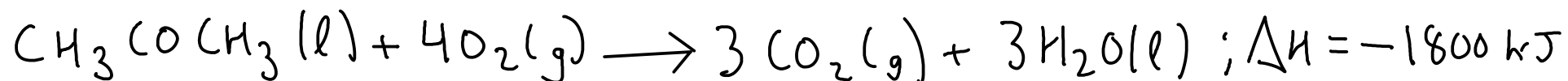
... we record the "enthalpy change of reaction" in our data books.

$$\Delta H_r$$

¹⁵⁷ 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.



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

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

$$1 \text{ mol CH}_3\text{COCH}_3 = -1800 \text{ kJ}$$

$$4 \text{ mol O}_2 = -1800 \text{ kJ}$$

$$3 \text{ mol CO}_2 = -1800 \text{ kJ}$$

$$3 \text{ mol H}_2\text{O} = -1800 \text{ kJ}$$

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



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

1 - Convert 25 g water to moles. Use FORMULA WEIGHT.

2 - Convert moles water to enthalpy change. Use THERMOCHEMICAL EQUATION.

$$\textcircled{1} \text{H}_2\text{O}: \begin{array}{r} 1 - 2 \times 1.008 \\ 0 - 1 \times 16.00 \\ \hline \end{array}$$

$$18.016 \text{ g H}_2\text{O} = 1 \text{ mol H}_2\text{O}$$

$$\textcircled{2} 3 \text{ mol H}_2\text{O} = -1800 \text{ kJ}$$

$$25 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.016 \text{ g H}_2\text{O}} \times \frac{-1800 \text{ kJ}}{3 \text{ mol H}_2\text{O}} = \boxed{-830 \text{ kJ}}$$

Some notes:

- 1) Negative sign - indicates process is EXOTHERMIC. (Not surprising for a COMBUSTION)
- 2) -830 kJ is also the HEAT (Q), provided pressure is constant.

A few more terms related to enthalpy:

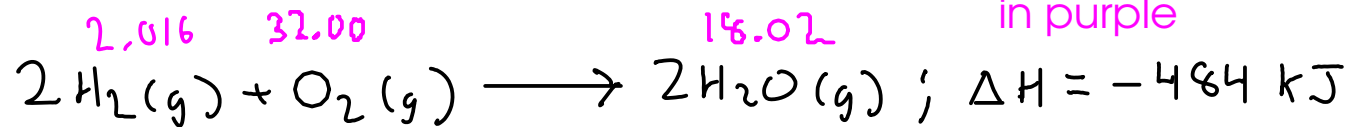
- Enthalpy of vaporization / heat of vaporization: The enthalpy change on vaporizing one mole of a substance. (from liquid to vapor)
- Enthalpy of fusion / heat of fusion: The enthalpy change when a mole of liquid changes to the solid state.



Phase changes require energy, too!

Example problems:

FORMULA WEIGHTS in g/mol
in purple



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

1 - Convert 1.00 kg hydrogen gas to moles. Use FORMULA WEIGHT.

2 - Convert moles hydrogen gas to enthalpy change. Use THERMOCHEMICAL EQUATION.

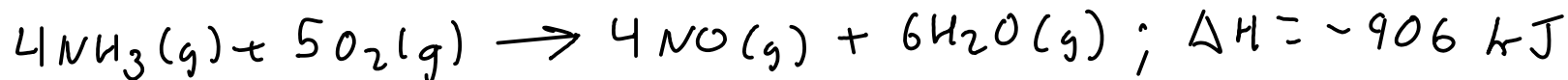
① $2.016 \text{ g H}_2 = 1 \text{ mol H}_2$ ② $2 \text{ mol H}_2 = -484 \text{ kJ}$

$$1000 \text{ g H}_2 \times \frac{1 \text{ mol H}_2}{2.016 \text{ g H}_2} \times \frac{-484 \text{ kJ}}{2 \text{ mol H}_2} = \boxed{-120000 \text{ kJ}} \text{ per kg H}_2$$

① ②

$\text{kg} = 10^3 \text{ g}$

$$1.00 \text{ kg H}_2 \times \frac{10^3 \text{ g}}{\text{kg}} = 1000 \text{ g H}_2$$



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?

1 - Convert 150. L of NO to moles. Use IDEAL GAS EQUATION.

2 - Convert moles NO to enthalpy change. Use THERMOCHEMICAL EQUATION.

$$\textcircled{1} \quad PV = nRT \quad \left| \quad P = 1.50 \text{ atm} \quad R = 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right.$$

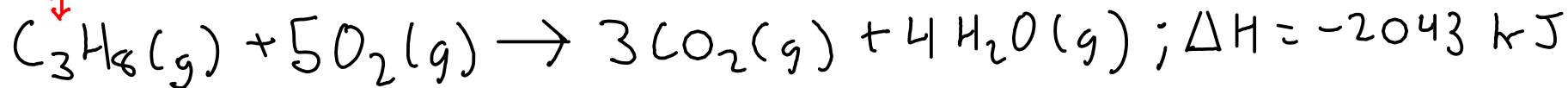
$$n = \frac{PV}{RT} \quad \left| \quad V = 150. \text{ L} \quad T = 25.0^\circ\text{C} = 298.2 \text{ K} \right.$$

$$n_{\text{NO}} = \frac{(1.50 \text{ atm})(150. \text{ L})}{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}\right)(298.2 \text{ K})} = 9.194822849 \text{ mol NO}$$

$$\textcircled{2} \quad 4 \text{ mol NO} = -906 \text{ kJ}$$

$$9.194822849 \text{ mol NO} \times \frac{-906 \text{ kJ}}{4 \text{ mol NO}} = \boxed{-2080 \text{ kJ}}$$

propane



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 mol propane. Use THERMOCHEMICAL EQUATION

2 - Convert moles propane to volume. Use IDEAL GAS EQUATION.

$$\textcircled{1} \text{ mol C}_3\text{H}_8 = -2043 \text{ kJ}$$

Since the calculation is from the point of view of the reaction, the reaction LOSES 565 kJ, so the number we start with will be -565 kJ

$$-565 \text{ kJ} \times \frac{\text{mol C}_3\text{H}_8}{-2043 \text{ kJ}} = 0.276554087 \text{ mol C}_3\text{H}_8$$

$$\textcircled{2} \begin{array}{l|l} PV = nRT & n = 0.276554087 \text{ mol C}_3\text{H}_8 \quad P = 1.08 \text{ atm} \\ V = \frac{nRT}{P} & R = 0.08206 \frac{\text{L-atm}}{\text{mol}\cdot\text{K}} \\ & T = 25.0^\circ\text{C} = 298.2 \text{ K} \end{array}$$

$$V = \frac{(0.276554087 \text{ mol C}_3\text{H}_8)(0.08206 \frac{\text{L-atm}}{\text{mol}\cdot\text{K}})(298.2 \text{ K})}{1.08 \text{ atm}}$$

$$= 6.27 \text{ L of C}_3\text{H}_8 @ 25.0^\circ\text{C}, 1.08 \text{ atm}$$

END OF CHAPTER 6