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 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!

USING A THERMOCHEMICAL EQUATION

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

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

$$25 \text{ g } H_2O \times \frac{\text{mol } H_2O}{18.016 \text{ g } H_2O} \times \frac{-1800 \text{ kJ}}{3 \text{ mol } H_2O} = -830 \text{ kJ}$$

(1) (2)

This would also equal the HEAT, provided the burning was done at constant pressure!

(This is an EXOTHERMIC process - since delta H is negative. Not really surprising, since this is the reaction for the burning of acetone!)

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

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

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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:

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

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

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

$$= \boxed{-2512.4}$$

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

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

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

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

(1) (2)