THERMOCHEMISTRY

1. **Enthalpy of Chemical Reaction**

$$\boxed{H = E + PV}$$

The change in Enthalpy:

$$\boxed{\Delta H = \Delta E + \Delta(PV)}$$

If the pressure is held constant:

$$\Delta H = \Delta E + P\Delta V$$

Enthalpy of Reaction
- Because most reactions are constant-pressure process, we can equate the heat change in these cases to the change in enthalpy.

$$\text{reaction} \longrightarrow \text{products}$$

→ The change in enthalpy, called the **Enthalpy of Reaction,**ΔH.

$$\boxed{\Delta H = H(products) - H(reactants)}$$

- $\Delta H > 0$, the reaction is an endothermic process.
- $\Delta H < 0$, the reaction is an exorthermic process.

Thermochemical Equations
$H_2O(s) \longrightarrow H_2O(l)$
Δ H = 6.01 kJ/mol.
A comparison of ΔH and ΔE:

2. **The change of internal energy:**

$$\begin{aligned} \Delta E &= \Delta H - P\Delta V && (1)\\ \Delta E &= \Delta H - \Delta(PV) && (2)\\ &= \Delta H - \Delta(nRT) && (3)\\ &= \Delta H - RT\Delta n && (4) \end{aligned}$$

For:

- $\Delta n = \Sigma n_{product} - \Sigma n_{reaction}$
- R = 8.314 J/mol $\cdot K$
- R = 0.08214 L $\cdot atm/mol \cdot K$

3. **Enthalpy of Formation** ($\Delta H°$)
   $\text{aA} + \text{bB} \longrightarrow \text{cC} + \text{dD}$
   Hess's law
   - When reaction are converted to products, the change in enthalpy is the **same** wheither the reaction takes place in one step or in the series of steps.ΔH **depends** only on the **initial** and **final state**.
   - We have a reaction:

$$\mathrm{CO\,(g)} + \frac{1}{2}\,\mathrm{O_2(g)} \longrightarrow \mathrm{CO_2(g)} \tag{5}$$

$$\Delta H = -283.0kJ/mol \tag{6}$$

$$\text{Then we inverse the equation:} \tag{7}$$

$$\mathrm{CO_2(g)} \longrightarrow \mathrm{CO\,(g)} + \frac{1}{2}\,\mathrm{O_2(g)} \tag{8}$$

$$\Delta H = +283.0kJ/mol. \tag{9}$$

   Example:

   Let's say we are interested in the standard enthalpy of formation of carbon monoxide (CO). We might represent the reaction as

$$\mathrm{C(graphite)} + \tfrac{1}{2}\mathrm{O_2}(g) \longrightarrow \mathrm{CO}(g)$$

   However, burning graphite also produces some carbon dioxide (CO_2), so we cannot measure the enthalpy change for CO directly as shown. Instead, we must employ an indirect route, based on Hess's law. It is possible to carry out the following two separate reactions, which do go to completion:

   (a) $\mathrm{C(graphite)} + \mathrm{O_2}(g) \longrightarrow \mathrm{CO_2}(g) \quad \Delta H^\circ_{\text{rxn}} = -393.5\ \text{kJ/mol}$

   (b) $\mathrm{CO}(g) + \tfrac{1}{2}\mathrm{O_2}(g) \longrightarrow \mathrm{CO_2}(g) \quad \Delta H^\circ_{\text{rxn}} = -283.0\ \text{kJ/mol}$

   First, we reverse Equation (b) to get

   (c) $\mathrm{CO_2}(g) \longrightarrow \mathrm{CO}(g) + \tfrac{1}{2}\mathrm{O_2}(g) \quad \Delta H^\circ_{\text{rxn}} = +283.0\ \text{kJ/mol}$

   Because chemical equations can be added and subtracted just like algebraic equations, we carry out the operation (a) + (c) and obtain

$$\begin{array}{llll}
\text{(a)} & \mathrm{C(graphite)} + \mathrm{O_2}(g) \longrightarrow \mathrm{CO_2}(g) & & \Delta H^\circ_{\text{rxn}} = -393.5\ \text{kJ/mol} \\
\text{(c)} & \mathrm{CO_2}(g) \longrightarrow \mathrm{CO}(g) + \tfrac{1}{2}\mathrm{O_2}(g) & & \Delta H^\circ_{\text{rxn}} = +283.0\ \text{kJ/mol} \\
\hline
\text{(d)} & \mathrm{C(graphite)} + \tfrac{1}{2}\mathrm{O_2}(g) \longrightarrow \mathrm{CO}(g) & & \Delta H^\circ_{\text{rxn}} = -110.5\ \text{kJ/mol}
\end{array}$$

4. **Entropy** (Phần quan trọng :)) - The change in entropy of the system:

$$\boxed{\Delta S_{sys} = \frac{q_{reversible}}{T}}$$

   The total change entropy is:

$$\Delta S = \Delta S_{surrounding} + \Delta S_{system}$$

   In reversible and irreversible process:

- Reversible Process: $\Delta S_{universe} = \Delta S_{system} + \Delta S_{surrounding} = 0$
- Irreversible Process $\Delta S_{universe} = \Delta S_{system} + \Delta S_{surrounding} > 0$

$\rightarrow$ The total entropy of the universe increases in any spontaneous process
Some properties of the change in entropy:

- **S** increases when **T** (temperature) increases
- when **M** increases then **S** increases.

And:

$$\boxed{S_g^\circ > S_l^\circ > S_s^\circ}$$

Example:F_2, Cl_2, Br_2, I_2.
$\rightarrow S_{I_2} < S_{Br_2} < S_{F_2} < S_{Cl_2}$