

# Theoretical representation of substitution reactions.

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## Abstract

When one functional group in a chemical molecule is replaced by another functional group, it is called a substitution reaction (also known as a single displacement reaction or a single substitution reaction). Substitution reactions are particularly essential in organic chemistry. Substitution reactions are classified as electrophilic or nucleophilic depending on the reagent employed, whether a reactive intermediate in the reaction is a carbocation, a carbanion, or a free radical, and if the substrate is aliphatic or aromatic. The ability to forecast the reaction's product outcome is aided by a thorough understanding of the reaction type. It may also be used to optimise a temperature and solvent selection reaction.

**Keywords:** Substitution reactions, Nucleophile, Electrophile, Nucleophilic substitution reaction, Electrophilic substitution reaction.

## Introduction

### Components

An electron-rich species donates a pair of electrons to an electron-poor species and forms a new product and a new base. Therefore, a substitution reaction contains four components [1].

- Nucleophile: the electron-rich species donating a pair of electrons to carbon
- Electrophile: the electron-deficient species accepting a pair of electrons
- Product: the species that is formed from a substitution reaction
- Leaving group: the group that leaves the compound

The substitution reaction is defined as a reaction in which the functional group of one chemical compound is substituted by another group or it is a reaction which involves the replacement of one atom or a molecule of a compound with another atom or molecule [2].

Substitution Reactions are of two types naming nucleophilic reaction and electrophilic reactions. These two types of reactions mainly differ in the kind of atom which is attached to its original molecule. In the nucleophilic reactions the atom is said to be electron-rich species, whereas, in the electrophilic reaction, the atom is an electron-deficient species [3].

Substitution reactions are among the most versatile and important reactions in all of organic chemistry.

## Types

### ➤ Nucleophilic Substitution Reaction

Nucleophiles are those species in the form of an ion or a molecule which are strongly attracted to the region of a positive charge. These are said to be fully charged or have negative ions present on a molecule. The common examples of nucleophiles are cyanide ions, water, hydroxide ions, and ammonia [4].

When an electron-rich species (nucleophile) provides an electron pair for bonding with the compound being transformed, it is called nucleophilic substitution. Some examples of nucleophiles are  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{OH}^-$ ,  $\text{RO}^-$ ,  $\text{CN}^-$ ,  $\text{H}_2\text{O}$ , and  $\text{NH}_3$ .

### ➤ Electrophilic Substitution Reaction

The electrophilic substitution reaction involves the electrophiles. Electrophiles are those which donate a pair of electrons in the formation of a covalent bond. The Electrophilic reactions occur mostly with the aromatic compounds. These compounds have about an excess of electrons that can be shared throughout the system of reaction [5].

When the substituent is electron-deficient (electrophile) and accepts an electron pair for bonding with the compound to be transformed, it is called electrophilic substitution. Some examples of electrophiles are  $\text{H}_3\text{O}^+$ ,  $\text{NO}_2^+$ , and  $\text{SO}_3$ .

## Conclusion

Substitution reactions are chemical processes in which a functional group in a molecule or ion is replaced by a

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functional group from another molecule or ion. The link between the functional group (ligand) and the reactive centre is broken during the substitution, and a new bond is created between the reactive centre and the new functional group (ligand). Substitution reactions are one of the most common types of organic chemistry reactions.

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