Petroleum chemistry

Crude is the name for a liquid mixture of different hydrocarbon connections found in the earth.

Petroleum, strictly speaking is crude oil, but it is used to describe all kinds of hydrocarbons.

Most petroleum is made of hydrocarbons (HC), hydrogen and carbon. HC contain relatively few impurities, mainly: Nitrogen (N), sulphur (S) and oxygen (O) called NSO components.

Content in % of weight:	83 to 87%	carbon
	11 - 15%	hydrogen
	0.1 - 7%	sulphur
	0.06 - 1.5%	oxygen
	0.1 - 0.5%	nitrogen

HC exist in all three states of matter, as natural gas, liquid crude and semi-solid asphalt.

Sulphur

Sulphur is most abundant in heavier crude oils and asphalt. It can also occur in natural gas mixtures such as the poisonous corrosive gas H_2S. Such gas is called "sour gas" as opposed to "sweet gas" with no or little H_2S.

Sulphur causes enormous problems in the oil industry as it is highly corrosive and the formation of H2S is deadly poisonous. In small and harmless quantities H_2S stinks terribly like rotten eggs.

Welltest operators at Maersk

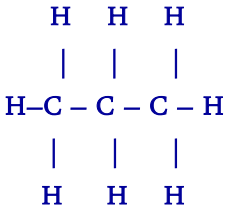
However, dangerous concentrations are heavier than air, odourless and require only one sniff to kill! As a safety precaution the oil industry set a concentration of 10 ppm as the maximum limit to operate in without a breathing aspirator.

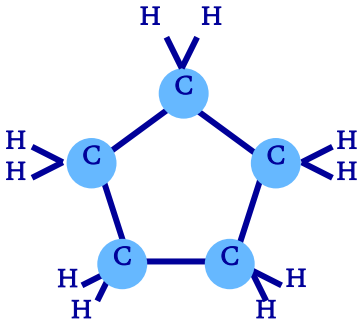
Basic hydrocarbon series in petroleum

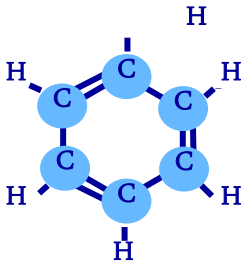
HC are grouped into four series:

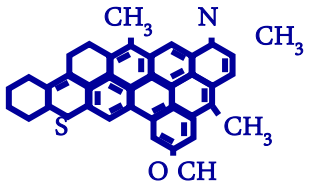
Paraffins, naphthenes, aromatics and resins / asphaltens.

Paraffines C_nH_{2n+2}	Straight and branched chains
Naphthenes C_nH_{2n}	Closed ring structure
Aromatics C_nH_{2n-6}	Basic hexagonal structure
Resins and Asphaltenes	Fused aromatic rings; NSO impurities







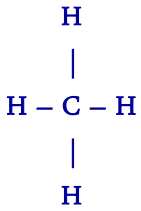


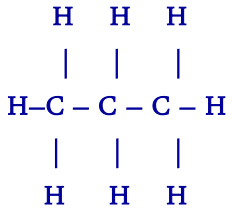
Paraffins

The carbon number (n) ranges from 4 to over 40.

Methane (n=4) is the lightest and natural gas the most important Paraffin.

C_nH_{2n+2}





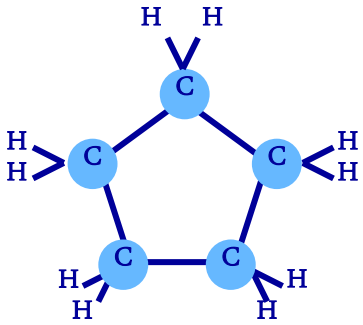
Natural gas composed of nearly pure methane is called "dry gas".

Other light weight paraffins, with carbon numbers up to 5, are also gaseous at normal pressure and temperature.

The mixture with methane is called "wet gas".

Higher molecular weight paraffins become viscous, waxy solids.

Naphthenes

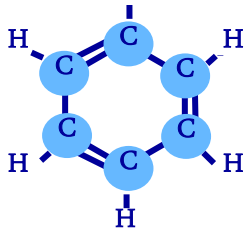


Naphthenes form as closed ring structures.

Compounds from naphthenes series have the same chemical and physical properties similar to paraffins with the same carbon number.

Together with paraffins, naphthenes form the major components of most crude oils.

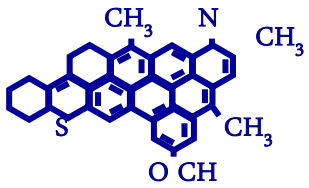
Aromatics



Aromatics have a structure based on a hexagonal ring of carbons, with alternate simple and double bonds. This basic unit is called the benzene ring. After the simplest and most abundant aromatic compound, benzene.

Other aromatic compounds are made by substituting paraffin chains or naphthenic rings at some of the hydrogen sites, or by fusing several benzene rings together.

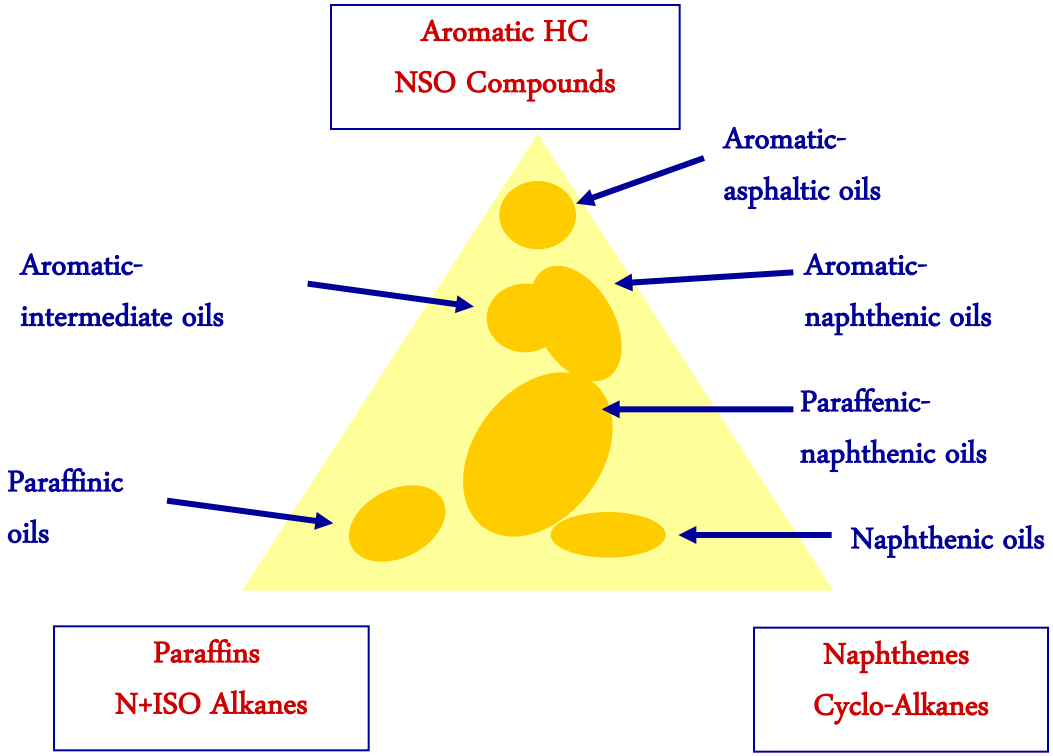
Resins and asphaltenes



Resins and asphaltenes are also composed of benzene-ring networks, but they contain impurity atoms and are not true hydrocarbons. These impurities are the high molecular weight compounds previously referred to as NSO compounds.

Resins and asphaltenes are the heaviest components of crude oil and the major components in many natural tars and asphalts.

Crude oils



Ternary diagram shows a composition of six classes of crude oils from 541fields.

Most normal crude oils fall within only three of the four fields. They can be either rich in paraffins (paraffinic oil), they can have nearly equal mounts of paraffins and naphthenes which together make up more than 50% of the crude (paraffinic-naphthenic oil) or they can have uneven amounts of paraffins and naphthenes, which total less than 50% and the composition is dominated by aromatics, resins and asphaltenes (aromatic intermediate oils).

API gravity

There are several measures of the weight or density of crude oil commonly used, two of which are relative density and API degrees.

Relative density refers to water or air as the reference.

Most commonly used classification for crude oils is by its specific gravity.

A simple procedure using a floating type hydrometer. API gravity is an inverse scale given by the relation:

$$°API = \{141.5/S.G.\ (at\ 60°\ F)\} - 131.5$$

0.800 - 0. 835 47° - 38°	Natural gas C_1 - C_5
0.840 - 0.876 37° - 30°	Liquid crude C_7 - C_{18} Increasing paraffins -- lighter Increasing Aromatics and NSO -- heavier
0.900 - 0.970 25° - 15° 1 10	Soild C_{18} - C_{20} to C_{60} Water

Classification of gases

Natural gas consists of 60% to 80% methane with the remainder made up primarily of the heavier gaseous hydrocarbons C_2, C_3, C_4 and C_5.

Exceptionally, natural gases have been found to contain as little as 7% methane.

Nitrogen, carbon dioxide, hydrogen sulphide and helium when present are considered impurities.

However, when present in sufficient large quantities, H_2S and He may be exploited commercially.

N_2 and CO_2 do not contribute to the thermal value of the gas and if present in large amounts, the gas may not burn.

CO_2 and H_2S with water are corrosive and cause embrittlement of ferrous material, while the latter is highly poisonous gas

Classification of natural gas by specific gravity, which is the ratio of gas compared to the density of air at the same temperature.

Methane	Ethane	Propane	Butane	Pentane
C_1	C_2	C_3	C_4	C_5

Bitumen

Naturally occurring, inflammable organic matter formed from kerogen in the process of petroleum generation that is soluble in carbon bisulfide.

Bitumen includes hydrocarbons such as asphalt and mineral wax.

Typically solid or nearly so, brown or black, bitumen has a distinctive petroliferous odour.

Kerogen

The naturally occurring, solid, insoluble organic matter that occurs in source rocks and can yield oil upon heating.

Typical organic constituents of kerogen are algae and woody plant material. Kerogen have a high molecular weight relative to bitumen, or soluble organic matter.

Bitumen forms from kerogen during petroleum generation.

Kerogen are described as
Type I, consisting of mainly algae and amorphous (but presumably algae) kerogen and is highly likely to generate oil;
Type II, mixed terrestrial and marine source material that can generate waxy oil; and
Type III, woody terrestrial source material that typically generates gas.

Saturated hydrocarbons (aka paraffins, alkanes)

Stable, the major component of gasolines, tend to burn in air with a clean flame

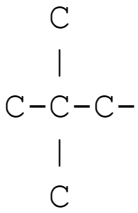
alkanes

normal = continuous chain of carbons ($C_n H_{2n+2}$)

normal heptane C-C-C-C-C-C-C C_7H_{16}

iso = branched chain of carbons ($C_n H_{2n+2}$)

iso octane = (aka 2,2,4-trimethylpentane)

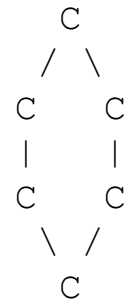


C_8H_{18}

cyclic = circle of carbons ($C_n H_{2n}$)

(aka Naphthenes)

cyclohexane =



C_6H_{12}

Unsaturated hydrocarbons

Unstable, are the remaining component of gasoline, tend to burn in air with a smoky flame.

Alkenes (aka olefins, have carbon=carbon double bonds)

These are unstable, and are usually limited to a few %.

```
                                C
                                |                   C5H10
      2-methyl-2-butene     C-C=C-C
```

C_5H_{10}

Alkynes (aka acetylenes, have carbon-carbon triple bonds)

These are even more unstable, are only present in trace amounts, and only in some poorly-refined gasolines .

```
                             _
      Acetylene               C=C                  C2H2
```

C_2H_2

Arenes (aka aromatics)

Used to be up to 40%, gradually being reduced to <20%.

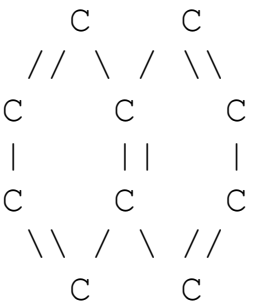
```
                   C                        C
                 // \                     // \
                C    C                 C-C    C
      Benzene   |    ||     Toluene      |    ||
                C    C                   C    C
                 \\ /                     \\ /
                   C                        C

                 C6H6                     C7H8
```

Polynuclear aromatics

Polynuclear Aromatics (aka PNAs or PAHs)

These are high boiling, and are only present in small amounts in gasoline. They contain benzene rings joined together, and the simplest is Naphthalene. The multi-ringed PNAs are highly toxic, and are not present in gasoline.

Naphthalene



C10H8

Octane is a hydrocarbon whose chemical formula is C8H18. It has a high anti-knock value. Octane rating of the fuel reflects the ability of the unburned end gases to resist spontaneous autoignition.

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