# Edexcel Chemistry A-level

## Topic 8: Energetics I

Detailed Notes

## Enthalpy Change ($\Delta H^o$)

Enthalpy change is heat energy change and is represented by the symbol $\Delta H^o$. 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.

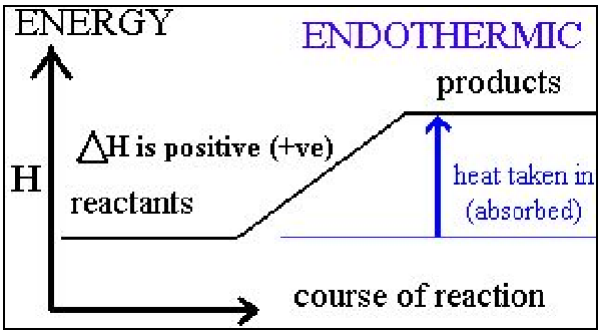
When energy is taken in from the surroundings, the **enthalpy change is positive**. When energy is released to the surroundings, the **enthalpy change is negative**.

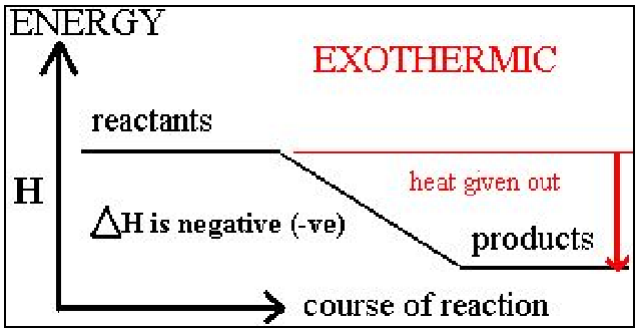
Overall enthalpy change ($\Delta H$) can be calculated as follows:

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

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

*Example:*




Images courtesy of Doc Brown's Chemistry

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

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 **$\Delta H$ is negative.**

## Measuring Enthalpy Change

### Enthalpy Change of Reaction ($\Delta H^o$)

This is defined as:

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

### Enthalpy Change of Formation ($\Delta_f H^o$)

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 ($\Delta_c H^o$)

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 ($\Delta_n H^o$)

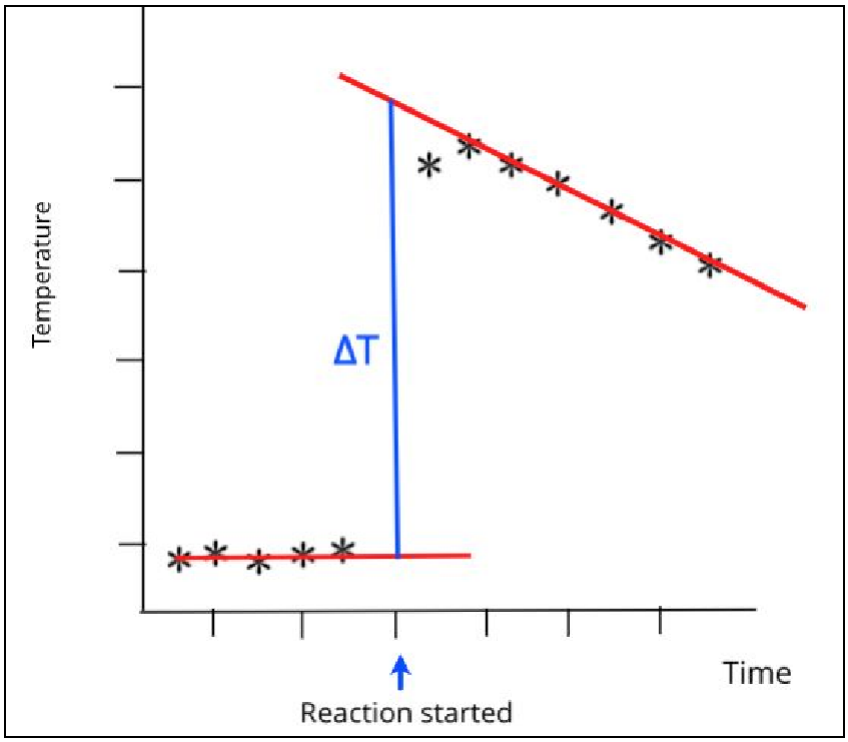
This is defined as:

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

## 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.

*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 (J $g^{-1}$ °$C^{-1}$), ΔT = temperature change (°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 substance by 1K without a change of state.**

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

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

### Sources of Error

$\Delta H$ 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.

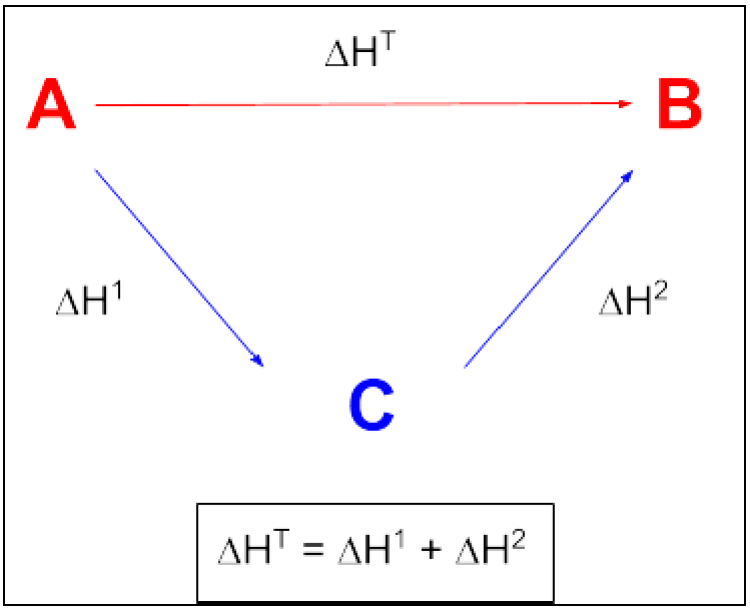
Also, the **specific heat capacity** of the solution is taken to be 4.18 kJ $mol^{-1}$, which is the value for water and not the **actual solution**. The specific heat capacity of the calorimeter is not taken into account so this leads to inaccuracies in the calculation.

## Hess's Law

Energy in a reaction system must be **conserved**, as energy 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:

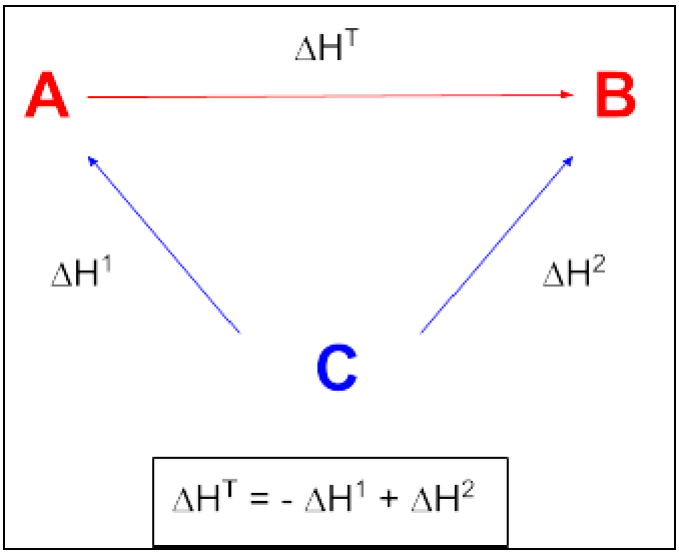
*Example:*



## 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 out from the central product C** as both A and B are formed from the elements at C.

*Example:*

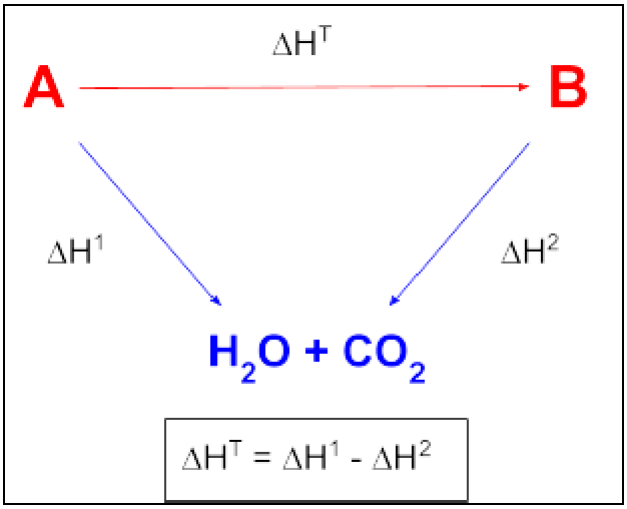



***Note:*** $\Delta H^1$ ***is subtracted as the reaction goes in the opposite direction to the arrow.***

## 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:*




***Note:*** $\Delta H^2$ ***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 **databook 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.

$$\Delta_r H = \sum \Delta H\,(bond\ breaking) - \sum \Delta H(bond\ forming)$$

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

**Chemical equation: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$**

**Bonds formed**

C=O x 2 = 799 x 2 = 1598

H-O x 4 = 464 x 4 = 1856

**Bonds broken**

C-H x 4 = 413 x 4 = 1652

O=O x 2 = 498 x 2 = 996

Enthalpy change = (1652+996) - (1856+1598)

= 2648 - 3454

= -806 kJ mol$^{-1}$