HW5

The **enthalpy change (ΔH)** of a chemical reaction describes the amount of heat energy released or absorbed during a reaction at constant pressure.
There are two types of reactions:

- **Exothermic reactions (ΔH < 0):** Release heat to the surroundings.
- **Endothermic reactions (ΔH > 0):** Absorb heat from the surroundings.

Two common methods for calculating the enthalpy change of a chemical reaction are **Hess's Law** and the **use of standard enthalpies of formation**.

1. Hess's Law

Hess's Law states that the total enthalpy change of a chemical reaction is the same regardless of whether the reaction occurs in one step or several steps.
This means that we can calculate the enthalpy change of a reaction by adding together the enthalpy changes of other reactions that produce the same overall result.

Example:

Let's look at the following problems:

Calculate enthalpy change for the following reaction

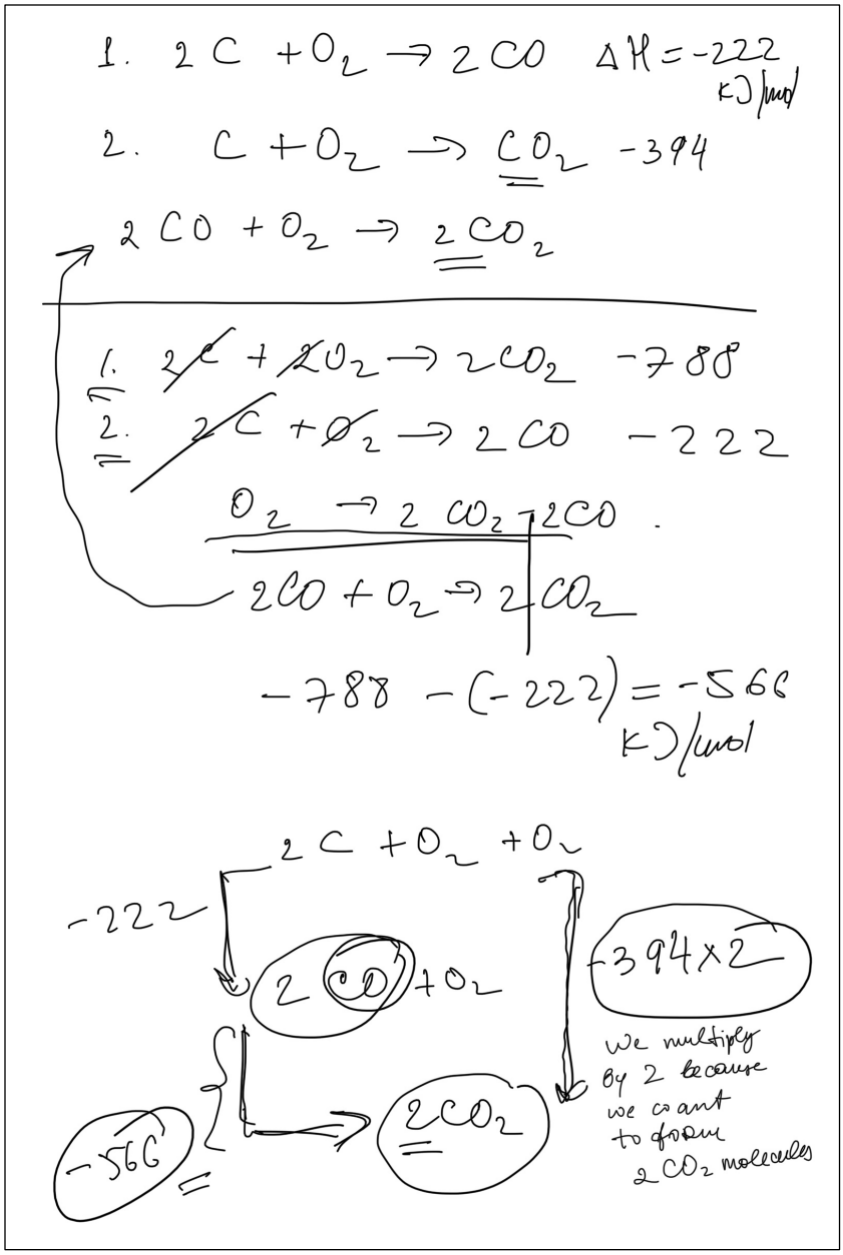
$2CO(g) + O_2(g) \rightarrow 2CO_2(g)$

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:



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

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

Important rules when using Hess's Law:

If we reverse a chemical reaction, we must reverse the sign of ΔH.

If we multiply a chemical reaction by a number, we must multiply its ΔH by the same number.

When adding reactions together, we also add their enthalpy changes.

2. Standard Enthalpy of Formation

The **standard enthalpy of formation (ΔH°f)** is the enthalpy change that occurs when exactly one mole of a substance is formed from its constituent elements in their standard states.

The standard state of an element is its most stable form at a specified temperature and standard pressure (1 atmosphere). Standard enthalpies of formation are commonly reported at 25°C (298 K).

Example: Formation of Water

$H_2(g) + ½O_2(g) \rightarrow H_2O(l)$

$\Delta H°f = -285.8$ kJ/mol

This means that when one mole of liquid water is formed from hydrogen and oxygen, 285.8 kJ of heat is released.

Important: The standard enthalpy of formation of an element in its standard state is always zero.

For example:

$\Delta H°f [O_2(g)] = 0$ kJ/mol

Calculating Reaction Enthalpy Using Standard Enthalpies of Formation

We can calculate the standard enthalpy change of a chemical reaction using the following equation:

$\Delta H°reaction = \Sigma(n \times \Delta H°f \text{ of products}) - \Sigma(n \times \Delta H°f \text{ of reactants})$

Where:

- $\Delta H°reaction$ = Standard enthalpy change of the overall reaction
- $\Delta H°f$ = Standard enthalpy of formation of each substance
- n = Coefficient of the substance in the balanced chemical equation
- Σ = Sum (add together)

In simple terms:

Enthalpy change = Products − Reactants

Example: Combustion of Methane

Calculate the standard enthalpy change for the following reaction:

$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$

The standard enthalpies of formation are:

Substance	ΔH°f (kJ/mol)
$CH_4(g)$	−74.8

$O_2(g)$	0
$CO_2(g)$	−393.5
$H_2O(l)$	−285.8

Step 1: Calculate the sum for the products.

Products: $CO_2 + 2H_2O$

$\Delta H°products = (-393.5) + 2(-285.8)$

$\Delta H°products = -965.1$ kJ

Step 2: Calculate the sum for the reactants.

Reactants: $CH_4 + 2O_2$

$\Delta H°reactants = (-74.8) + 2(0)$

$\Delta H°reactants = -74.8$ kJ

Step 3: Subtract the reactants from the products.

$\Delta H°reaction = \Delta H°products - \Delta H°reactants$

$\Delta H°reaction = -965.1 - (-74.8)$

$\Delta H°reaction = -890.3$ kJ

The negative value indicates that the reaction is exothermic. This means that burning one mole of methane releases approximately 890.3 kJ of heat under standard conditions when liquid water is produced.

Key Points to Remember

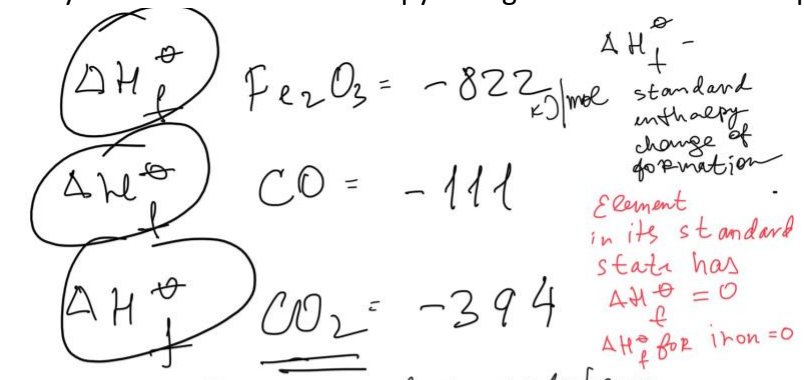
1. Enthalpy change (ΔH) describes the heat energy absorbed or released during a reaction at constant pressure.
2. Hess's Law states that the total enthalpy change is independent of the reaction pathway.
3. Standard enthalpy of formation ($\Delta H°f$) describes the enthalpy change when one mole of a substance forms from its constituent elements in their standard states.
4. The standard enthalpy of formation of an element in its standard state is zero.
5. To calculate reaction enthalpy using standard enthalpies of formation, use:

$\Delta H°reaction = \Sigma(n \times \Delta H°f\ products) - \Sigma(n \times \Delta H°f\ reactants)$

6. A negative ΔH indicates an exothermic reaction, while a positive ΔH indicates an endothermic reaction.

Remember: Calculating a reaction's enthalpy change using standard enthalpies of formation is actually an application of Hess's Law. Both methods are based on the idea that the overall enthalpy change depends only on the initial and final states, not on the pathway taken.

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



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. $2Fe + \frac{3}{2}O_2 \rightarrow Fe_2O_3$ $\Delta H = -822$
formation of Fe_2O_3

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

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

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
   $BrF\ (g) + F_2\ (g) \rightarrow BrF_3\ (l)$ **Δ** H=- 242 kJ/mol
   $BrF_3\ (g) + F_2\ (g) \rightarrow BrF_5\ (l)$ **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