

# Thermochemistry Notes

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April 29, 2025

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# 1 Definitions

## 1.1 Conservation of energy

Energy cannot be created or destroyed; it can only be converted from one form to another.

## 1.2 Thermal energy

Thermal energy refers to the kinetic energy of molecular motion. It is measured by finding the **temperature** of an object.

## 1.3 Heat

Heat refers to the amount of thermal energy transferred from one object to another as the result of a **temperature difference** between the two.

## 1.4 First law of thermodynamics

The total internal energy  $E$  of an isolated system is constant.

$$\Delta E = E_{final} - E_{initial}$$

## 1.5 State function

A state function is a function or property whose value depends only on the present state or condition of the system, not on the path used to arrive at that state.

## 1.6 Expansion work

Expansion work is the work done as the result of a volume change in the system.

## 1.7 Enthalpy

Enthalpy refers to the total heat content of a system. It is equal to the internal energy of the system plus the work done on the system. It is also a state function.

$$\Delta H = \Delta E + w$$

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

## 1.8 Thermodynamic standard state

The thermodynamic standard state is the most stable form of a substance. The conditions are:

1. Pressure of 1 atm
2. Temperature of 25 °C
3. Concentration of 1 M for all substances in solution

Values at this state are denoted with a superscript circle, like  $\Delta H^\circ$ ,  $\Delta S^\circ$  and  $\Delta G^\circ$ .

## 1.9 Enthalpy change of fusion ( $\Delta H_{fusion}$ )

The enthalpy change of fusion is the amount of heat required to **melt** a substance **without changing its temperature**.

## 1.10 Enthalpy change of vaporisation ( $\Delta H_{vap}$ )

The enthalpy change of vaporisation is the amount of heat required to **vaporise** a substance **without changing its temperature**.

## 1.11 Enthalpy change of sublimation ( $\Delta H_{subl}$ )

The enthalpy change of sublimation is the amount of heat required to convert a substance from a **solid to a gas without going through a liquid phase**.

At constant temperature:

$$\Delta H_{subl} = \Delta H_{fusion} + \Delta H_{vap}$$

## 1.12 Exothermic reaction

An exothermic reaction is a reaction that releases heat, which means its enthalpy change is negative, i.e.  $\Delta H < 0$ .

## 1.13 Endothermic reaction

An endothermic reaction is a reaction that absorbs heat, which means its enthalpy change is positive, i.e.  $\Delta H > 0$ .

### 1.14 Heat capacity ( $C$ )

Heat capacity refers to the amount of heat necessary to raise the temperature of an object or substance a given amount.

$$C = \frac{q}{\Delta T}$$
$$q = C \times \Delta T$$

### 1.15 Specific heat capacity ( $c$ )

Specific heat capacity refers to the amount of heat required to raise the temperature of 1 g of a substance by 1 °C.

$$q = mc\Delta T, \text{ where } m \text{ is the mass of the substance in g}$$

### 1.16 Molar heat capacity ( $C_m$ )

Molar heat capacity is the amount of heat necessary to raise the temperature of 1 mol of a substance by 1 °C.

$$q = C_m \times n \times \Delta T, \text{ where } n \text{ is the number of moles of the substance}$$

### 1.17 Hess's law

Hess's law states that the overall enthalpy change for a reaction is equal to the sum of the enthalpy changes for the individual steps in the reaction.

Essentially:

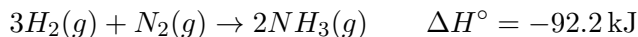
$$\Delta H_{overall} = \Delta H_1 + \Delta H_2 + \Delta H_3 + \dots + \Delta H_n$$

### 1.18 Haber process

The Haber process is just the industrial process to create ammonia ( $NH_3$ ) from  $H_2$  and  $N_2$  to form ammonia ( $NH_3$ ).

The conditions are:

1. Pressure of 200 atm
2. Temperature of 450 °C
3. Presence of iron ( $Fe$ ) catalyst



### 1.19 Standard enthalpy change of formation ( $\Delta H_f^\circ$ ) (Standard heat of formation)

The standard enthalpy change of formation is the enthalpy change for the formation of 1 mol of a substance in its **standard state** from its constituent elements in their **standard states**.

### 1.20 Bond dissociation energies

Bond dissociation energies is the **standard enthalpy changes** for the corresponding **bond-breaking** reactions.

Essentially, it is  $\Delta H_{Bond-breaking}^\circ$ .

### 1.21 Spontaneous process

A spontaneous process is a process that, once started, proceeds on its own **without** a continuous **external influence**.

### 1.22 Entropy ( $S$ )

Entropy is the amount of molecular randomness in a system.

### 1.23 Change in Gibbs Free Energy ( $\Delta G$ )

$$\Delta G = \Delta H - T\Delta S$$

- When  $\Delta G < 0$ , the reaction is **spontaneous**.
- When  $\Delta G = 0$ , the reaction is at **equilibrium**.

- When  $\Delta G > 0$ , the reaction is **not spontaneous**.

## 2 Formulas

### 2.1 Change in internal energy due to change in pressure or volume

$q$  = Heat transferred

Work done:  $w = -P\Delta V$

$$\Delta E = q + w$$

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

For constant volume ( $\Delta V = 0$ ):

$$q_v = \Delta E$$

For constant pressure:

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

Since enthalpy change ( $\Delta H$ ) is equal to the heat transferred:

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

Since enthalpy is a state function whose value depends only on the current state of the system:

$$\begin{aligned}\Delta H &= H_{final} - H_{initial} \\ &= H_{products} - H_{reactants} \\ &= \Delta(H_f)_{products} - \Delta(H_f)_{reactants} \\ &= \Delta H_{Bond-breaking} - \Delta H_{Bond-forming}\end{aligned}$$