

Edexcel IAL Chemistry A-Level

Topic 6: Energetics

Detailed Notes

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Enthalpy Change (ΔH°)

Enthalpy change is heat energy change and is represented by the symbol ΔH° . Enthalpy is measured under standard conditions of **100 kPa pressure** and a specified temperature, generally **298 K**.

In a reaction, bonds are broken and then bonds are made. For bonds to be **broken**, energy is **taken in** from the surroundings and when bonds are **formed**, energy is **given out**. The overall energy change of the reaction depends on how much energy is transferred in these processes.

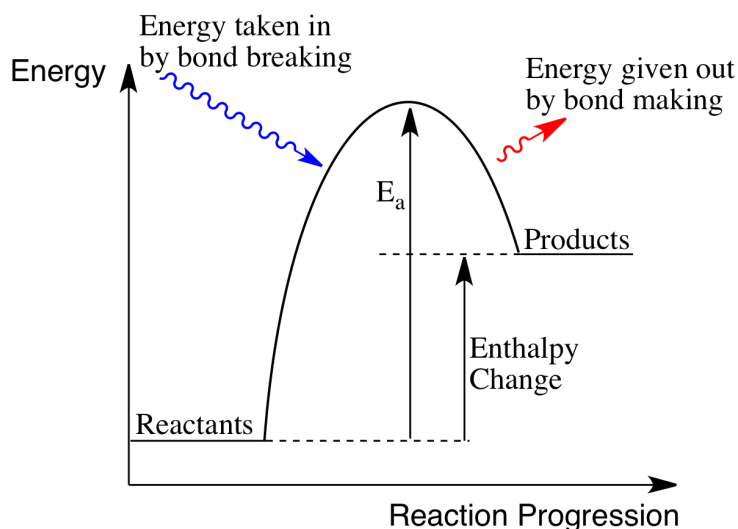
When energy is taken in from the surroundings, the **enthalpy change is positive**. When energy is released to the surroundings, the **enthalpy change is negative**.

Overall enthalpy change (ΔH) can be calculated as follows:

$$\Delta H = \text{energy to break bonds (+ve)} + \text{energy to make bonds (-ve)}$$

Enthalpy changes in a reaction can be shown on an **energy level diagram**. These also indicate if the reaction is endothermic or exothermic.

Example: Endothermic energy level diagram

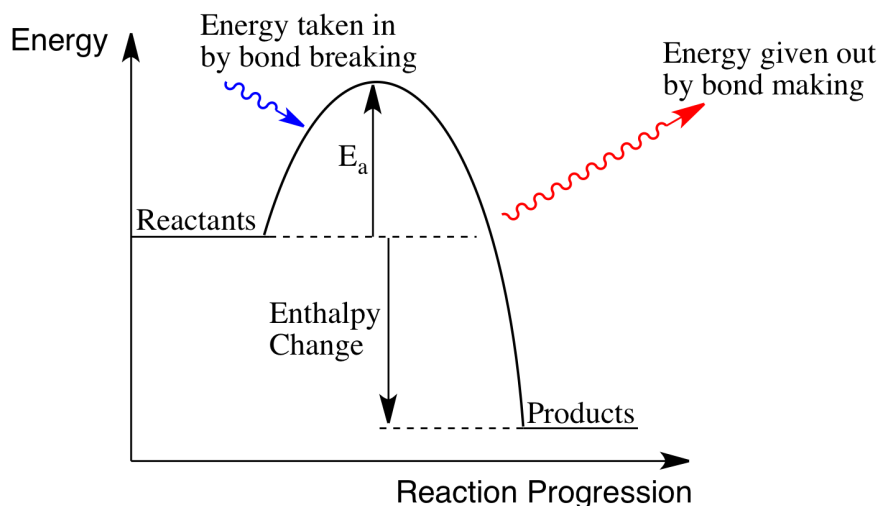


In **endothermic** reactions more energy is needed to break bonds than make new ones. Therefore, the overall **ΔH is positive** and **heat is taken in** from the surroundings.





Example: Exothermic energy level diagram



In **exothermic** reactions the opposite is true, with more energy being needed to make new bonds than break existing ones. Therefore **heat is given out** and **ΔH is negative**.

Measuring Enthalpy Change

Enthalpy Change of Reaction ($\Delta_r H^\circ$)

This is defined as:

The enthalpy change when quantities of substances in standard states react completely under standard conditions.

Enthalpy Change of Formation ($\Delta_f H^\circ$)

This is defined as:

The enthalpy change when one mole of a substance is produced from its elements under standard conditions.

Enthalpy Change of Combustion ($\Delta_c H^\circ$)

This is defined as:

The enthalpy change when one mole of a substance is burned completely in oxygen under standard conditions.

Enthalpy Change of Neutralisation ($\Delta_{\text{neut}} H^\circ$)

This is defined as:





The enthalpy change when solutions of acid and alkali react together under standard conditions to produce one mole of water.

Enthalpy Change of Atomisation ($\Delta_{\text{at}}H^\ominus$)

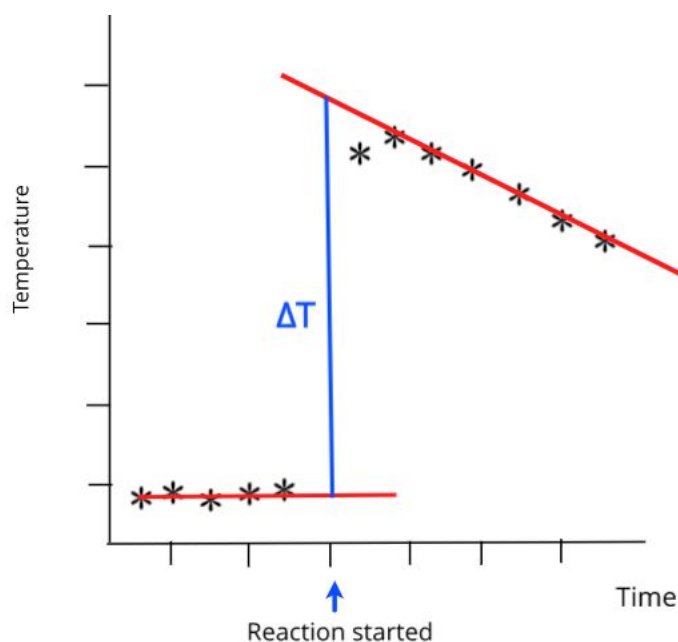
This is defined as:

The enthalpy change when one mole of gaseous atoms is formed from an element in its standard state.

Calorimetry

Calorimetry is an **experimental method** for finding enthalpy change by measuring **temperature change over time**. When recorded and plotted on a graph, data can be **extrapolated** to give an accurate value for the change in temperature at the beginning of the reaction.

Example: Graph showing the extrapolated line of best fit



This measured change in temperature, ΔT , is **proportional** to the energy change:

$$q = mc\Delta T$$

(where q = energy change (J), m = mass (g), c = specific heat capacity ($\text{J g}^{-1} \text{ }^\circ\text{C}^{-1}$), ΔT = temperature change ($^\circ\text{C}$))



This equation allows the energy change of a substance of known mass to be calculated. It depends on its **specific heat capacity**, defined as:

**The energy required to raise 1g of the substance by
1K without a change of state.**

Using this energy value (q), **enthalpy change per mole** (J mol^{-1}) of substance can be calculated:

$$\Delta H = \frac{q}{\text{moles}}$$

Sources of error

ΔH values found using calorimetry are **never completely accurate** as energy is easily lost from the system. Heat loss can occur due to **conduction**, **convection** or inaccuracies in measuring temperatures. The heat loss to the surroundings can be reduced by putting a **lid** on the calorimeter and **insulating** the outsides of the calorimeter using an insulator like polystyrene.

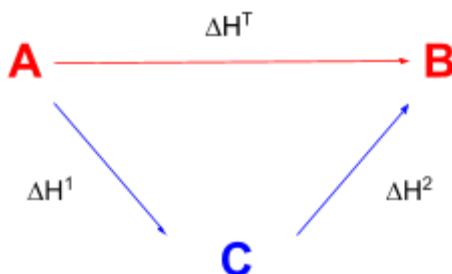
Also, the **specific heat capacity** of the solution is taken to be 4.18 kJ mol^{-1} , which is the value for water and not the **actual solution**. The specific heat capacity of the calorimeter is not taken into account so this leads to inaccuracies in the calculation.

Hess's Law

Energy in a reaction system must be **conserved**, as it cannot be created or destroyed. Therefore, the **overall enthalpy change** for a reaction is **the same**, regardless of the **route taken**.

This is **Hess's Law** and it is used to determine the enthalpy changes for reactions that cannot be found directly using an experimental method. To do this, a **triangular cycle method** is used with an intermediate product. The direction of the arrows indicates whether the values should be added or taken away. They can be treated like vectors:

Example:



$$\Delta H^{\ddagger} = \Delta H^1 + \Delta H^2$$

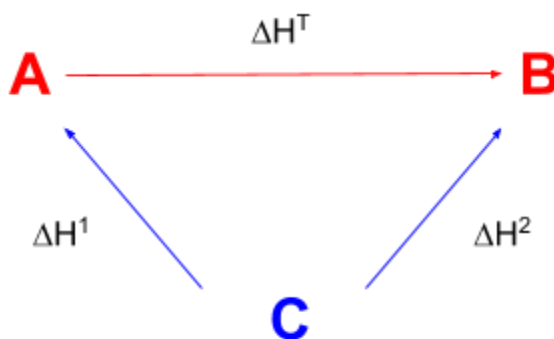




Enthalpies of Formation

Hess's law can be used to calculate an enthalpy change using given enthalpies of formation. When setting up the triangular diagram, the **arrows point up from the central product C** as both A and B are formed from the elements at C.

Example:



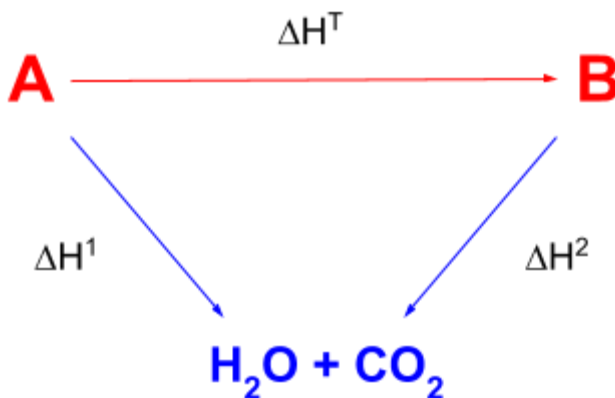
$$\Delta H^T = -\Delta H^1 + \Delta H^2$$

Note: ΔH^1 is subtracted as the reaction goes in the opposite direction to the arrow.

Enthalpies of Combustion

Hess's law can also be used to calculate an enthalpy change using given enthalpies of combustion. When setting up the triangular diagram, the **arrows point towards the central product (which is always H_2O and CO_2)** as both A and B burn to form the products at C.

Example:



$$\Delta H^T = \Delta H^1 - \Delta H^2$$

Note: ΔH^2 is subtracted as the reaction goes in the opposite direction to the arrow.





Bond Enthalpies

Bond enthalpy data is an **averaged** value representing:

The energy required to break one mole of the stated bond in a gaseous state, under standard conditions.

Different covalent bonds require different amounts of energy to be broken. Values can be found experimentally using **calorimetry** methods. The bond enthalpy values calculated in this way often differ from the **data book values** as they are **not exact** and **vary in each situation**. This means the databook values are **averaged values**.

Mean bond enthalpy values tell you how much energy is required to break a particular bond, averaged out across the range of compounds containing that bond. These values relate to how **strong** a bond is, so they can be used to infer which bonds might **break first** in a chemical reaction. Bonds with **lower** bond enthalpy values would be expected to break first.

If a reaction requires the breaking of many strong bonds or the reaction is endothermic overall, then it is likely that the reaction will occur **slowly** at **room temperature**.

Bond enthalpy calculations

Mean bond enthalpy values can be used to calculate the **overall enthalpy change** for a reaction.

$$\Delta H_{\text{reaction}} = \sum H_{\text{bonds broken}} - \sum H_{\text{bonds formed}}$$

This means that the enthalpy change for a reaction is equal to the **sum** of the bond enthalpies for the bonds **broken** in the reaction, minus the **sum** of the bond enthalpies for the bonds **formed** in the reaction.

Mean bond enthalpy values are often **tabulated**. You need to identify the bonds broken and formed during the reaction in order to calculate the overall enthalpy change.

Example:

Calculate the enthalpy change when methane undergoes complete combustion in oxygen using the bond enthalpies given.





Bond	Bond enthalpy (kJ mol ⁻¹)
C-H	413
O=O	498
O-H	464
C=O	799



Bonds formed

$$\text{C=O} \times 2 = 799 \times 2 = 1598$$

$$\text{H-O} \times 4 = 464 \times 4 = 1856$$

Bonds broken

$$\text{C-H} \times 4 = 413 \times 4 = 1652$$

$$\text{O=O} \times 2 = 498 \times 2 = 996$$

$$\begin{aligned} \text{Enthalpy change} &= (1652+996) - (1856+1598) \\ &= 2648 - 3454 \\ &= -806 \text{ kJ mol}^{-1} \end{aligned}$$

