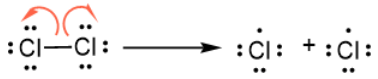
4.1: What is a reaction mechanism

What is a chemical reaction?

Chemical reactions involve rearranging atoms in a substance or substances called reactants resulting in new substances called products. In other words, chemical reactions involve breaking and/or making bonds. There are two major ways of breaking and making bonds, i.e., hemolytic and heterolytic bond breaking and making.

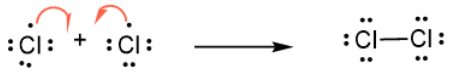
Hemolytic bond breaking and making

A covalent bond is a shared pair of electrons. In hemolytic bond breaking or hemolytic cleavage, the two elections are divided equally between the products as represented by the following reaction of a chlorine molecule (Cl_2) splitting into two chlorine atoms.



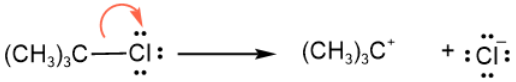
Recall that the half-headed curvy arrow represents the movement of one electron, pair of dots represents lone pair of electrons, a line represents a pair of bonding electrons, and a single dot represents an unpaired valance electron. A specie with an unpaired valence electron is called a free radical, e.g., $:\dot{\underset{\cdot\cdot}{Cl}}:$ in the above reaction is a free radical. Free radicals are usually reactive species.

The Reverse of the above reaction is a hemolytic bond making where two reactants contribute one electron each to make a covalent bond, as shown in the following reaction between two chlorine atoms.

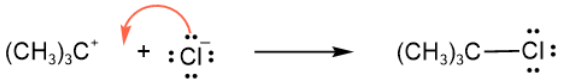


Heterolytic bond breaking and making

Heterolytic bond breaking happens so that a shared pair of electrons in the covalent bond are retained by one of the bonded atoms decreasing the charge by one, and the other bonded atom loses the shared electron increasing the charge by one, as shown in the following reaction.



Note that a regular curvy arrow represents the movement of two electrons, in this case, a bonding pair of electrons ending up as the fourth lone pair on the chlorine atom. Usually, the more electronegative atom receives the bonding pair of electrons and the less electronegative atom loses it in the heterolytic bond breaking. The reverse of the above reaction is heterolytic bond making, where the bonding pair of electrons are donated by one of the reactants, as shown in the following reaction.



Reaction mechanism

Chemical reactions often involve more than one bond-making and/or bond-breaking event. Further, reactions often happen in a sequence of steps that add up to yield the overall reaction equation. Individual reaction steps in the sequence are called **elementary reactions**.

Description of the step-by-step sequence of elementary reaction by which the overall chemical change occurs is called a **reaction mechanism**. There are two major reaction mechanisms, i) free radical reaction mechanisms that involve hemolytic bond breaking and making and ii) polar reaction mechanisms that involve heterolytic bond breaking and making. Some of the important reaction mechanisms are described in the following sections.