

Converting kerogen to crude oil

Step 1: Diagenesis forms Kerogen

- Diagenesis is a process of compaction under mild conditions of temperature and pressure.

When organic aquatic sediments (proteins, lipids, carbohydrates) are deposited, they are very saturated with water and rich in minerals.

- Through chemical reaction, compaction, and microbial action during burial, water is forced out and proteins and carbohydrates break down to form new structures that comprise a waxy material known as "kerogen" and a black tar like substance called "bitumen".

All of this occurs within the first several hundred meters of burial.

The bitumen comprises the heaviest components of petroleum, but the kerogen will undergo further change to make hydrocarbons

Step 2: Catagenesis (or "cracking") turns kerogen into petroleum and natural gas

As temperatures and pressures increase (deeper burial) the process of catagenesis begins, which is the thermal degradation of kerogen to form hydrocarbon chains.

Importantly, the process of catagenesis is catalyzed by the minerals that are deposited and persist through marine diagenesis.

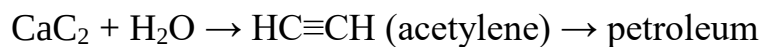
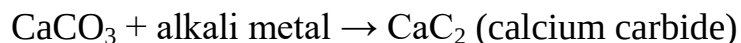
The conditions of catagenesis determine the product, such that higher temperature and pressure lead to more complete "cracking" of the kerogen and progressively lighter and smaller hydrocarbons.

Petroleum formation, then, requires a specific window of conditions;

too hot and the product will favor natural gas (small hydrocarbons), but too cold and the plankton will remain trapped as kerogen.

Inorganic Theory:

This theory assumes the oil hydrocarbon compounds are produced from the reaction of hot water vapor with carbides, which will form the hydrocarbon substances under high pressure and temperature as follows:

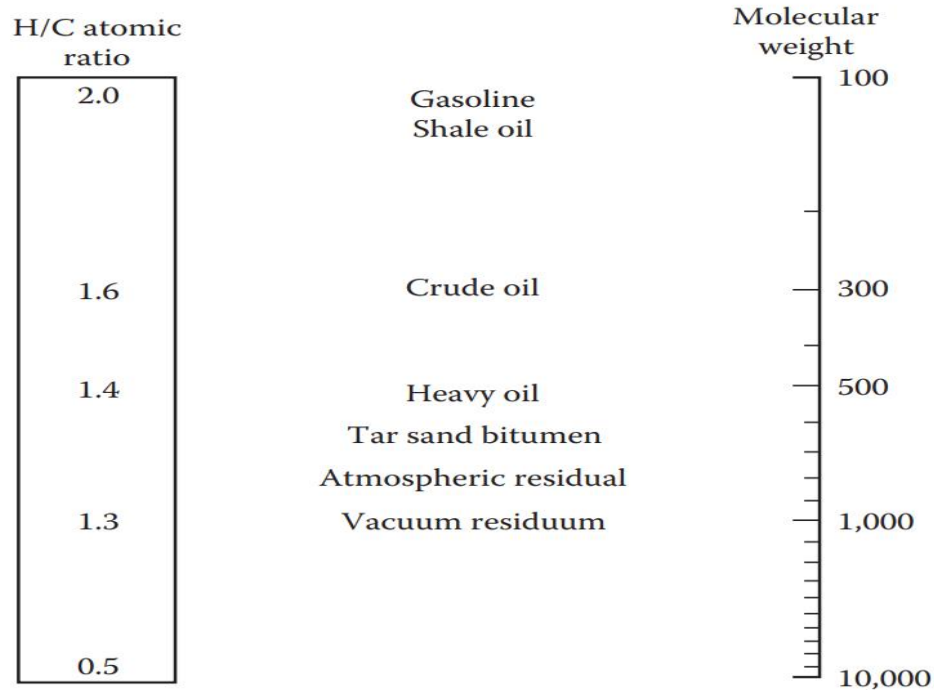


Composition of Crude Oils

Crude oil is a complex liquid mixture made up of a vast number of hydrocarbon compounds that consist mainly of carbon and hydrogen in different proportions. In addition, small amounts of organic compounds containing Sulphur, oxygen, nitrogen and metals such as vanadium, nickel, iron and copper are also present.

Hydrogen to carbon ratios affect the physical properties of crude oil:

- As the H/C ratio decreases, the gravity and boiling point of the hydrocarbon compounds increases.
- the higher the H/C ratio of the feedstock, the higher its value is to a refinery because less hydrogen is required.

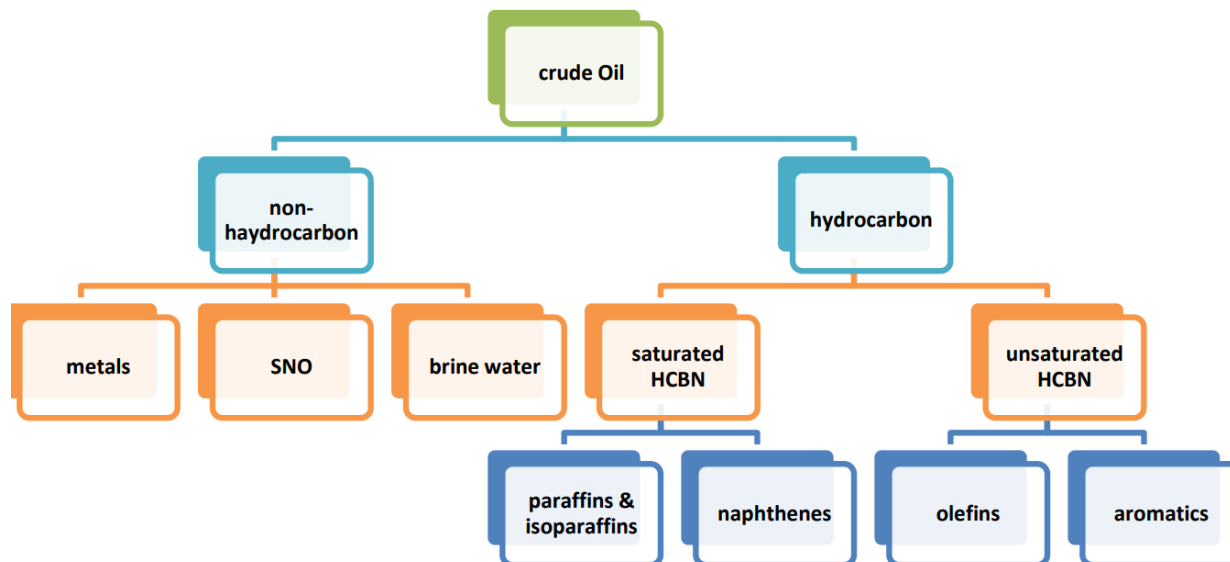


H/C ratio of various feedstocks

There are three main classes of hydrocarbons. These are based on the type of carbon–carbon bonds present.

These classes are:

- Saturated hydrocarbons contain only carbon–carbon single bonds. They are known as paraffins (or alkanes) if they are acyclic, or naphthenes (or cycloalkanes) if they are cyclic.
- Unsaturated hydrocarbons contain carbon–carbon multiple bonds (double, triple or both). These are unsaturated because they contain fewer hydrogens per carbon than paraffins. Unsaturated hydrocarbons are known as olefins. Those that contain a carbon–carbon double bond are called alkenes, while those with carbon–carbon triple bond are alkyenes.
- Aromatic hydrocarbons are special class of cyclic compounds related in structure to benzene.



Crude Oil Composition Scheme

Paraffins

Paraffins, are saturated compounds that have the general formula C_nH_{2n+2} , where n is the number of carbon atoms. also known as alkanes, The simplest alkane is methane (CH_4), which is also represented as C_1 .

Normal paraffins (n-paraffins or n-alkanes) are unbranched straight chain molecules. Each member of these paraffins differs from the next higher and the next lower member by a $-CH_2-$ group called a methylene group (Table 1).

They have similar chemical and physical properties, which change gradually as carbon atoms are added to the chain.

Isoparaffins (or isoalkanes) are branched-type hydrocarbons that exhibit structural isomerization.

Structural isomers are the molecules have the same formulas but different arrangements of atoms, known as isomers. Butane and all succeeding alkanes can exist as straight-chain molecules (n-paraffins) or with a branched-chain structure (isoparaffins). For example, butane and pentane have the following structural isomers:

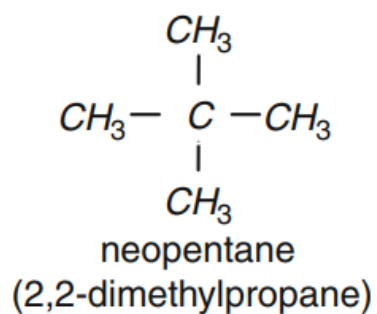
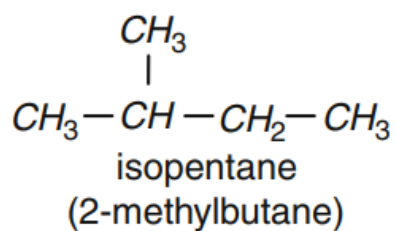
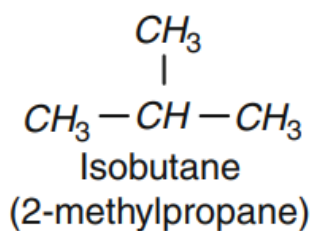
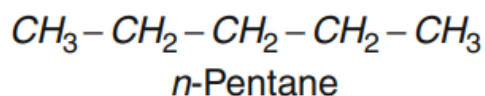
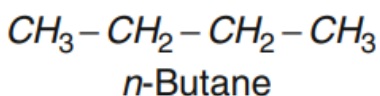


Table1 Names and formulas of the first ten paraffins (alkanes)

Name	Number of carbon atoms	Molecular formula	Structural formula	Number of isomers
Methane	1	CH ₄	CH ₄	1
Ethane	2	C ₂ H ₆	CH ₃ CH ₃	1
Propane	3	C ₃ H ₈	CH ₃ CH ₂ CH ₃	1
Butane	4	C ₄ H ₁₀	CH ₃ CH ₂ CH ₂ CH ₃	2
Pentane	5	C ₅ H ₁₂	CH ₃ (CH ₂) ₃ CH ₃	3
Hexane	6	C ₆ H ₁₄	CH ₃ (CH ₂) ₄ CH ₃	5
Heptane	7	C ₇ H ₁₆	CH ₃ (CH ₂) ₅ CH ₃	9
Octane	8	C ₈ H ₁₈	CH ₃ (CH ₂) ₆ CH ₃	18
Nonane	9	C ₉ H ₂₀	CH ₃ (CH ₂) ₇ CH ₃	35
Decane	10	C ₁₀ H ₂₂	CH ₃ (CH ₂) ₈ CH ₃	75

The number of isomers increases geometrically with the carbon number. While there are two isomers for butane and three for pentane, there are 75 isomers for decane ($C_{10}H_{22}$). For paraffins in the range of C_5 – C_{12} , there are more than 600 isomers with only 200–400 that are identified in petroleum fractions. Because of their different structures, these isomers have different properties. For instance, the presence of isoparaffins in gasoline is essential for increasing the octane number of gasoline fuels.

The properties of straight chain are:

- High molecular weight.
- High boiling point.
- Low octane number

The properties of branch paraffins are:

- Low boiling point.
- High octane number therefore is favorite in cars fuel.
- The common in crude oil is one branch and less tow branches.

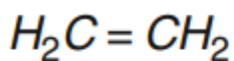
Olefins

Olefins are unsaturated hydrocarbons containing carbon–carbon double bonds, also known as alkenes. The general formulas of olefins are $C_nH_{2n}(R-CH=CH-R')$. When Compounds containing carbon–carbon triple bonds are known as acetylenes, The general formulas of acetylenes $C_nH_{2n-2}(R-C\equiv C-R')$.

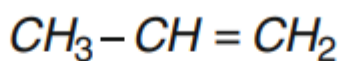
Unsaturated compounds may have more than one double or triple bond. If two double bonds are present, the compounds are called alkadienes or, more commonly, dienes ($R-CH=CH-CH=CH-R'$). There are also trienes, tetraenes and even polyenes.

Olefins are not naturally present in crude oils but they are formed during the conversion processes. They are more reactive than paraffins. The lightest alkenes

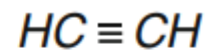
are ethylene (C_2H_4) and propylene (C_3H_6), which are important feedstocks for the petrochemical industry. The lightest alkyne is acetylene.



Ethylene
(ethene)

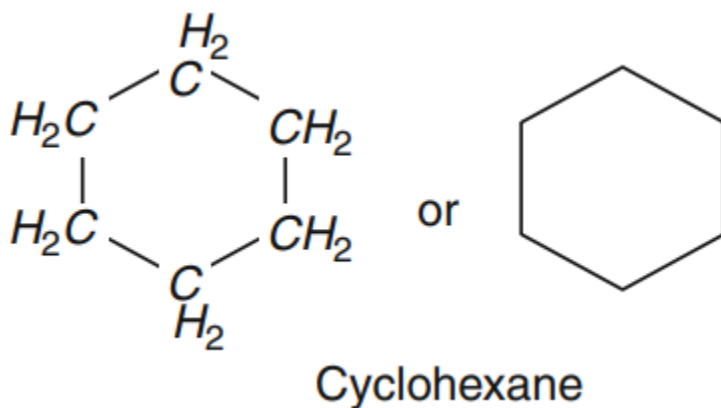


Propylene
(propene)



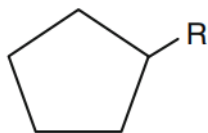
Acetylene
(ethyne)

Naphthenes (cycloalkanes) **Naphthenes**, also known as cycloalkanes, are saturated hydrocarbons that have at least one ring of carbon atoms. They have the general formula C_nH_{2n} . A common example is cyclohexane (C_6H_{12}).

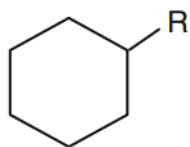


The boiling point and densities of naphthenes are higher than those of alkanes having the same number of carbon atoms.

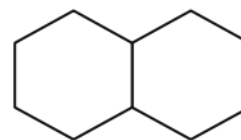
Naphthenes commonly present in crude oil are rings with five or six carbon atoms. These rings usually have alkyl substituents attached to them. Mutli-ring naphthenes are present in the heavier parts of the crude oil. Examples of naphthenes are shown below.



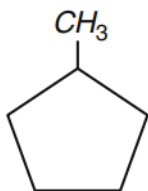
Alkylcyclopentanes



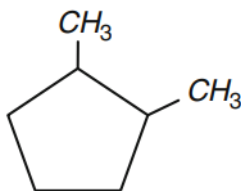
Alkylcyclohexanes



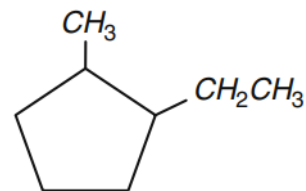
Bicycloalkanes



methylcyclopentane



1,2-dimethylcyclopentane

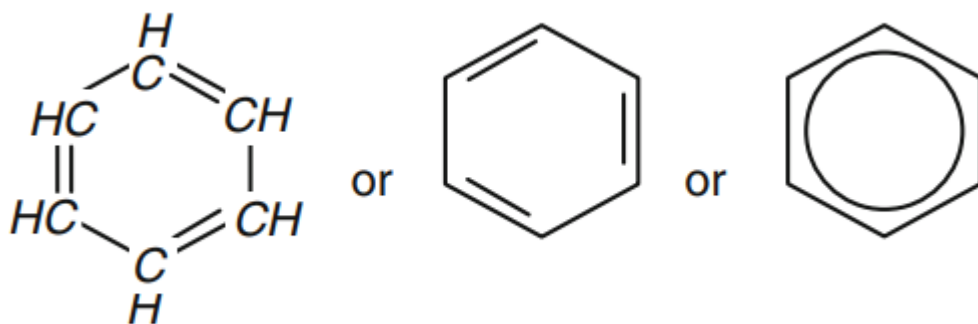


1-ethyl-2-methylcyclopentane

Cycloalkanes have similar properties to alkanes but have higher boiling points

Aromatics

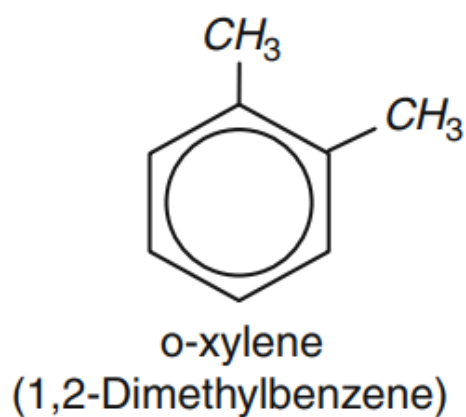
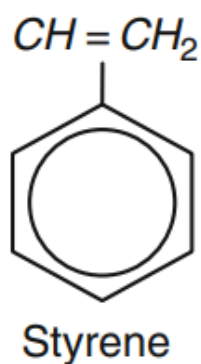
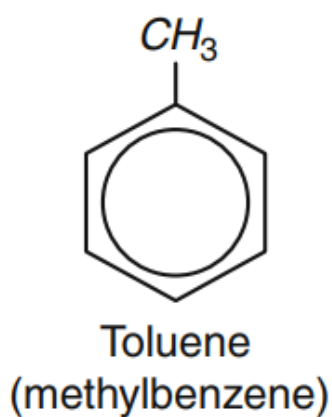
Aromatics are unsaturated cyclic compounds composed of one or more benzene rings. The benzene ring has three double bonds with unique electron arrangements that make it quite stable



Benzene

Crude oils from various origins contain different types of aromatic compounds in different concentrations.

Light petroleum fractions contain mono-aromatics, which have one benzene ring with one or more of the hydrogen atoms substituted by another atom or alkyl groups. Examples of these compounds are toluene and xylene. Together with benzene, such compounds are important petrochemical feedstocks, and their presence in gasoline increases the octane number.

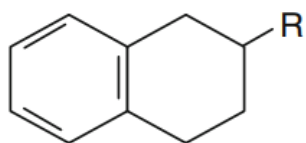


More complex aromatic compounds consist of a number of “fused” benzene rings. These are known as polyromantic compounds.

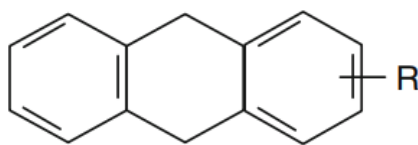
They are found in the heavy petroleum, their presence is undesirable because

- 1- they cause catalyst deactivation
- 2- coke deposition during processing
- 3- causing environmental problems when they are present in diesel and fuel oils.

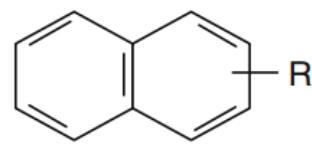
The heaviest portion of the crude oil contains asphaltenes, which are condensed polyromantic compounds of complex structure. Examples of polyromantic compounds are shown below.



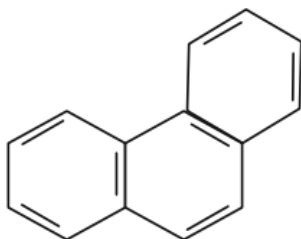
Aromatic-cycloalkanes



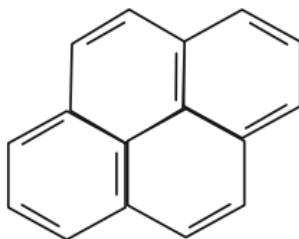
Fluorenes



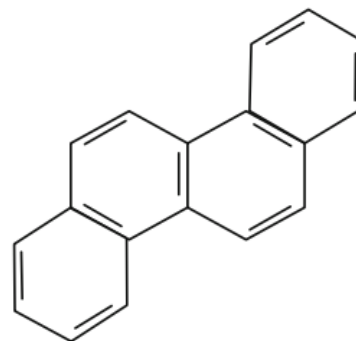
Binuclear aromatics



Phenanthrene



Pyrene



Chrysene

The amount of aromatics in different crude oils varies from 15 to 50%. The highest amounts of aromatics are typically found in naphthenic oils.

Aromatic compounds rarely amount to more than 15% of the crude oils. These are concentrated in heavy fractions such as gas oil, lubricating oils and the residuum.