

# Electrophilic Aromatic Substitution

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## DESCRIPTION

Aromatic rings don't go through the electrophilic addition processes that alkenes do. Instead, they form a substitution product by reacting with electrophiles—and only in the presence of a catalyst. An electrophile ( $E^+$ ) replaces  $H^+$  in these processes.

In textbooks, monographs, and reviews, the classic SEAr mechanism of electrophilic aromatic substitution (EAS) reactions includes the creation of arenium ion intermediates (complexes) in a two-stage process. The generality of this mechanistic paradigm is called into question by our findings from multiple studies of EAS reactions. The focus of this report is on new computational and experimental results for three types of EAS reactions: halogenation with molecular chlorine and bromine, nitration with mixed acid (a combination of nitric and sulfuric acids), and sulfonation with  $SO_3$ .

The chlorination of anisole with molecular chlorine in  $CCl_4$  was investigated using a combination of computational and experimental methods. Direct substitution mechanisms compete with routes. The development of addition byproducts was discovered during a detailed NMR investigation of the course of experimental anisole chlorination at various temperatures. Furthermore, in the absence of Lewis acid catalysis, direct halogenation processes proceed via concerted single transition states rather than arenium ion intermediates. In nonpolar solvents, we found similar results for chlorination and bromination of numerous arenes. The classic reaction of benzene nitration by mixed acid was investigated using theoretical computations and experimental spectroscopic measurements. In this method, the structure of the first intermediate has been a source of contention. The production of the first intermediate in this reaction has been demonstrated experimentally using UV/vis spectroscopy. The impacts of the medium as a bulk solvent are considered in our broader theoretical modelling of the process, as well as the precise interactions of an  $H_2SO_4$  solvent molecule with intermediates and transition states along the chemical route. Our theoretical results show that the structure of the initial complex limits electronic charge transfer from the benzene system to the nitronium unit, which is consistent with the reported spectroscopic evidence. In contrary to commonly held beliefs, our computational findings show that in nonpolar, non-complexing media, and in the absence of catalysts, Aromatic sulfonation with sulphur trioxide has a coordinated method that avoids the use of the traditional  $\pi$ -complex (Wheland) intermediates.  $(SO_3)_2$  dimers react with benzene significantly more quickly

than monomeric sulphur trioxide under such conditions because they are more stable. The reaction follows the conventional two-stage SEAr mechanism in polar (complexing) media. The rate-controlling transition state, however, entails, the electrophile affinity (E), which measures the stabilization energy related with the production of arenium ions, is used to quantify the reactivity and regioselectivity in EAS reactions that follow the standard mechanistic framework. There are few application examples offered.

An aromatic ring can be replaced by a variety of electrophiles. In a halogenation reaction, a halogen atom, commonly chlorine or bromine, is added to the ring. Nitration and sulfonation reactions are aided by the nitro group ( $NO_2$ ) and the sulfonic acid group ( $SO_3H$ ). Alkylation and acylation processes add alkyl (R) and acyl (COR) groups to molecules. All of these reactions are triggered by the same mechanism.

## Electrophilic aromatic substitution mechanism

The electrophile accepts a pair of electrons from the aromatic ring in the first phase of electrophilic aromatic substitution, which is similar to the addition of electrophiles to alkenes. Aromatic compounds, on the other hand, are substantially less reactive than alkenes because this electron pair is part of a delocalized aromatic sextet. Because they are so much less reactive, a Lewis acid, such as  $FeBr_3$  in bromination and  $AlCl_3$  in alkylation and acylation, is needed as a catalyst to form an electrophile robust enough to react with the aromatic ring.

When the electrophile reacts with the aromatic ring, a carbocation intermediate is formed. The rate-determining step in electrophilic aromatic substitution is frequently the first. The intermediate is called a sigma complex because it produces a new sigma bond in the first phase.

## Electrophilic aromatic substitution reactions: substituent effects

To this point, we've simply talked about benzene's electrophilic substitution reactions. Now we'll look at how a substituent already linked to the aromatic ring affects an electrophile's ability to bind a second substituent to the ring. Only one product emerges from a benzene substitution process. When a second substituent is added to substituted benzene, one of three isomers can be produced: Ortho, Meta, or para. We'd like to know how the initial substituent impacts the rate at which these products are formed and the distribution of these products.

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