Grade - XI

Content Area: Organic Chemistry

Unit-12 Basic Concepts of Organic Chemistry (6 TH) New Syllabus

- Introduction to organic chemistry and organic compounds
- Reason for the separate study of organic compounds from inorganic compounds
- Tetra-covalency and catenation properties of carbon
- Classification of organic compounds
- Alkyl groups, functional groups and homologous series
- Idea of structural formula, contracted formula and bond line structural formula
- Preliminary idea of cracking and reforming, quality of gasoline, octane number, cetane number and gasoline additive

Introduction to Organic Chemistry and Organic Compounds

The branch of chemistry that deals with the study of compounds of carbon and hydrogen (i.e. hydrocarbons) and their derivatives is called organic chemistry.

Organic Compound (Old Definition)

The compounds that can be obtained from living things (plants & animals) are called organic compounds.

The compounds that can be obtained from non-living things (rocks, minerals) are called inorganic compounds.

Vital Force Theory

This theory was given by Swedish chemist **John Jacob Berzelius in 1815.**

According to this theory,

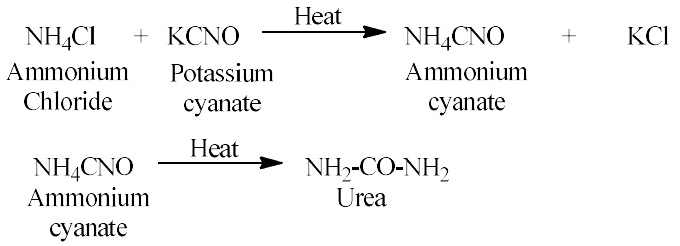
"Organic compounds are synthesized within the body of plant or animals and which requires some mysterious force or live force or vital force that is responsible to keep the living beings alive."

Limitations of Vital Force Theory

The hypothetical model of vital force theory came to an end when some chemists were able to synthesize organic compounds from inorganic substances outside the body of living beings & proved that vital force has no significant role in the synthesis of organic compounds.

For example:

Friedrich Wohler (German Chemist) in 1828 accidently synthesizes urea (organic compound) from inorganic compound.



Later on other organic compounds were also synthesized in the lab. Such as;

In 1845, Herman Kolbe synthesizes acetic acid.

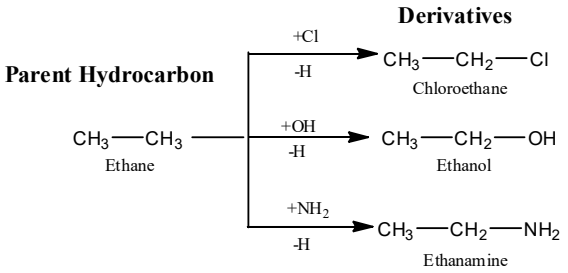
In 1856, Berthelot synthesizes methane.

By this time, the concept of vital force theory was completely disproved and was discarded.

Modern Definition of Organic Compound

The compounds of carbon and hydrogen (hydrocarbons) and their derivatives in which covalently bonded carbon atom is essential constituent are called organic compounds.

i.e.



Note: *Compounds of carbon such as CO, CO_2, H_2CO_3, metal carbonates & bicarbonates (like Na_2CO_3, $NaHCO_3$), carbides (like CaC_2), cyanides (like HCN) etc. are studied under inorganic chemistry because of their great resemblance with inorganic compounds*

Reasons for the separate study of organic compounds from inorganic compounds

1. **Existence of large number of organic compounds**
   There are large numbers of organic compounds possible due to the existence of self-linking property of carbon (i.e. catenation) to form chains and rings through covalent bond. The C-atom also forms C=C & C≡C bonded compounds. C-atom also forms compounds with other elements.

2. **Unique physical and chemical properties**
   There is a marked difference between composition, bonding, structure and properties of organic and inorganic compounds

Tetra-covalency and catenation properties of carbon

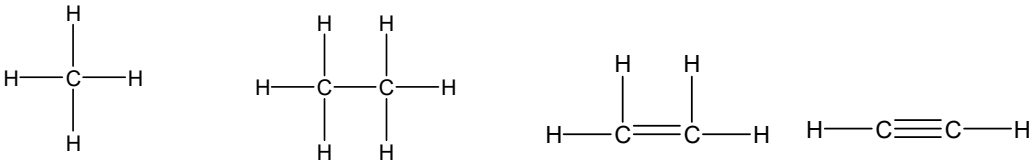
➢ Tetra-covalency of Carbon atom

The property of carbon atom by which it can forms four covalent bonds is called tetracovalency of carbon.

The electronic configuration of carbon atom is

C-atom $= 1\mathbf{s}^2\ 2\mathbf{s}^2\ 2\mathbf{p}_x^1\ 2\mathbf{p}_y^1\ 2\mathbf{p}_z^0$ (Ground state configuration)
C-atom $= 1\mathbf{s}^2\ 2\mathbf{s}^1\ 2\mathbf{p}_x^1\ 2\mathbf{p}_y^1\ 2\mathbf{p}_z^1$ (Excited state configuration)

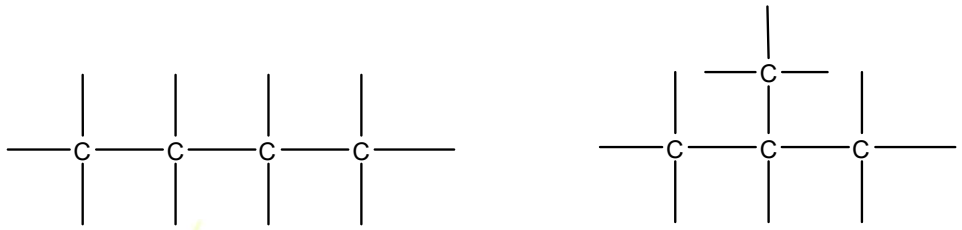
The C-atom shows the tetracovalency because during the formation of covalent bonds the C-atom gets excited and the electron from 2s is promoted to vacant $2p_z$ orbital to form four equivalent half-filled orbitals which is responsible to form four covalent bonds (single, double or triple covalent bonds) around central carbon atom.

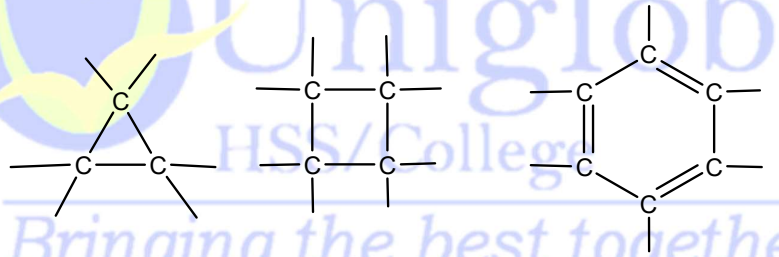


➢ Catenation property of Carbon atom

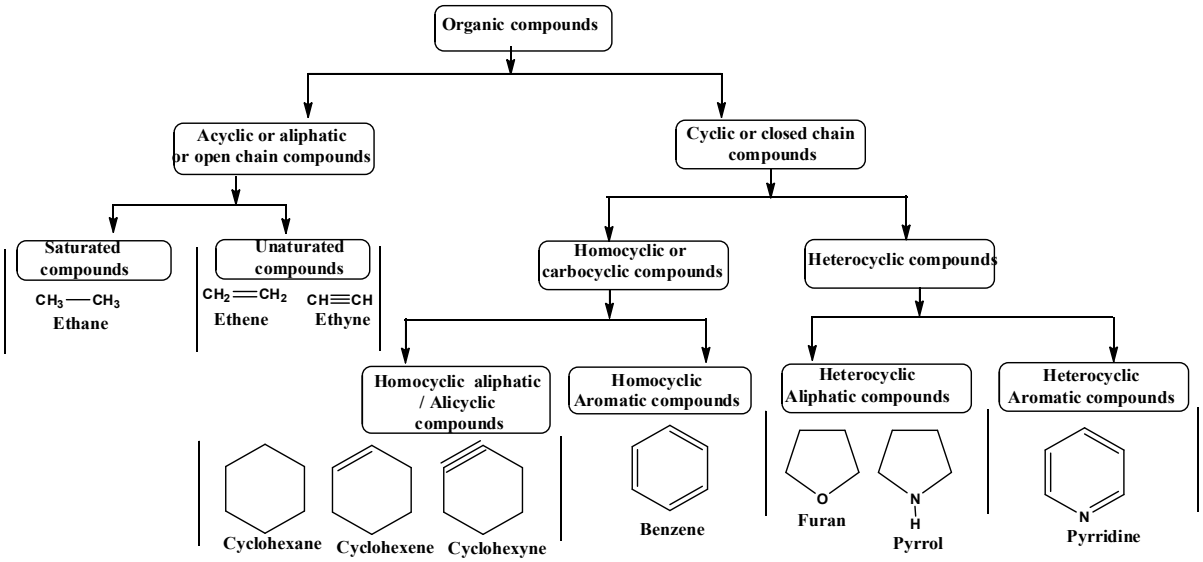
The property of carbon atom to form linear (straight) carbon chains or branched carbon chains or closed carbon rings by self-linking with another carbon atoms through covalent bonds is called **catenation property of carbon.**

The extent of catenation depends on strength of bond between atoms (Strength of C-C covalent bond is very high i.e. 355 KJ/mol than Si-Si bond (200KJ/mol))





Classification of Organic Compounds

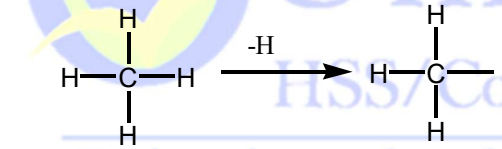


Alkyl group, Aryl group, Functional groups

Derivatives of hydrocarbons mainly consist of two groups:

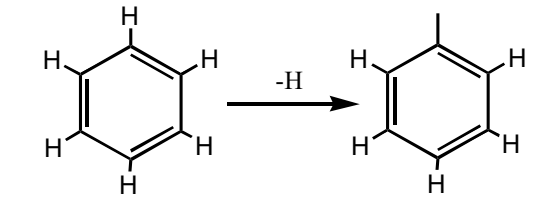
a) Less reactive group **[Alkyl (R-) or aryl (Ar-) group]**

The group formed by removing one hydrogen atom from saturated hydrocarbon (i.e. alkanes) is called alkyl group. It is represented by 'R—'.



Methane (aliphatic hydrocarbon) → Methyl (alkyl group)

The group formed by the removal of one hydrogen atom from aromatic hydrocarbons (arenes) like Benzene are called aryl group. It is represented by 'Ar—'.



Phene/benzene (aromatic hydrocarbon) → **Phenyl (aryl group)**

b) More reactive group **(Functional group)**

An atom or group of atoms present in organic compound which determines the characteristics properties of that compound is called **functional group**.

Characteristics of Functional group

i. It provides information for the identification of class or family of organic compounds.

For example:

Organic compounds with functional group –OH are called alcohols, -CHO are aldehydes & -COOH are carboxylic acids, etc.

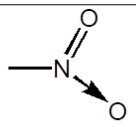
ii. It is the site of chemical reactivity in organic compound.

For example: In aldehyde, -CHO group is the site where chemical reaction takes place.

iii. It is specific in nature.

Some important examples of Functional groups are as follows

S.N.	Name of Functional Group	Structure
1.	Sulphonic acid	—SO_3H or —S(=O)(=O)—OH
2.	Carboxylic acid	—COOH or —C(=O)—OH
3.	Acid anhydride	>$(CO)_2O$ or —C(=O)—O—C(=O)—
4.	Ester	—COOR or —C(=O)—OR
5.	Acid halide	—COX or —C(=O)—X
6.	Acid amide	—$CONH_2$ or —C(=O)—NH_2
7.	Cyanide/Nitrile	—CN or —C≡N
8.	Aldehyde	—CHO or —C(=O)—H
9.	Ketone	>CO or —C(=O)—
10.	Alcohol	—OH
11.	Amine	—NH_2
12.	Alkene	—C=C—
13.	Alkyne	—C≡C—
14.	Ether	—O—

15.	Halo	—X (Where X= F, Cl, Br I)
16.	Nitro	—NO_2 or 
17.	Nitrite	—ONO
18.	Nitroso	—NO
19.	Thiols	—SH
20.	Isocyanides / Isonitriles / Carbylamines	—NC
21.	Cyanates	—CNO
22.	Isocyanates	—NCO
23.	Azo	—N=N—

Homologous Series

A systematic arrangement or series of organic compounds in the increasing order of molecular mass in which the adjacent members differ each other by methylene group (–CH_2 – unit) or 14 amu is called **homologous series**.

- An individual member of homologous series is called **homologue** and the process is called **homology.**

Examples:

Homologous series of Alkane (C_nH_{2n+2})

1st member	CH_4	Methane
2nd member	$CH_3—CH_3$	Ethane
3rd member	$CH_3—CH_2—CH_3$	Propane
4th member	$CH_3—CH_2—CH_2—CH_3$	Butane

Homologous series of Alcohol ($C_nH_{2n+1}OH$)

1st member	$CH_3—OH$	Methanol
2nd member	$CH_3—CH_2—OH$	Ethanol
3rd member	$CH_3—CH_2—CH_2—OH$	Propanol
4th member	$CH_3—CH_2—CH_2—CH_2—OH$	Butanol

Characteristics of Homologous Series

i. Each members of a homologous series contain the same elements and same functional group.
ii. Two adjacent members of a homologous series are different by a methylene group (–CH_2 – unit) or 14 amu.
iii. All the members of a homologous series can be represented by same general formula.

For example:

C_nH_{2n+2} is the general formula for alkanes.

$C_nH_{2n+1}OH$ *or* $C_nH_{2n+2}O$ is the general formula for alcohols.

iv. Each members of a homologous series have similar chemical properties due to presence of same functional group.
v. Each members of a homologous series may have different physical properties such as boiling point, melting point, solubility, etc. i.e. there is gradual increase or decrease of physical properties on increase in the molecular mass.
vi. The first member of some homologous series shows unusual or different behavior than other members.

Idea of Structural formula, Contracted formula and Bond-line / Skeletal formula

1) **Empirical formula:** The formula which represent simplest possible whole number ratio of different atoms in organic compound.
   Example: C_2H_4O is the empirical formula of butanoic acid.
   CH is the empirical formula of Benzene

2) **Molecular formula:** The formula which represent the actual/exact number of different atoms present in organic compound.
   Example: Molecular formula of butanoic acid is $C_4H_8O_2$
   Molecular formula of Benzene is C_6H_6

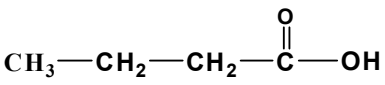
   NOTE: Relation between empirical and molecular formula is
   Molecular formula = empirical formula X n
   Where, n= molecular wt/ empirical formula wt.

3) **Condensed / Contracted Formula:** The formula which represents the carbon atoms separately with other atoms attached to it with some exceptions in cyclic compound like benzene where carbon atoms are written in group.

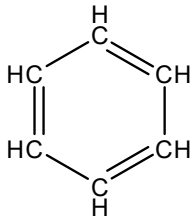
   $CH_3CH_2CH_2COOH$ (Butanoic acid)
   C_6H_6 (benzene)

4) **Structural Formula:** The formula which represent the only fewer details about the bonds.

Example:

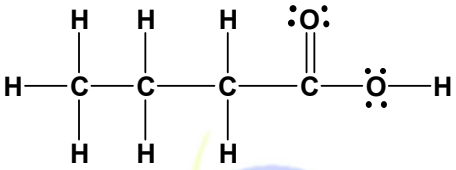


(Butanoic acid)

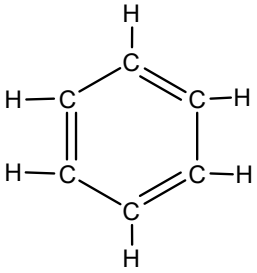


Benzene

5) <u>Displayed Formula</u>: The formula which represents all the atoms and all the bonds in details.

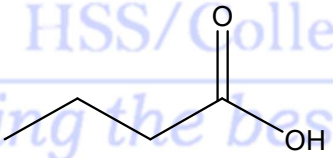


(Butanoic acid)

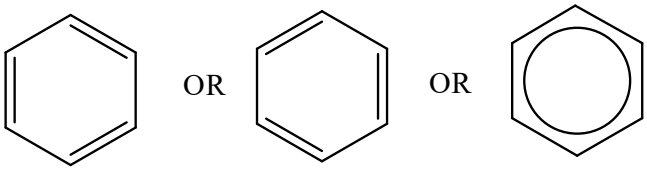


Benzene

6) <u>Skeletal / Bond-line Formula</u>: The formula which is represented in such a way that only line and vertices with fewer heteroatoms like O, N, S, etc. are shown & hydrogens, carbons are omitted.



(Butanoic acid)



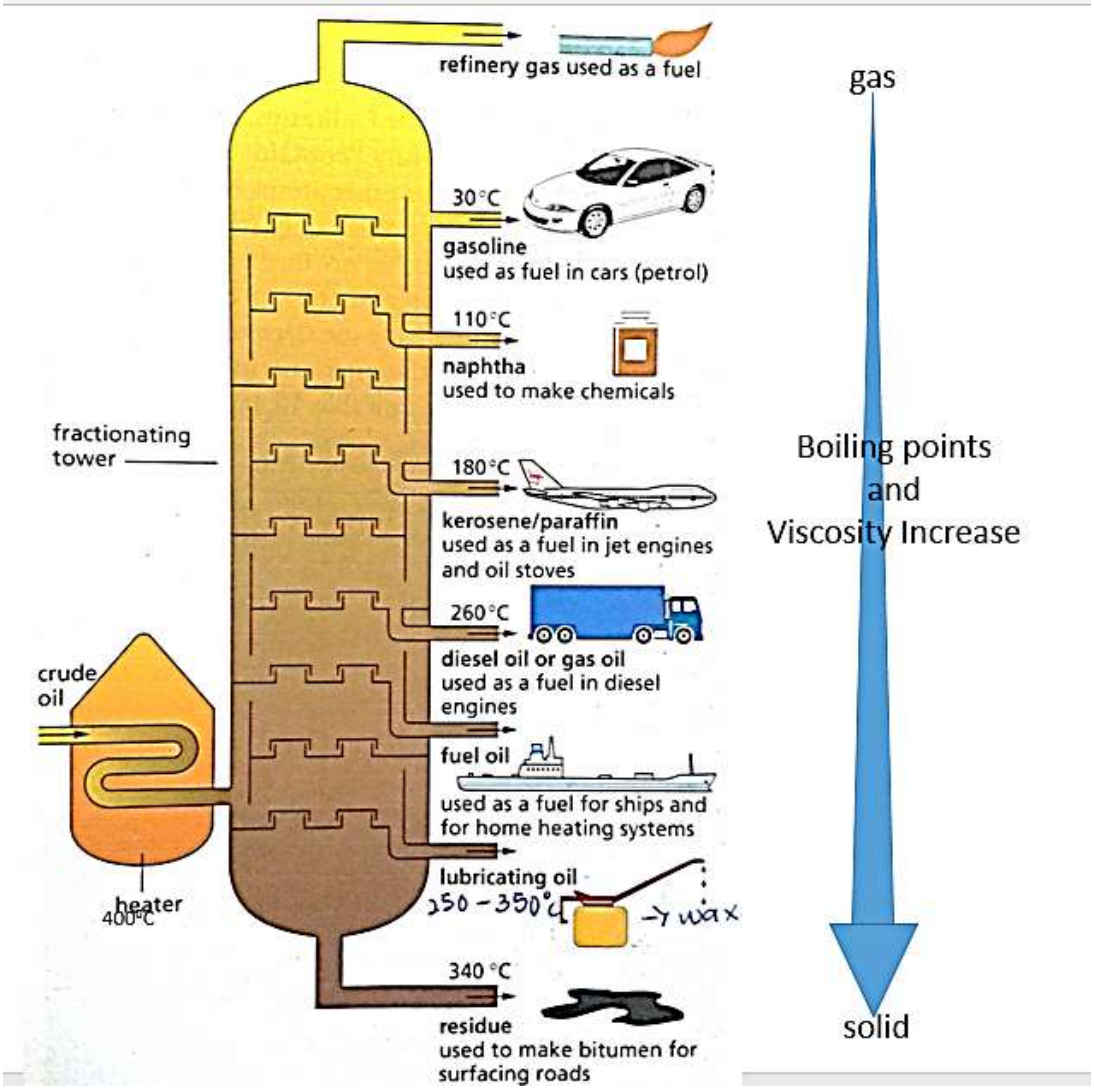
Benzene

Preliminary idea of Cracking and Reforming

- Coal & petroleum are the promising source of fossil fuel & very important across society, including in economy, politics and technology.
- The rise in importance was due to the invention of the internal combustion engine (petrol & diesel engines) the rise in commercial aviation (jet engines) and the importance of petroleum to industrial organic chemistry, particularly the synthesis of plastics, fertilizers, solvents, adhesives, pesticides, dyes, drugs, etc.
- Coal & petroleum are originated from decayed organic matter (plants & animals) occur beneath earth crust trapped below the sedimentary rocks**. (Greek: "Petra"= Rock & "Oleum"= oil)**
- These coal and petroleum are the excellent sources of aliphatic and aromatic hydrocarbons.
- Petroleum (crude oil) is very complex mixtures of several hydrocarbons (aliphatic and aromatic hydrocarbons) & organic compound containing oxygen, sulphur, nitrogen, etc.
- Petroleum (crude oil) can be separated into the useful fractions (LPG gas, petrol, aviation fuel, kerosene, diesel, lubricating oils, etc.) by **fractional distillation.**
- This process of separating crude oil into useful petroleum fractions is called **refining of petroleum (crude oil)** & carried out industrially in large **fractionating columns**.

Cracking (Deforming)

The process of breaking down or decomposition of higher molecular weight hydrocarbons into mixture of lower molecular weight hydrocarbons under suitable condition of temperature and catalyst in absence of air is called cracking.



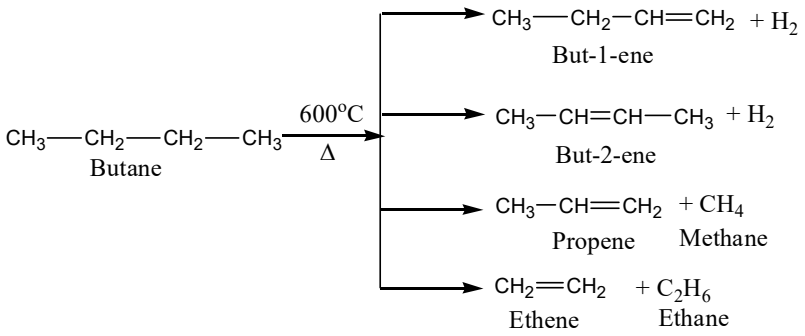
- Cracking is very important to yield lower boiling fractions (gasoline) from less useful high boiling fractions.

- Cracking yields lower boiling by products such as ethene which can be converted into polyethene (thermos plastic) by polymerization reaction.

Cracking is mainly of two types;

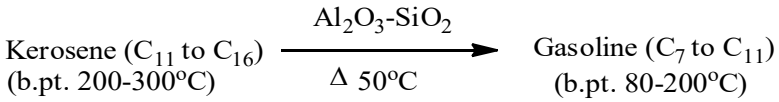
A) <u>Thermal Cracking (Pyrolysis)</u>: **(Pyro= heat ; lysis= break down)**

The process of conversion of higher molecular weight alkanes into mixture of lower molecular weight alkanes, alkenes, hydrogen gas, etc. by the application of heat in absence of air is called thermal cracking or pyrolysis.



B) <u>Catalytic Cracking</u>: The process of conversion of higher molecular weight alkanes into mixture of lower molecular weight alkanes, alkenes, hydrogen gas, etc. by the application of heat and catalyst in absence of air is called catalytic cracking.

Kerosene (C_{11} to C_{16}) can be converted **into gasoline (C_7 to C_{11})** by cracking process.



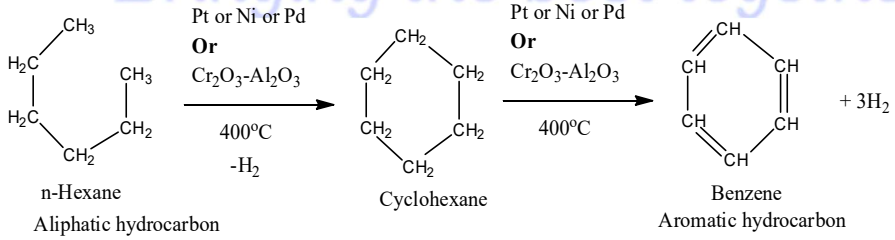
<u>Reforming (Aromatization)</u>

The process of converting aliphatic (open chain) straight chain hydrocarbons and close chain hydrocarbons (cycloalkanes) into aromatic hydrocarbons under the suitable conditions of temperature and catalyst in absence of air is known as **reforming** or **aromatization.**

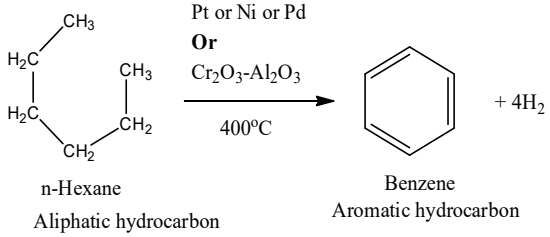
This process is important to increase the quality of gasoline.

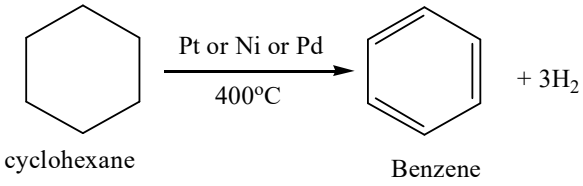
Examples:

n-Hexane and Cyclohexane produce aromatic compound, benzene after reforming. Benzene can be used further to produce dyes, drugs, explosives, etc.



Or Simply,





Quality of Gasoline, Octane number, Cetane number and Gasoline additive

Quality of Gasoline

Gasoline is an important fraction of petroleum product mainly contains a complex mixture of hydrocarbons from C_7 to C_{11}, which is used in internal combustion engines.

The quality of gasoline is determined by its knocking property or octane number.

Knocking

The pre-ignition or irregular combustion of air-gasoline mixture that gives jerks in the engine, which produces violent metallic noise known as knocking (also known as pinging or pinking).

- The quality of gasoline can be checked by knowing the extent of knocking. A good fuel produces the minimum knocking.
- The quality of gasoline is measured in terms of **"Octane number or Octane rating."**

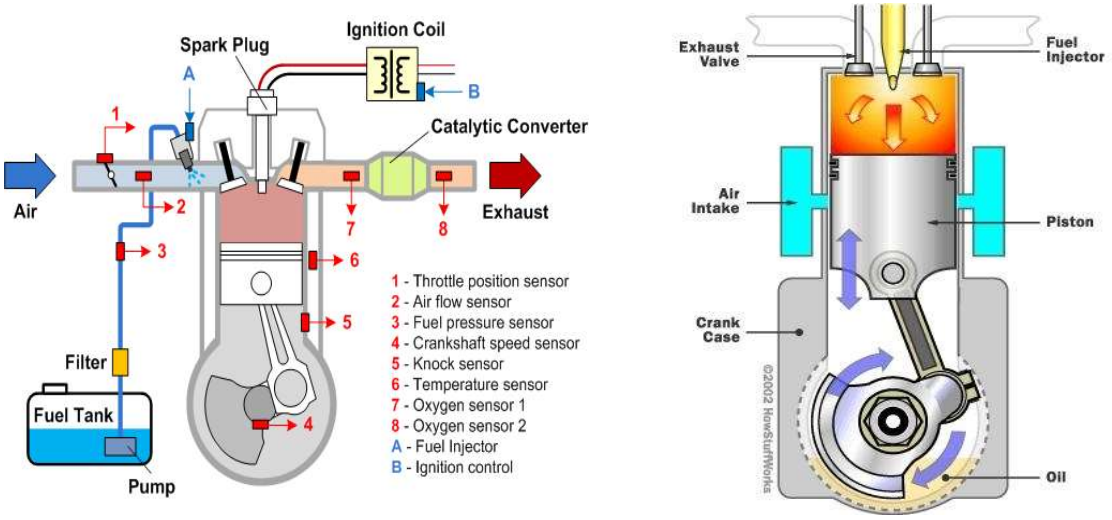


Figure: Engine

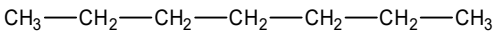
Octane Number or Octane ratings

It is the arbitrary unit or scale used to determine the quality of gasoline (petrol).

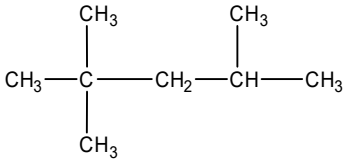
Definition:

Octane number is defined as the percentage by volume of iso-octane present in the mixture of iso-octane & n-heptane which has same knocking property as the fuel under examination.

- Octane number depends on the structure of hydrocarbons i.e. branched chain alkanes, alkenes and aromatic hydrocarbons have high octane number whereas straight chain alkanes have low octane number. i.e.



n- Heptane
Straight chain hydrocarbon
Octane Number is assigned as 0
High Knocking
Low Anti-knocking



Iso-octane (2,2,4-trimethylpentane)
Branched chain hydrocarbon
Octane Number is assigned as 100
Low Knocking
High Anti-knocking

For Example

Gasoline(petrol) with the same knocking characteristics as a mixture of 90% iso-octane and 10% n-heptane would have an octane number of 90.

Question. A fuel has octane number 80. What does it mean?

Ans: The Octane number of fuels under examination is 80 means it has same knocking property as a mixture of 80% by volume of iso-octane & 20% by volume of n- heptane.

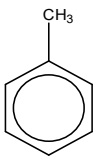
Gasoline additives or Antiknocking agents

The chemical substances added to gasoline to enhance (increase) the octane number of fuels by decreasing the knocking are called gasoline additives or anti knocking agents.

- The gasoline containing tetraethyl lead is called leaded gasoline (petrol).

Examples of gasoline additives are as follows:

a. Tetraethyl lead (TEL), $(C_2H_5)_4Pb$
b. Toluene
c. BTEX (a hydrocarbon mixture of Benzene, Toluene, Ethylbenzene & Xylene)
d. MTBE (**Methyl *tert*-butyl ether**)
e. ETBE (**Ethyl *tert*-butyl ether),** etc.



Toluene

$(CH_3)_3COCH_3$
MTBE

$(CH_3)_3COCH_2CH_3$
ETBE

Cetane Number or Cetane Ratings

The quality of diesel is measured in terms of cetane number.

Definition:

Cetane number is defined as the percentage by volume of cetane present in the mixture of cetane & α-methyl naphthalene which has same ignition property as the fuel under examination.

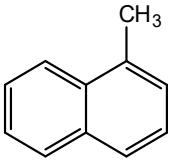
$CH_3(CH_2)_{14}CH_3$

Cetane

n-Hexadecane

Cetane Number is assigned as 100

Ignites rapidly



1-Methyl-naphthalene

or alpha methyl napthalene

Cetane Number is assigned as 0

Ignites slowly

For Example:

Diesel under the examination with the ignition quality as a mixture of 70% cetane and 30% α-methyl naphthalene would have cetane number of 70.

Question. A fuel has cetane number 75. What does it mean?

Ans: The cetane number of fuel (diesel) under examination is 75 means it has same ignition property as a mixture of 75% by volume of cetane & 25% by volume of α-methyl naphthalene.