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
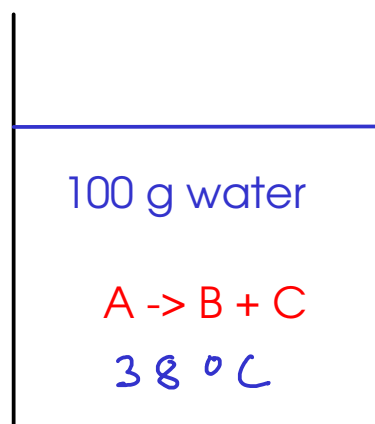
Specific heat of water:

$4.184 \, \frac{J}{g \cdot °C}$

$Q_r + Q_w = 0$

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

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

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

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

We often call this kind of number a "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.

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

- 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!

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

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 $3\,mol\ H_2O = -18004\,J$

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

* This is an EXOTHERMIC reaction!  (830 kJ transferred to the SURROUNDINGS)
* The enthalpy change (-830 kJ) is the same as the heat, Q ... provided pressure is constant.
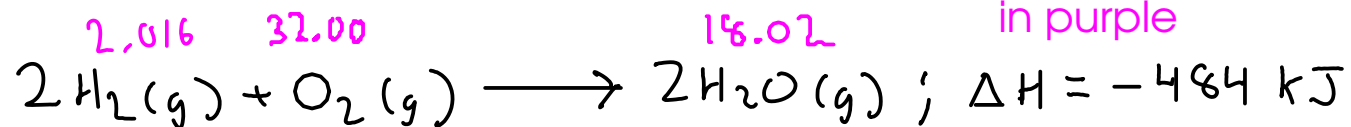
A few more terms related to enthalpy:

- 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.

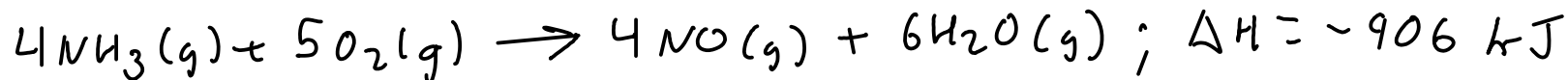Phase changes require energy, too!

Example problems:

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

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

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

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

$$1.00 \, kg \; H_2 \times \underset{①}{\frac{10^3 g}{kg}} \times \underset{①}{\frac{mol \; H_2}{2.016 \, g \; H_2}} \times \underset{②}{\frac{-484 \, kJ}{2 \, mol \; H_2}} = \boxed{\begin{array}{c} -120000 \, kJ \\ per \; kg \; H_2 \end{array}}$$

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

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?

1 - Convert 150. L of NO to moles.  Use IDEAL GAS EQUATION.
2 - Convert moles NO to enthalpy change.  Use THERMOCHEMICAL EQUATION

① $PV = nRT$ | $P = 1.50 \, atm$    $R = 0.08206 \, \frac{L \cdot atm}{mol \cdot K}$

$n = \frac{PV}{RT}$ | $V = 150. \, L$    $T = 25.0 \, °C = 298.2 \, K$

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

② $4 \, mol \, NO = -906 \, kJ$

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

②

propane
↓

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g) \; ; \; \Delta H = -2043 \, kJ$$
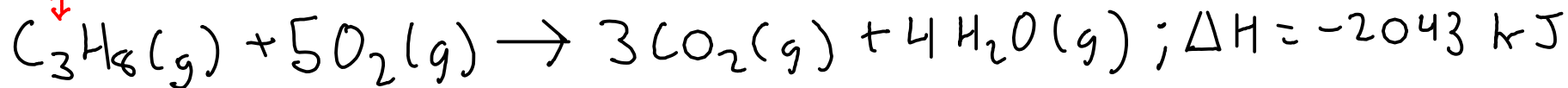
Calculate the volume of propane gas at 25.0 C and 1.08 atm required to provide 565 kJ of heat using the reaction above.

1 - Convert 565 kJ energy requirement to moles of propane. Use THERMOCHEMICAL EQUATION.
2 - Convert moies propane to volume. Use IDEAL GAS EQUATION.

① $mol \; C_3H_8 = -2043 \, kJ$

Since the REACTION is the system in the calculation, the energy requirement is going to be NEGATIVE from the system's point of view. The reaction is losing 565 kJ !

$$-565 \, kJ \times \frac{mol \; C_3H_8}{-2043 \, kJ} = 0.27655408771 \, mol \; C_3H_8$$

② $PV = nRT$

$V = \dfrac{nRT}{P}$

$n = 0.27655408771 \, mol \; C_3H_8 \qquad P = 1.08 \, atm$

$R = 0.08206 \dfrac{L \cdot atm}{mol \cdot K}$

$T = 25.0^\circ C = 298.2 \, K$

$$V = \frac{(0.27655408771 \, mol \; C_3H_8) \times \left(0.08206 \frac{L \cdot atm}{mol \cdot K}\right)(298.2 \, K)}{(1.08 \, atm)} =$$

$= \boxed{6.27 \, L \; propane \; @ \; 25.0^\circ C, \; 1.08 \, atm}$

# END OF CHAPTER 6