HW5

We can describe enthalpy as H = U + PV, where U – internal energy of the system, P – pressure of the system, V – volume of the system. Since we don't know the absolute value of U for our "chemical" purposes this equation is useless. But we can presume that our system in under constant pressure (pressure does not change), that is true for the most chemical reactions, and then we can calculate the enthalpy change (it is basically heat added or taken out from the system, system in our case is chemical reaction)

Enthalpy change (**Δ** H) of the reaction – amount of chemical heat energy taken in (giving out) in a reaction. If we know the sign of enthalpy change we can describe if a reaction endothermic or exothermic.

The most common theoretical methods for calculating the enthalpy change of a reaction are Hess's Law and the use of standard enthalpies of formation.
Hess's Law states that the total enthalpy change for a reaction is the same regardless of the number of steps or the path taken, provided the initial and final conditions are the same.

The **enthalpy change of formation** (ΔH_f) refers to the heat energy change that occurs when **one mole** of a substance is formed from its constituent elements in their **standard states** under standard conditions (298 K, 1 atmosphere pressure). It is a type of **enthalpy change**, a thermodynamic quantity used to describe the energy change in chemical reactions.

Let's look at the following problems:
Calculate enthalpy change for the following reaction
$2CO(g) + O_2(g) \rightarrow 2CO_2(g)$
The enthalpy change for the following reactions are known
$2C(s) + O_2(g) \rightarrow 2CO(g)$ **Δ** H=- 222 kJ/mol
$C(s) + O_2(g) \rightarrow CO_2(g)$ **Δ** H=- 394 kJ/mol

Let's use the Hess's Law:

1. $2C + O_2 \rightarrow 2CO$ $\Delta H = -222$ kJ/mol
2. $C + O_2 \rightarrow \underline{CO_2}$ -394

$2CO + O_2 \rightarrow \underline{2CO_2}$

Multiply reaction number 2 by 2, because we need to count 2 CO_2 in the final reaction. Delta H we will multiply as well -394x2

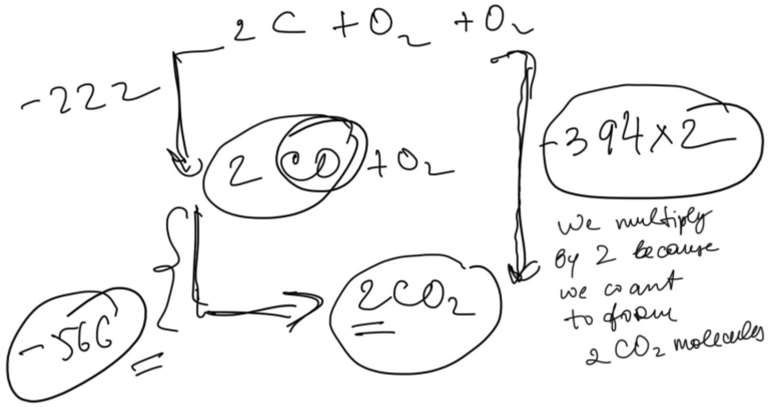
1. $\cancel{2C} + \cancel{2}O_2 \rightarrow 2CO_2$ -788
2. $\cancel{2C} + \cancel{O_2} \rightarrow 2CO$ -222

$O_2 \rightarrow 2CO_2 - 2CO$

$2CO + O_2 \rightarrow 2CO_2$

$-788 - (-222) = -566$ kJ/mol

Subtract reaction 2 from reaction1 including enthalpy changes, we will get our final reaction and the enthalpy change.



We can also draw the scheme of the reaction to see more clearly how it goes.

Let’s use the enthalpy change of formation to solve the same problem:

$\Delta H_f (CO_2(g)) = -393.5$ kJ/mol

$\Delta H_f (CO(g)) = -110.5$ kJ/mol

$\Delta H_f (O_2(g)) = 0$ kJ/mol

ΔH_r = sum of ΔH_f of products – sum of ΔH_f of reactants

For the reaction $2CO(g) + O_2(g) \rightarrow 2CO_2(g)$

The calculation is: (2x-393.5)- (2x-110.5 + 1x0)= -566 kJ/mol

Another example: Calculate enthalpy change for the reaction **Fe_2O_3 + 3CO → 2Fe + $3CO_2$**
When you know standard enthalpy change of formation of the products and reactants.

$\Delta H_f^\ominus$ $Fe_2O_3 = -822$ kJ/mol

$\Delta H_f^\ominus$ $CO = -111$

$\Delta H_f^\ominus$ $CO_2 = -394$

$\Delta H_f^\ominus$ - standard enthalpy change of formation.

Element in its standard state has $\Delta H_f^\ominus = 0$

$\Delta H_f^\ominus$ for iron $= 0$

Knowing $\Delta H_f^\ominus$ for the above substances calculate enthalpy change for the following reaction: $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$.

1. $2Fe + \frac{3}{2}O_2 \rightarrow Fe_2O_3$

formation of Fe_2O_3

$\Delta H = -822$

2. $C + \frac{1}{2}O_2 \rightarrow CO$ -111

formation of CO

3. $C + O_2 \rightarrow CO_2$ -394

formation of CO_2

ΔH_r = sum ΔH_f (products) − Sum ΔH_f (reactants)

symbol for sum Σ

$\Delta H_r = \Sigma\, \Delta H_f(\text{products}) - \Sigma\, \Delta H_f(\text{reactants})$

our products 2 Fe and 3 CO_2

$2 \times 0 + 3 \times (-394)$

our reactants Fe_2O_3 and 3 CO

$-822 + (3 \times -111)$

$\Delta H_r = 3 \times (-394) - (-822 + (3 \times -111)) =$

$= -27$ kJ/mol

Questions:

1. Calculate the enthalpy change for the reaction
   $BrF (g) + 2F_2 (g) \rightarrow BrF_5 (l)$
   We know that
   $BrF (g)+ F_2 (g) \rightarrow BrF_3 (l) (g)$ Δ H=- 242 kJ/mol
   BrF_3 (gl+ F_2 (g) $\rightarrow$ BrF_5(l) (g) Δ H=- 158 kJ/mol
2. Calculate the enthalpy change for the reaction
   $ClF_3 (g) + F_2 (g) \rightarrow ClF_5 (g)$
   We know that
   $Cl_2 (g) + 3F_2 (g) \rightarrow 2ClF_3 (g)$ Δ H=- 328 kJ/mol
   $Cl_2(g) + 5F_2 (g) \rightarrow 2ClF_5 (g)$ Δ H=- 510 kJ/mol
3. Calculate the enthalpy change for the reaction
   $4NH_3(g) + 5O_2 (g) \rightarrow 4NO (g) + 6H_2O (g)$
   Standard enthalpy change of formation for NH_3(g) = -46 kJ/mol, for NO (g) = 90 kJ/mol, for H_2O (g) = -242 kJ/mol