Thermochemistry Cheat Sheet

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September 19, 2023

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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 ΔG° .

1.9 Enthalpy change of fusion (ΔH_{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 (ΔH_{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 (ΔH_{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 $1\,\mathrm{g}$ of a substance by $1\,\mathrm{^{\circ}C}$.

 $q = mc\Delta T$, where m 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.

 $q = C_m \times n \times \Delta T$, where n 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:

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

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

$$3H_2(g) + N_2(g) \to 2NH_3(g)$$
 $\Delta H^{\circ} = -92.2 \,\text{kJ}$

1.19 Standard enthalpy change of formation (ΔH_f°) (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 (ΔG)

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

- 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

$$q = {\it Heat transferred}$$

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 (ΔH) 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:

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