16.2 - Reaction Mechanism

16.2.1 - Explain that reactions can occur by more than one step and that the slowest step determines the rate of reaction (the rate-determining step)

Reaction will take place in a series of steps, forming **intermediate products** in the process. This is because most reactions involve more than two molecules. The chance of multiple particles colliding simultaneously is extremely low, so instead, the reaction will occur in stages, each involving one or two molecules. This step-by-step process is called the reaction mechanism.

The equations for these steps, when added together, will give the overall balanced equation for the reaction. For example:

$$\textit{Step } 1: O_{3\,(g)} \rightarrow O_{2\,(g)} + O\cdot_{(g)}$$
$$\textit{Step } 2: O_{3\,(g)} + O\cdot_{(g)} \rightarrow 2O_{2\,(g)}$$

Added together, the overall equation is:

$$2O_{3\,(g)} \rightarrow 3O_{2\,(g)}$$

The overall rate of reaction is affected by both steps; however, it is the slowest step that determines how fast the reaction will proceed. Hence, it is called the **rate-determining step**. The rate expression for this step will therefore be the same as the rate expression for the whole reaction.

When proposing a reaction mechanism, it is important to ensure that none of the steps involve more than two molecules colliding, as this is extremely unlikely. A step involving two molecules is bimolecular; a step involving one molecule is unimolecular.

During a bimolecular reaction, the species collide and form an **activated complex**, which consists of the two reactants as they are in the process of breaking and forming bonds. This will go on to break down into the products, or revert back to the reactants.

16.2.2 - Describe the relationship between reaction mechanism, order of reaction and rate-determining step

The order of reaction always matches the number of molecules involved in the rate-determining step: a unimolecular reaction will be first order; a bimolecular reaction will be second order.

As a result, if the rate expression is given, then it can be used to check that the correct mechanism has been deduced. Remember that the IB will only ever ask you about reaction mechanisms that have one or two steps.

For example, the reaction:

$$2NO_{(g)} + 2H_{2\,(g)} \rightarrow N_{2\,(g)} + 2H_2O_{(g)}$$

The reaction mechanism is:

$$NO_{(g)} + NO_{(g)} \rightarrow N_2O_{2\,(g)}$$
$$N_2O_{2\,(g)} + H_{2\,(g)} \rightarrow N_2O_{(g)} + H_2O_{(g)} \; (rate\ determining\ step)$$
$$N_2O_{(g)} + H_{2\,(g)} \rightarrow N_{2\,(g)} + H_2O_{(g)}$$

The rate expression for the second step would be: **rate = $k[N_2O_2][H_2]$**

However, since the concentration of N_2O_2 depends on the first step, it is instead:

rate = $k[NO]^2[H_2]$

This is a bimolecular reaction, since there are two molecules in the rate-determining step.