

Reaction Mechanisms

In reactions, we generally know the particles we start with as reactants and can identify the products, but is there anything in between?

It is difficult to determine the **REACTION MECHANISM**

definition: the exact collision processes that occur as the reactant particles change into product particles. It gives us a detailed description of the pathway followed during a chemical reaction.

The reaction mechanism is a series of **elementary processes** which determine the reaction rate and, when added together, result in an overall balanced equation. An elementary process is a single step reaction in a multi-step reaction mechanism.

Some reactions are simple and generally proceed as one step.

Example: $\text{H}_2(\text{g}) + \text{Cl}_2(\text{g}) \rightarrow 2\text{HCl}(\text{g}) + \text{energy}$

Others are more complex and could not proceed in just one step.

Example:

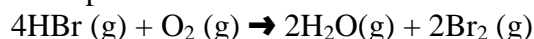


This is more complex and occurs as two steps

1. $\text{N}_2\text{O} \rightarrow \text{N}_2 + \text{O}$ (Elementary process)
 2. $\text{N}_2\text{O} + \text{O} \rightarrow \text{N}_2 + \text{O}_2$ (Elementary process)
- $$2\text{N}_2\text{O} \rightarrow 2\text{N}_2 + \text{O}_2$$

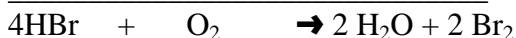
* Note that the O atoms shown occur as both products and reactants of the two elementary processes. These CANCEL. Any species on both sides of the arrow can cancel. Add the two reactions together to get the overall reaction.

Example:



This has three steps that proceed at different rates.

1. $\text{HBr} + \text{O}_2 \rightarrow \text{HOBr}$ slow
2. $\text{HOBr} + \text{HBr} \rightarrow 2\text{H}_2\text{O}$ fast
3. $2\text{HOBr} + 2\text{HBr} \rightarrow 2\text{H}_2\text{O} + 2\text{Br}_2$ fast



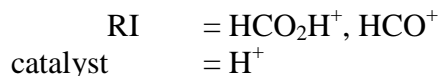
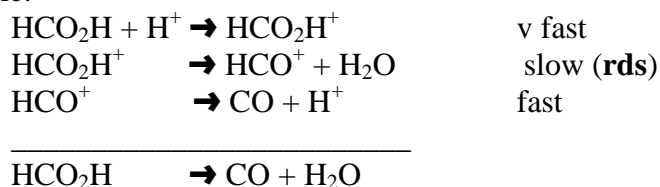
*** Note the presence of HOBr and HBr. These are called **reaction intermediates**.

Definition : a species that is generated or produced by an elementary process and is consumed by a later elementary process.

THE RATE OF A CHEMICAL REACTION IS ONLY AS FAST AS THE SLOWEST STEP.
This step is called the rate determining step (RDS)

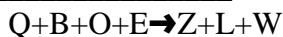
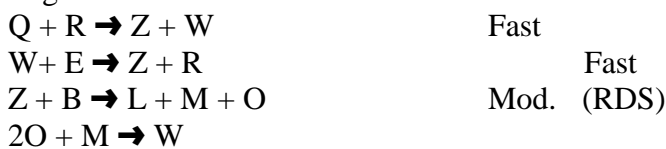
REACTION MECHANISMS AND CATALYSTS

example:



Catalyst in a Reaction Mechanism is a species that is added and then produced in a later step. It is not seen in the overall reaction and is re-useable (p.477)

In general terms:



The RI is M

The catalyst is R

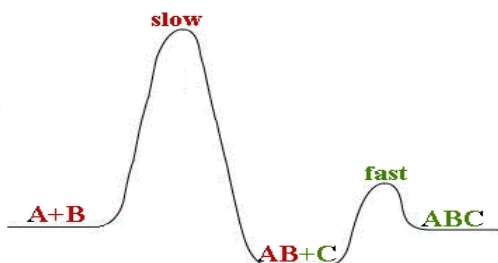
(You can tell the difference between a catalyst and a reaction intermediate because a catalyst is first introduced as a reactant and cancels out on the product side, but a reaction intermediate first appears as a product and then cancels out on the reactant side)

POTENTIAL ENERGY DIAGRAMS AND REACTION MECHANISMS

All our E_p diagrams so far have been for reactions that occur in one step.

If a reaction mechanism occurs through more than one elementary process, each one can be represented on an E_p diagram.

Rate Determining Step



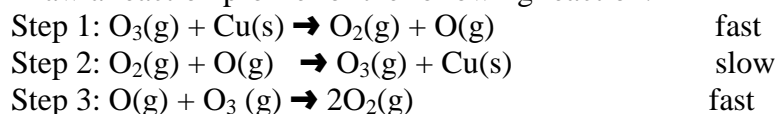
NOTE:

- Each process has its own activation energy... it's from the top of its bump to the valley previous to it.
- The elementary process with the largest E_a is the rate determining step (RDS)
- the reaction profile remains unchanged even if it occurs in more than one step- an exothermic reaction remains an exothermic reaction.

You might be asked to draw the reaction profile for a given mechanism. To do this follow these rules:

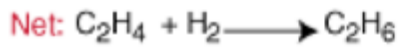
1. There must be a bump for each elementary process
2. Decide which step is the RDS **before** you begin to draw - it has to have the highest E_a
3. Determine before you start (if possible) if the overall reaction is exo- or endothermic.
4. Even though the profile is not drawn to scale, check that the bumps look correct - that the fast bump is smaller than the slow bump.

Draw a reaction profile for the following reaction:



Look at the overall effect of a catalyst

Uncatalyzed mechanism:



Pd catalyzed mechanism

