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Class: S. Y. B. Sc, Paper-II course-302
Sem.-III (First term)

Name of Paper: Inorganic and organic Chemistry

According to the new revised syllabus of Savitribai

Phule University from June 2020

Name of Teacher: Prof. Kolekar S.S.

Topic-Aromatic hydrocarbons

Aromatic hydrocarbons

Introduction

The hydrocarbons which are ring compounds are cyclic compounds they may be aromatic or nonaromatic.

The homocyclic compounds may be monocyclic aromatic like benzene or polycyclic aromatic like naphthalene, Anthracene, Phenanthrene.

The homocyclic compounds may be monocyclic non aromatic like cyclo-propane cyclo-butane, cyclo- pentane or polycyclic nonaromatic like Decalin.

The monocyclic aromatic compound like benzene having molecular formula C_6H_6

Benzene is aromatic compound obey the Huckel rule it is planer cyclic and fully conjugated molecule containing (4n+2) pi electrons, i.e. 6 pi electrons.

Each carbon atoms uses two of its sp2 orbitals to

form two sigma bonds with other two carbons and one with hydrogen to form the third sigma bond, Each carbon then has one unhybridized p orbital containing one unpaired electron. All these p orbitals then overlap to form three pi bonds

The derivative of benzene is three types

Mono-substituted benzene
Di-substituted benzene
Poly-substituted benzene

Mono-substituted benzene- The mono substituted benzene derivatives named by starting the name of substituent followed by the word the benzene

Di-substituted benzene-The disubstituted benzene derivatives shows ortho, meta and para substituted isomeric compounds

Poly -substituted benzene – The relative positions of the group is indicated by numbering

Preparation of the benzene

From Acetylene - The dry and pure acetylene gas is allowed to pass over red hot tube of iron or copper at 873^0K The cyclic polymerization is take place gives benzene.

From phenol- At high temperature, the phenol is treated with reducing agent like Zn dust gives the benzene

From sodium benzoate- The sodium salt of carboxylic acid treated with NaOH and lime it gives the benzene

From benzene sulphonic acid –

The hot steam is allowed to pass through benzene sulphonic acid gives benzene

Electrophilic substitution reaction

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Aromatic compound like benzene undergoes the substitution reaction rather than addition reaction under normal condition because the benzene got special stability, it obey the Huckel rule and it is aromatic. Benzene undergoes electrophilic

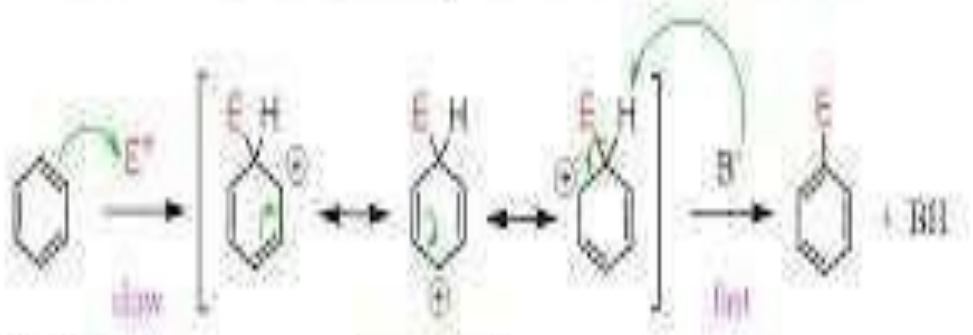
substitution reaction like nitration, sulphonation, halogenation Friedel –craft alkylation, friedel -craft acylation.

- Electrophile- It is electron deficient species havingpositive charge.
- Nucleophile- It is electron rich species having negative charge or lone pair

General mechanism of electrophilic substitution reactions.

1) Formation of Pi complex.
2) Formation of sigma complex. (Arenium ion)

The Mechanism of Electrophilic Aromatic Substitution



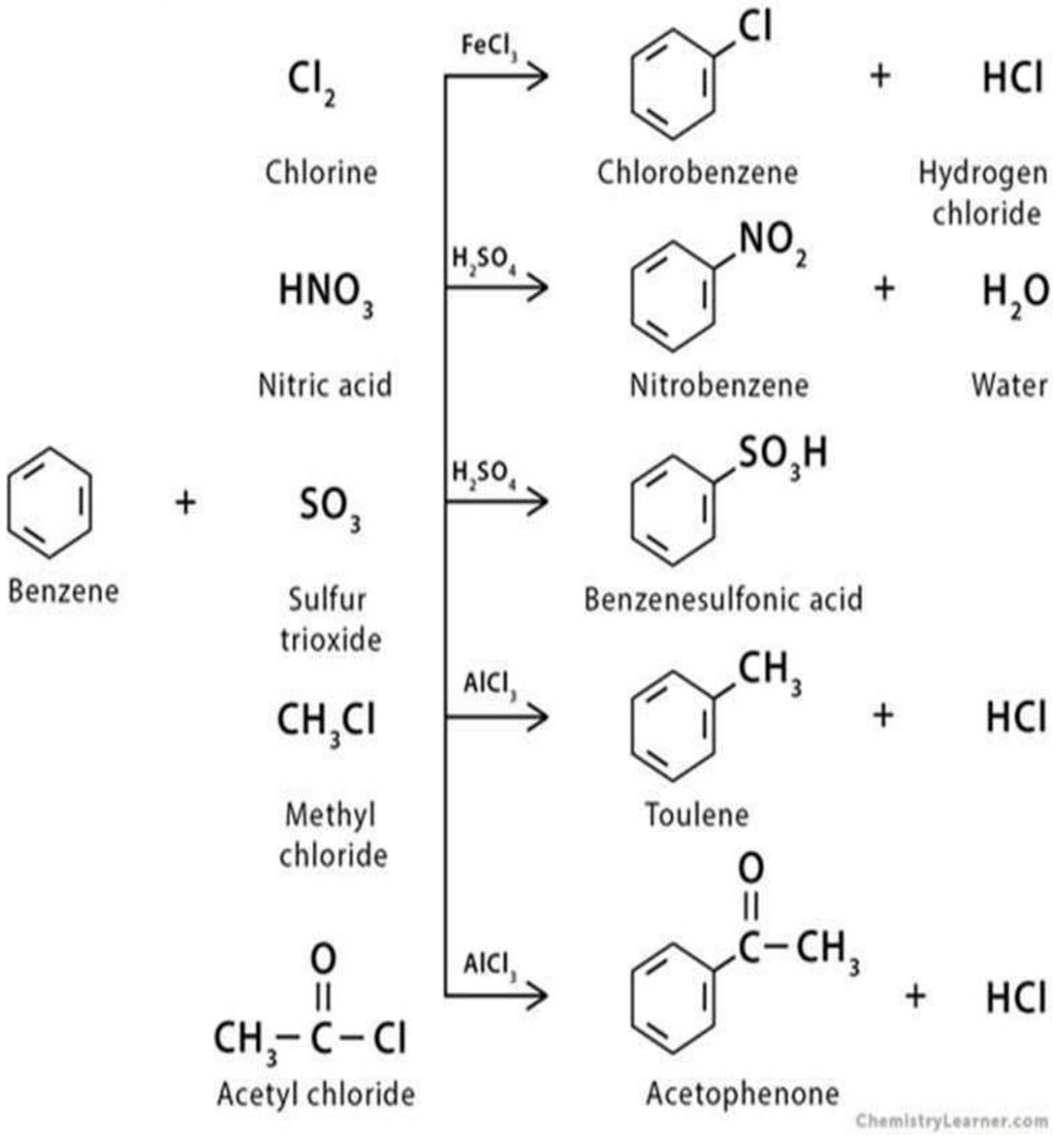
Step1. Addition of the electrophile- Making the C-E bond

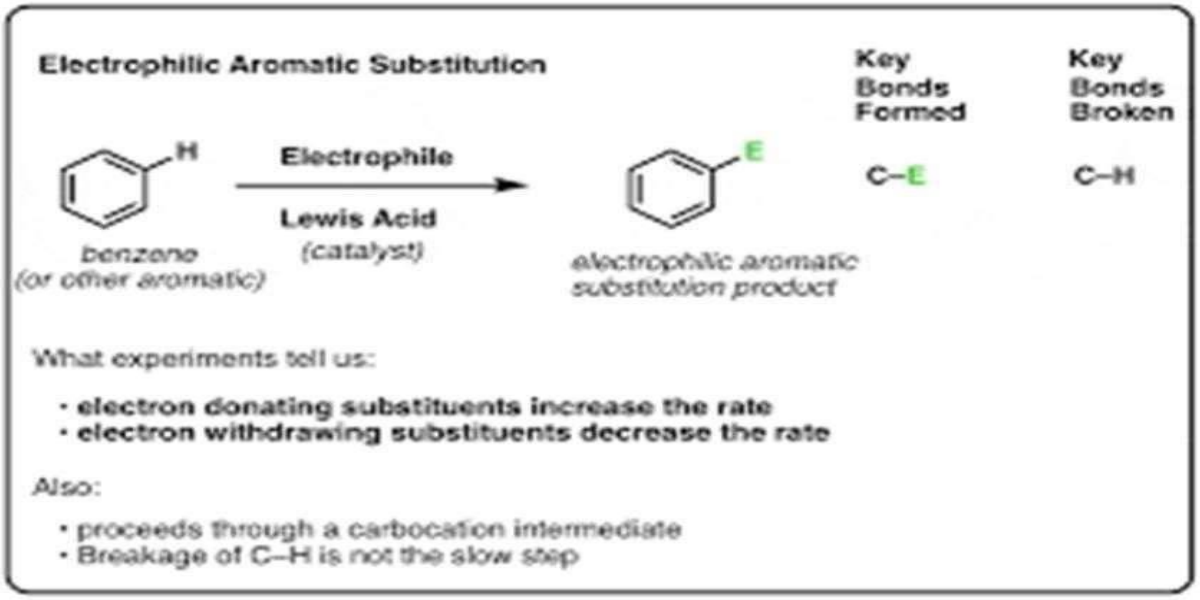
Sigma Complex

Resonance stabilized Arenium ion

Step 2. Proton transfer- Restoring Aromaticity

Electrophilic Aromatic Substitution of Benzene



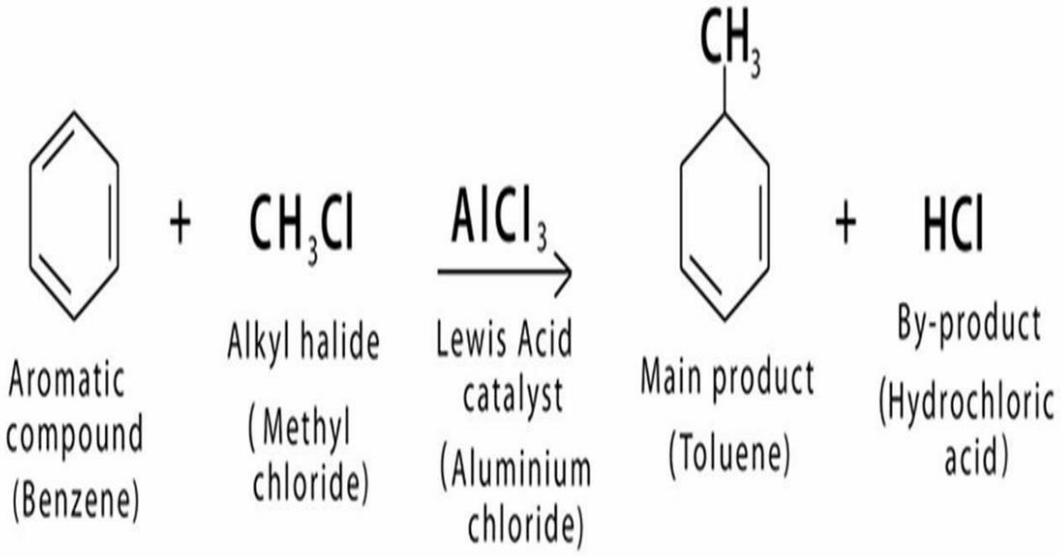


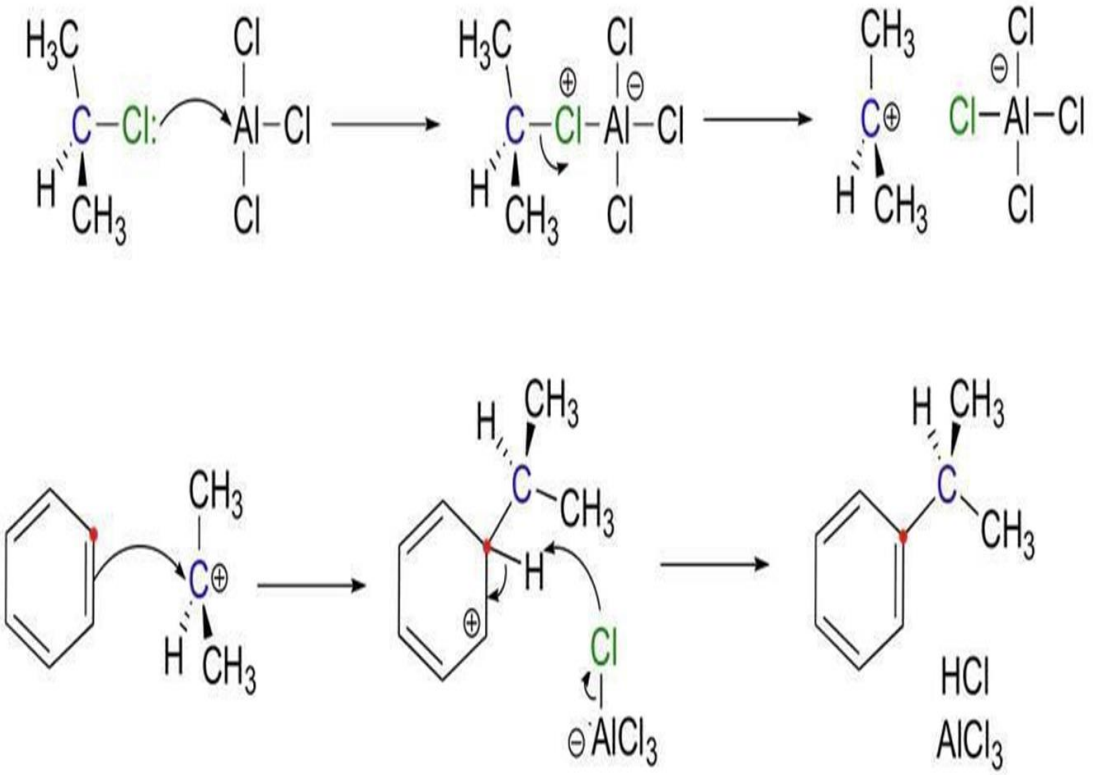
Friedel –Craft alkylation of benzene and Friedel –Craft Acylation of benzene

It is an electrophilic substitution reaction in which an alkyl group –R is introduced in the benzene ring., the Lewis acid is the catalyst is used to generate the electrophilic carbonium ion from alkyl halide.

Friedel –Craft alkylation carried out by using different alkylating agents like Lewis acid ,alkene,alcoholsto generate electrophilic carbonium ion.

Friedel-Crafts Alkylation Reaction




H3C
C
Cl:
H
CH3
Cl
Al
Cl
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CH3
C⊕
H
CH3
Cl
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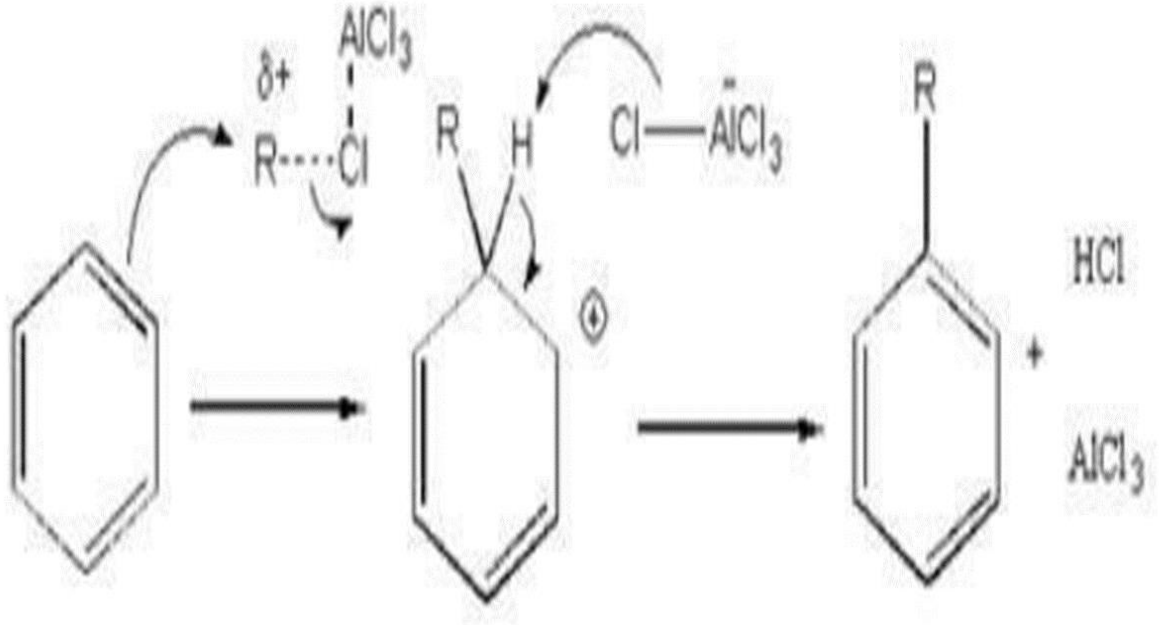
HCl
AlCl3



Limitation of F.C. Alkylation

It have number of serious drawbacks.

1) **Poly-alkylation**- F.C. alkylation never stops after mono alkylation. ,it gives poly alkylated products this because when an alkyl group is introduce in the benzene ring it activate the benzene ring by

+I effect and hyperconjugation effect

as a result

of it mono alkylated benzene become more reactive than benzene. So it do not stop the reaction at mono-
alkylation and shows poly- alkylation .

2) **Rearranged product**- The electrophile involved is a carbonium ion ,many alkylated product are formed due to the rearrangement of carbonium ion. , because initially form carbonium ion try to obtain more stable form. Tertiary carbonium ion more stable than secondary and secondary carbonium ion more stable than primary

Friedel –Craft Acylation of benzene

Friedel –Craft acylation is also an electrophilic substitution reaction in which an acyl group -COR acts as the electrophile becomes attached to the aromatic ring thus forming a ketone , the process is called acylation.

Mechanism- The effective electrophile in acylation reaction may be acylium group or a polarized complex and hence the mechanism involves two different route under different conditions

References: According to the new revised syllabus of Savitribai Phule Pune University from June 2020 , Text book of Inorganic and organic chemistry for S.Y. B.Sc. course (CH-302), Sem-II Manali Publication and google images