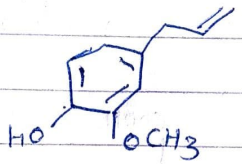
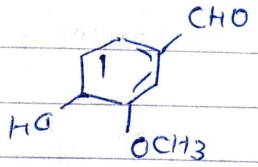
AROMATICS COMPOUNDS

In general Aromatic = ~~Aromatic~~ fragrance

"Aromatic compounds are benzene or compound that resembles benzene in chemical behaviour"



Eugenol
(In oil of cloves)



Vanillin

Nomenclature of Benzene derivatives:

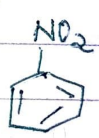
Two system are used in naming monosubstituted benzenes:

* In many simple compound, benzene is the parent name and the substituent is simply indicated by a prefix.

Fluorobenzene

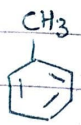
Chlorobenzene

Bromobenzene



Nitrobenzene

* Simple and common compound, the substituent and the benzene ring taken together, may form a commonly accepted parent name.



Toluene

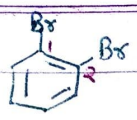
Phenol

Aniline

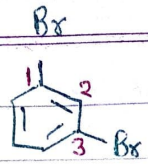
Anisole

Benzoic acid

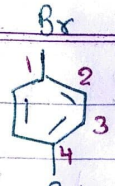
* When two substituent are present, their relative position are indicated by prefix ortho-, meta-, and para- (abbreviated o-, m- and p-) or by the use of the numbers.



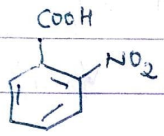
1,2 - Dibromobenzene
or
o - dibromobenzene



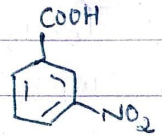
1,3 - dibromobenzene
or
m - dibromobenzene



1,4 - Dibromobenzene
or
p - dibromobenzene

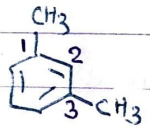


2 - Nitrobenzoic acid
or
o - nitrobenzoic acid

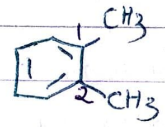


3 - Nitrobenzoic acid
or
m - nitrobenzoic acid

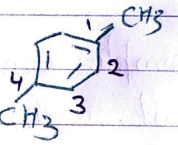
4 - nitrobenzoic acid
or
p - nitrobenzoic acid



1,3 - Dimethyl benzene
or
m - xylene



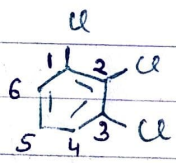
o - xylene



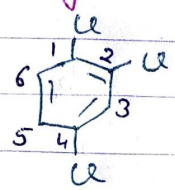
p - xylene

Dimethyl benzene are often called as xylene.

* If more than two group are present on the benzene ring, their positions must be indicated by the use of the numbers.



1,2,3 - Trichlorobenzene

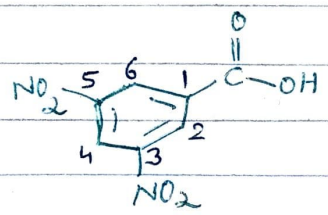


1,2,4 - Trichlorobenzene

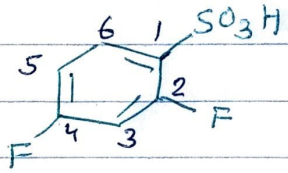
* The benzene ring is numbered so as to give the lowest possible number to the substituents.

* When more than two substituent are present and the substituent are different, they are listed in alphabetical order.

* When a substituent is one that together with benzene ring gives a new base name, that substituent is assumbed to be in position 1 and the new parent name is used.



3,5 - Dinitrobenzoic acid

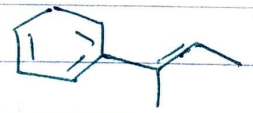


2,4 - Difluorobenzene sulfonic acid

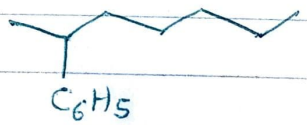
* When the C_6H_5- group is named as a substituent, it is called a phenyl group. The phenyl group is often abbreviated as C_6H_5- or Ph-.

* A Hydrocarbon composed of one saturated chain and one benzene ring is usually named as a derivative of larger structural unit. However, if the chain is unsaturated, the compound may be named as a derivative of that chain, regardless the ring size.

Butyl benzene

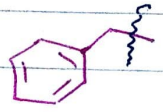


(E) - 2-Phenyl-2-butene



2-Phenyl Heptane

* Benzyl is an alternative name of phenylmethyl group and abbreviated as Bn.



Benzyl group
or
phenyl methyl group

Benzyl chloride
or
BnCl

Benzene: Benzene was discovered in 1825 by Michael Faraday and called this new hydrocarbon "bicarburet of hydrogen".

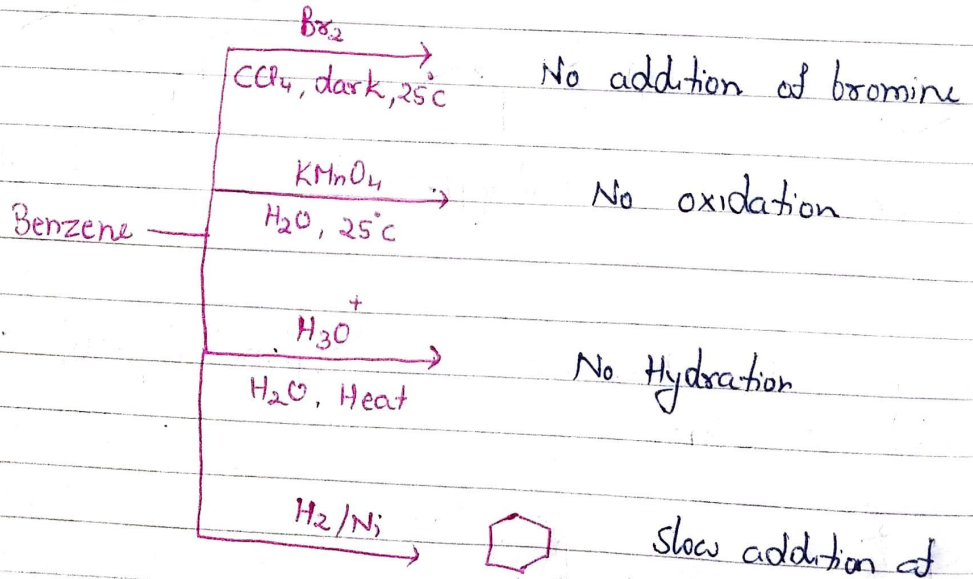
In 1834, Eilhardt Mitscherlich prepared the same compound by heating the benzoic acid with lime.

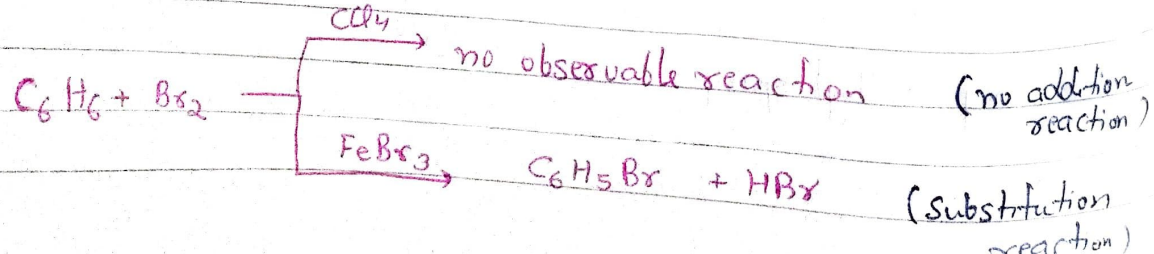
$$C_6H_5CO_2H + CaO \xrightarrow{heat} C_6H_6 + CaCO_3$$

Because of its relationship to benzoic acid, this hydrocarbon came to be named benzin, then later benzene.

Degree of unsaturation = 4
or
Index of Hydrogen dificiency

Reaction of Benzene Since benzene was a highly unsaturated compound and scientists were expected it to react accordingly.





Benzene does react with bromine but only in the presence of a lewis acid catalyst such as $FeBr_3$. it reacts not by addition but by substitution.

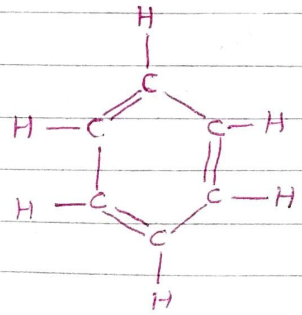
When benzene reacts with bromine, only one monobromo benzene is formed. Similarly, when benzene is chlorinated, only monochloro benzene results.

Two possible explanation can be given for these obseruation.

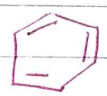
i) Only one of the six hydrogen atoms in benzene is reactive towards these reagent.

ii) All six hydrogen atoms in benzene are equivalent and replacing any one of them with a substituent results in the same product. (We shall see the second explanation is correct).

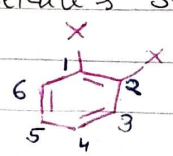
The Kekule Structure of Benzene According to Kekule, "The carbon atoms of benzene are in a ring, that they are bonded to each other by alternating singe and double bonds. One Hydrogen atom is attached to each carbon atom"



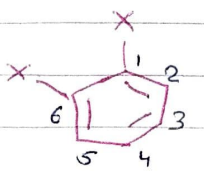
or



Flaws of Kekule's Structure:



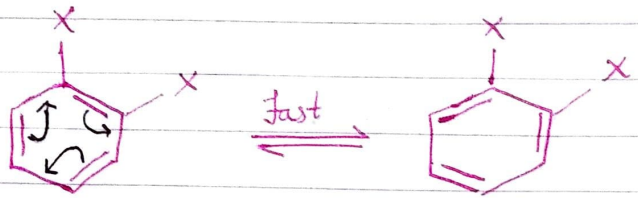
1,2-Disubstituted derivative of benzene



1,6-Disubstituted derivative of Benzene

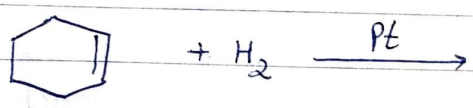
According to Kekule structure 1,2- and 1,6- disubstitution pattern creat different compound (isomer)
The two substituted carbons are connected by a double bond in one but by a single bond in other.

Kekule suggested that two isomeric structure could exist but interconvert too rapidly to be seprated.



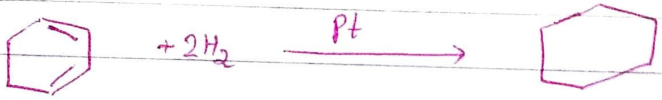
Now, we know that this idea of equilibrium was also incorrect.

Thermodynamic Stability of Benzene



Cyclohexene — Cyclohexane

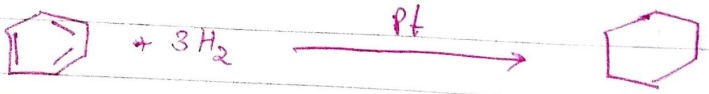
$\Delta H^\circ = -120\ KJ\ mole^{-1}$



1,3-Cyclohexadiene

Calculated
$\Delta H^\circ = 2 \times -120 = -240\ KJ\ mole^{-1}$

Observed
$\Delta H^\circ = -232\ KJ/mole$



Benzene

Calculated
$\Delta H^\circ = 3 \times (-120)$
$= -360\ KJ\ mole^{-1}$

Observed
$\Delta H^\circ = -208\ KJ\ mole^{-1}$

Difference = 152 KJ mole^{-1}

Thus Benzene is much more stable than the calculated value. It is more stable than the hypothetical 1,3,5-cyclohexatriene by 152 KJmole^{-1}. The difference between the amount of heat actually released and the calculated value is known as resonance energy of the compound

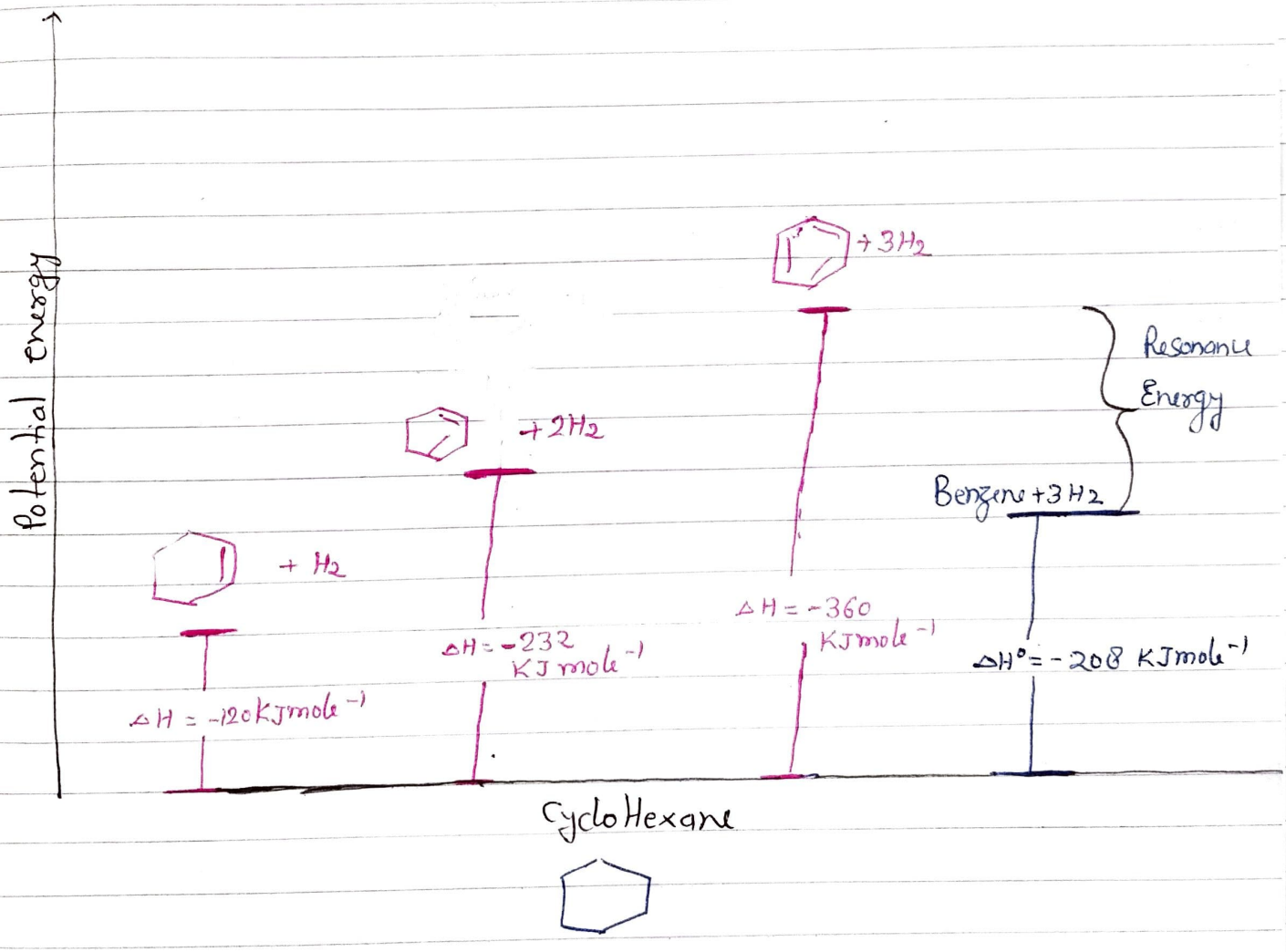


Figure: Relative stability of cyclohexene, 1,3-cyclohexadiene, 1,3,5-cyclohexatriene (hypothetical), and benzene