Al-Mustaqbal University
College of Science
Forensic Evidence Department

جامعة المستقبل
AL MUSTAQBAL UNIVERSITY

كلية العلـــوم
قـسـمـــــــم الادلة الجنائية

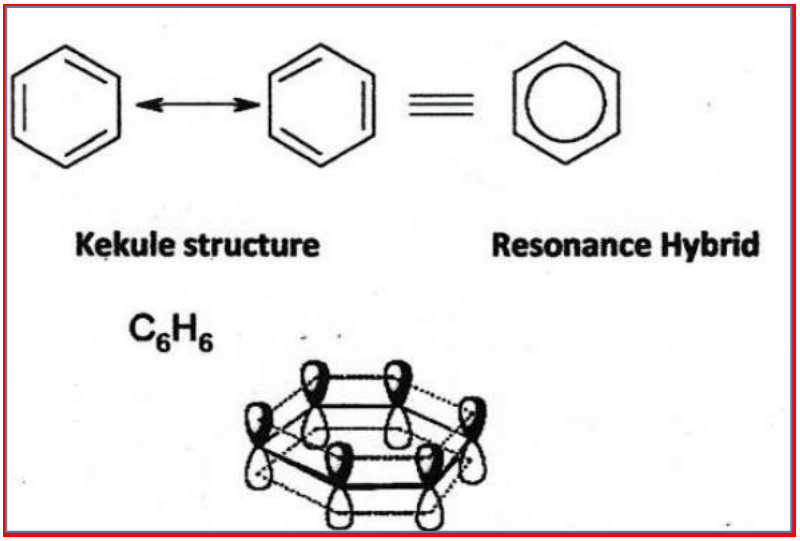
المحاضرة السادسة

Aromatic compound

المادة : عضوية
المرحلة : الثانية
اسم الاستاذ: م.د. كرار مجيد عبيد

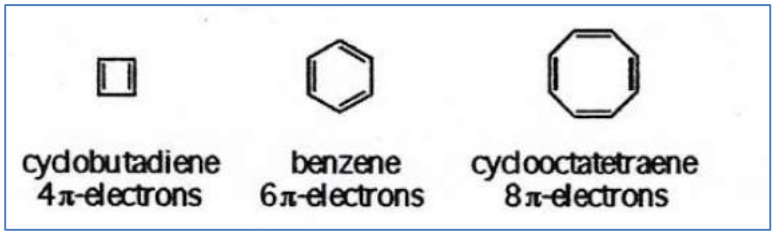
Benzene

a molecule of benzene consists of a ring of six carbon atoms with only drogen atom attached to each carbon. It has the molecular formula C_6H_6. The real molecule of benzene is a resonance hybrid of the two Lewis structures (a unique feature that makes benzene chemically stable).



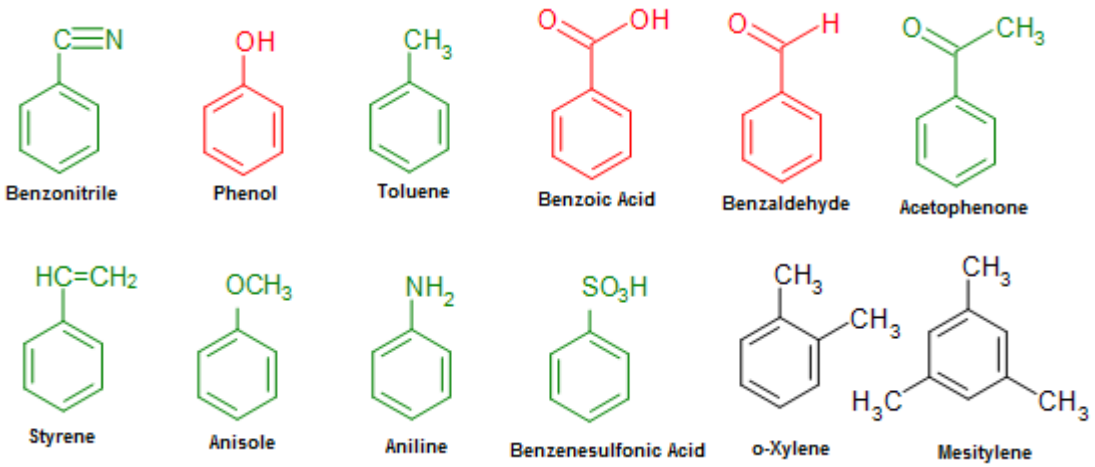
Aromaticity and the Hückel 4n + 2 Rule

Cyclic conjugated molecules: not all cyclic conjugated systems are aromatic (no special stability)



Nomenclature of benzene derivatives

we simply prefix the name of the substituent group to the word - benzene, as, for example, in

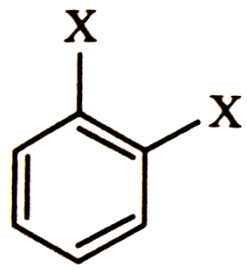


Other derivatives have special names which may show no resemblance to the name of the attached substituent group. For example, methyl benzene is always known as toluene, aminobenzene as aniline, hydroxybenzene as phenol.

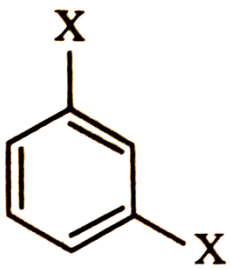
If several groups are attached to the benzene ring, the three possible isomers of a disubstituted benzene are:

The three isomers are typically referred to as:

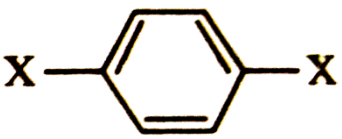
- **Ortho-** (o-): The two substituents are on adjacent carbon atoms (positions 1 and 2).
- **Meta-** (m-): The two substituents are separated by one carbon atom (positions 1 and 3).
- **Para-** (p-): The two substituents are on opposite sides of the ring (positions 1 and 4).



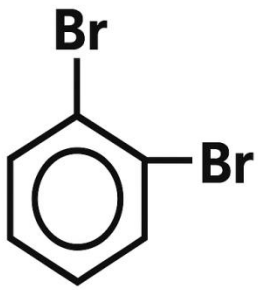
ortho (1, 2–)



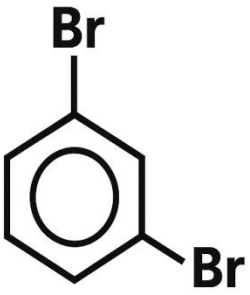
meta (1, 3–)



para (1, 4–)



ibromobenzene
ortho

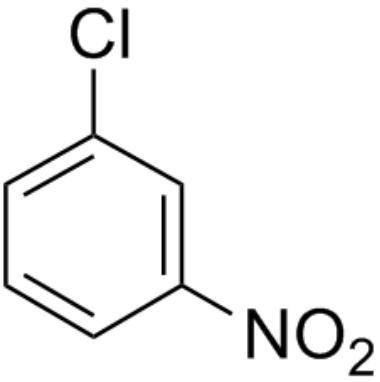


m-Dibromobenzene
meta

p-Dibromobenzene
para

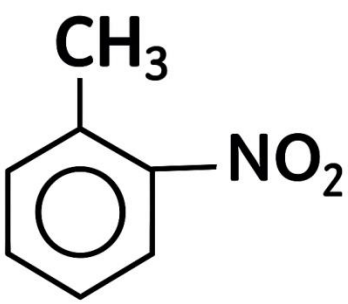
If the two groups are different, and neither is a group that gives a special name to the molecule, we simply name the two groups successively and end the word with -benzene, as, for example, chloronitrobenzene, bromoiodobenzene, etc."

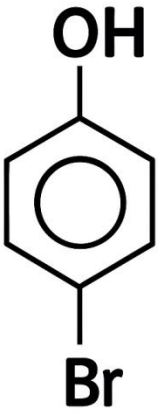
p-Bromoiodobenzene



m-Chloronitrobenzene

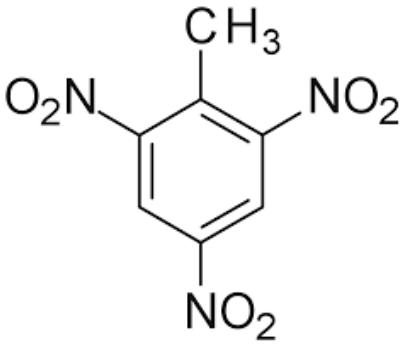
If one of the two groups is the kind that gives a special name to the molecule, then the compound is named as a derivative of that special compound, as, for example, nitrotoluene, bromophenol, etc.



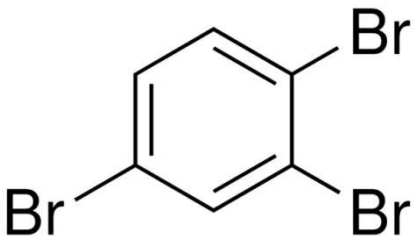


o-Nitrotoluene *p*-Bromophenol

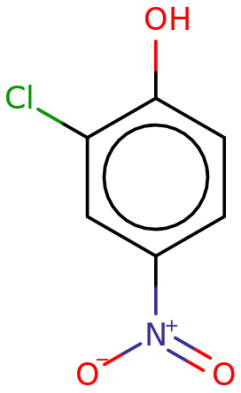
If more than two groups are attached to the benzene ring, numbers are used to indicate their relative positions with the lowest possible value and list the substituent alphabetically with hyphenated number.



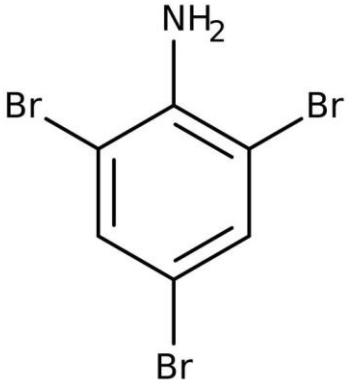
2,4,6-Trinitrobenzen(TNT)



1,2,4-Tribromobenzen



2-chloro 4-nitro phenol

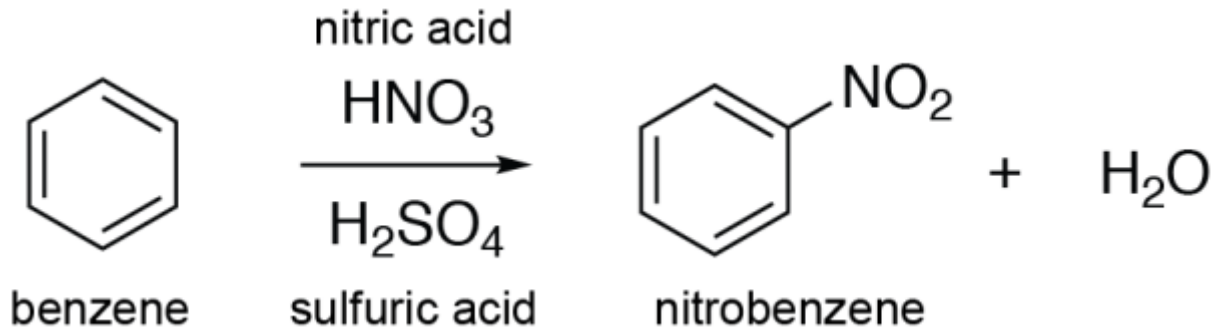


2,4,6-tribromoaniline

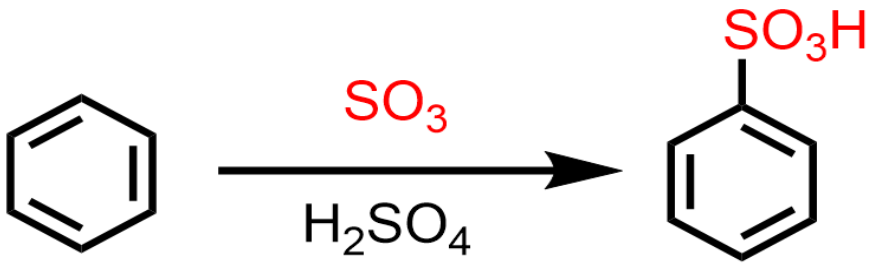
Reactions of Benzene (Substitution)

We have already seen that the characteristic reactions of benzene involve substitution, in which the resonance-stabilized ring system is preserved.

1-Nitration

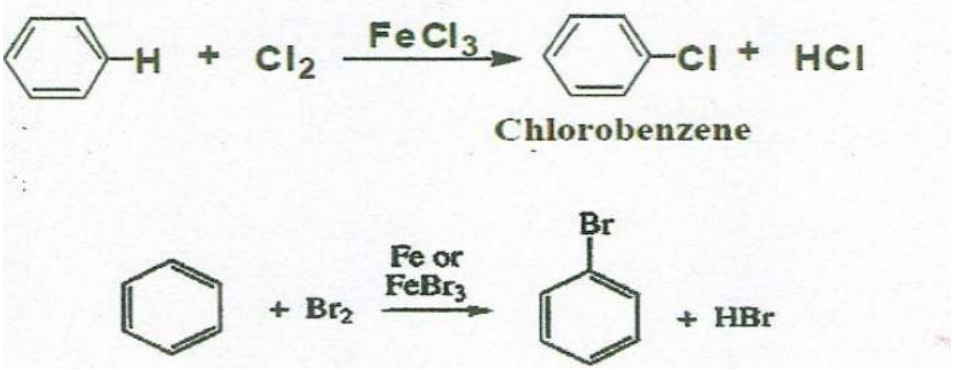


2-Sulfonation

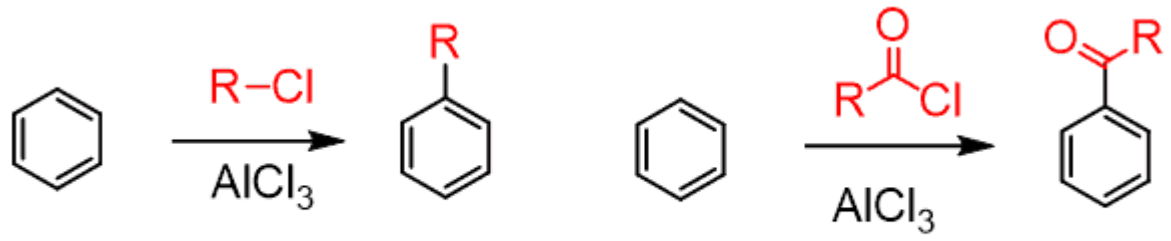


Benzene Benzenesulfonic acid

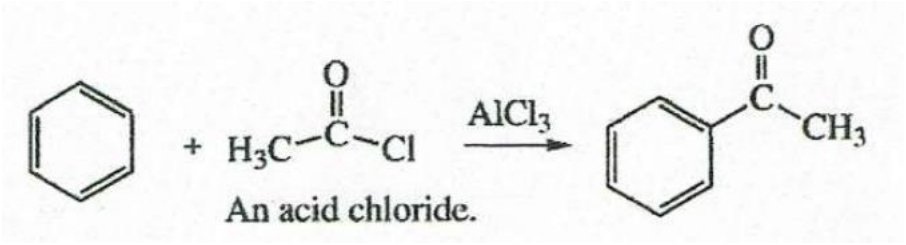
3- Halogenation



4- Friedel crafts alkylation and Friedel crafts acylation



Friedel-Crafts Alkylation **Friedel-Crafts Acylation**

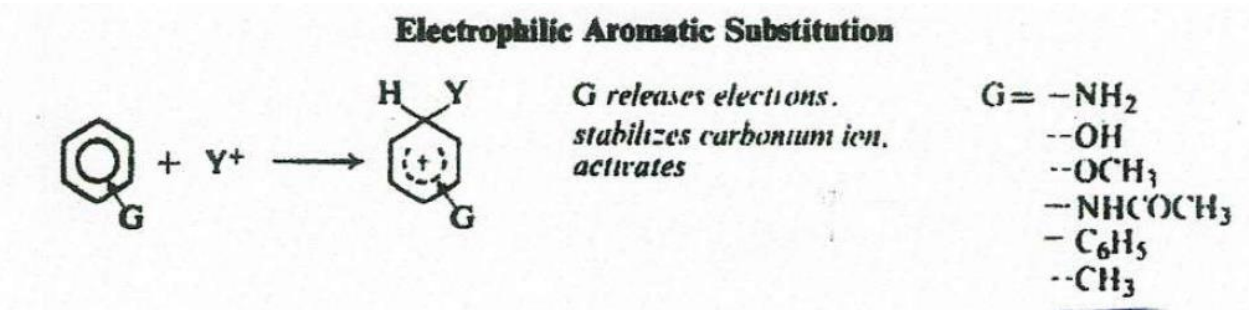


An acid chloride.

Orientation in Monosubstituted Benzenes

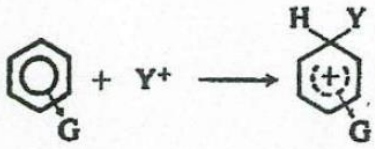
✓ **Effect of Substituent Groups**

Any group attached to a benzene ring affects the reactivity of the ring and determines the orientation of the next substitution. When an electrophilic reagent attacks an aromatic ring, a group that makes the ring more reactive than benzene is called an activating group, and causes attack to occur chiefly at positions ortho and para to it is called an ortho,para director.



A group that makes the ring less reactive than benzene is called a deactivating group, and causes attack to occur chiefly at positions meta to it is called a meta director.

Electrophilic Aromatic Substitution



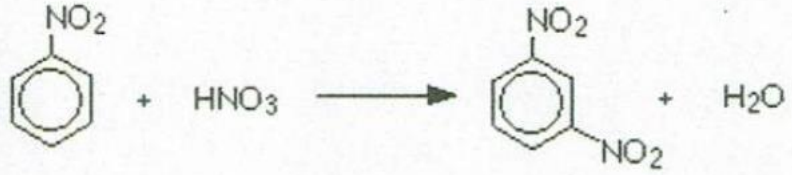
G withdraws electrons · destabilizes carbonium ion, deactivates

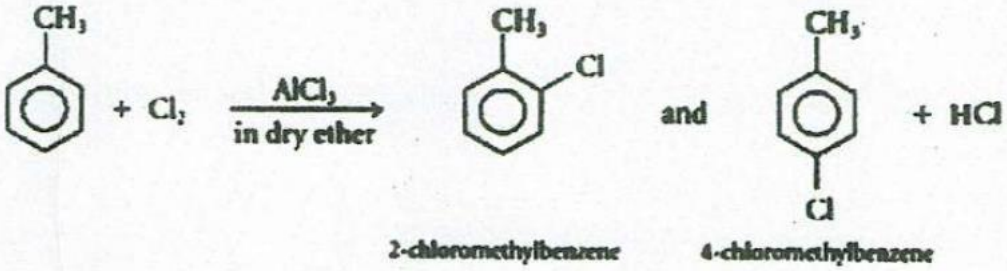
G=

Deactivating: *Meta* Directors
—NO_2
—$N(CH_3)_3^+$
—CN
—COOH (—COOR)
—SO_3H
—CHO, —COR

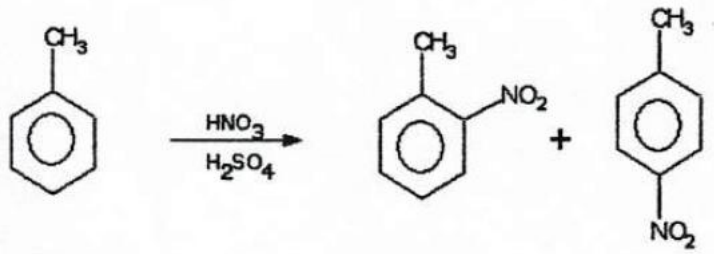
Deactivating: *Ortho,para* Directors
—F, —Cl, —Br, —I

Examples on orientation in monostituted benzene:

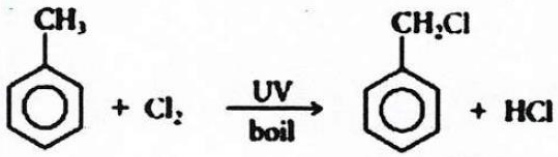




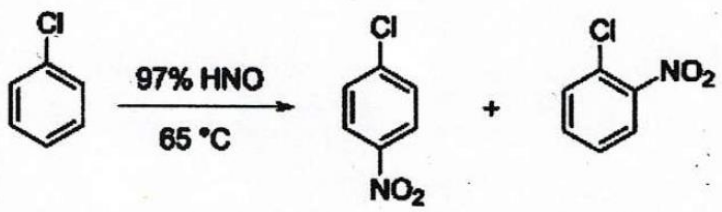
2-chloromethylbenzene 4-chloromethylbenzene

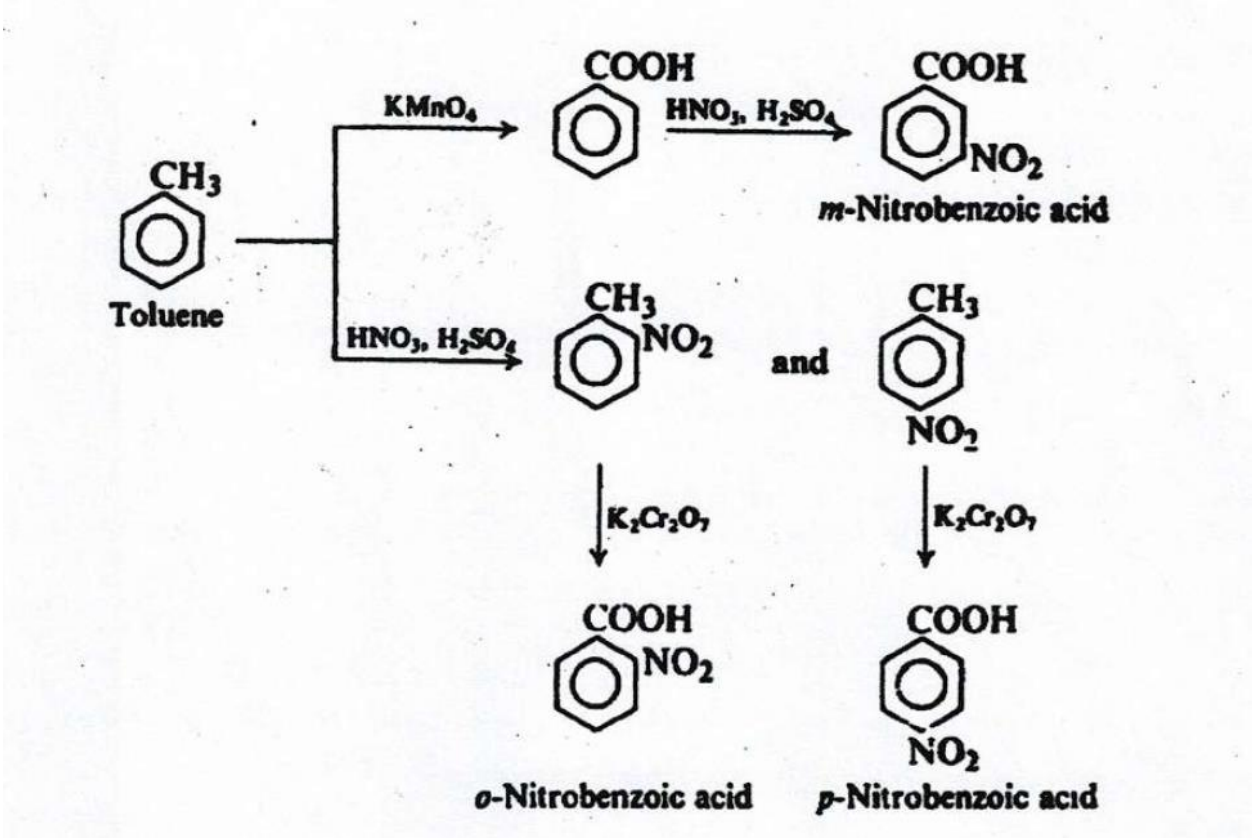


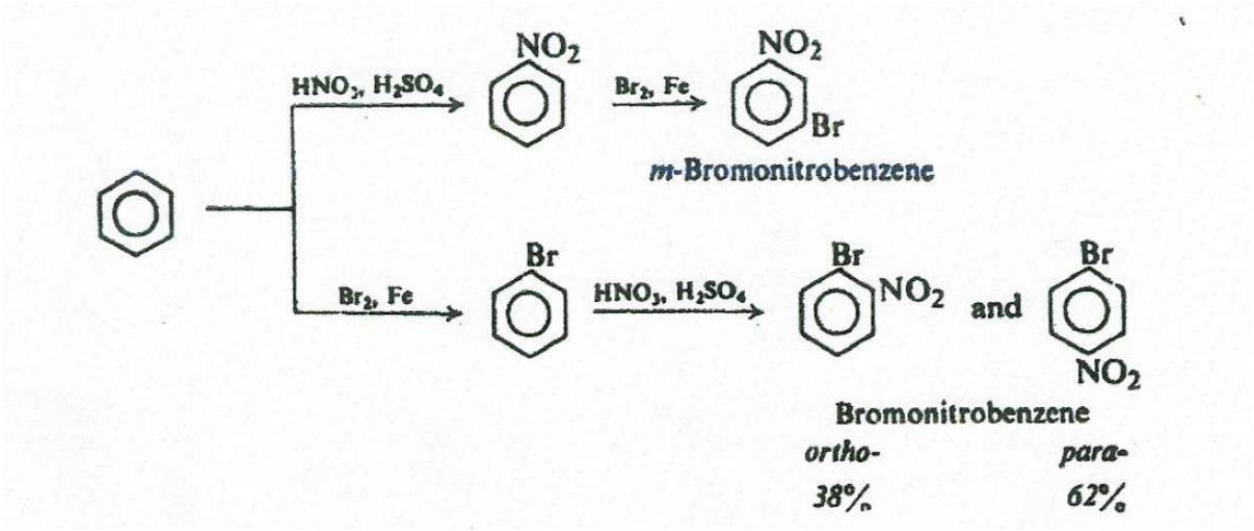
NOTE:



chloromethylbenzene




CH3
Toluene
KMnO4
COOH
HNO3, H2SO4
COOH
NO2
m-Nitrobenzoic acid
HNO3, H2SO4
CH3
NO2
and
CH3
NO2
K2Cr2O7
K2Cr2O7
COOH
NO2
COOH
NO2
o-Nitrobenzoic acid
p-Nitrobenzoic acid


HNO3, H2SO4
NO2
Br2, Fe
NO2
Br
m-Bromonitrobenzene
Br2, Fe
Br
HNO3, H2SO4
Br
NO2
and
Br
NO2
Bromonitrobenzene
ortho-
38%
para-
62%