

Chemical Composition of Petroleum

Petroleum is a mixture of hundreds of hydrocarbons of all type with water, salts, sulfur and nitrogen containing compounds and some metal complexes.

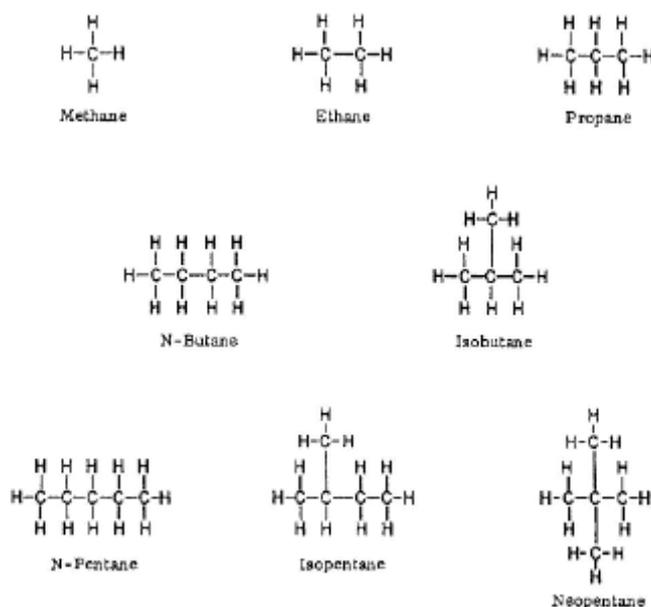
The elementary composition of crude oil usually falls within the following ranges.

Element	Percent by weight
Carbon	84–87
Hydrogen	11–14
Sulfur	0–3
Nitrogen	0–0.6

The three different types of hydrocarbons that crude has are paraffins, aromatics, cyclo-alyphatic or naphthenes and olefins.

Paraffins

The paraffin series of hydrocarbons is characterized by the rule that the carbon atoms are connected by a single bond and the other bonds are saturated with hydrogen atoms. The general formula for paraffins is C_nH_{2n+2} . The simplest paraffin is methane, CH_4 , followed by the homologous series of ethane, propane, normal and isobutane, normal, iso-, and neopentane, etc. (Fig. 1).



Figure(1) Paraffins in crude oil.

Saturated alkanes: (n-alkane and i-alkane)

- ✚ General formula C_nH_{2n+2}
- ✚ Boiling point and density increase with increasing # of C atoms.
- ✚ Branched alkanes (iso-alkanes) is very small in quantity
- ✚ Boiling point of straight chains > iso-alkanes with the same # of C

Naphthenes or cycloparaffins

Cycloparaffin hydrocarbons in which all of the available bonds of the carbon atoms are saturated with hydrogen are called naphthenes. Typical examples of these are cyclopentane, cyclohexane, etc. (Figure 2).

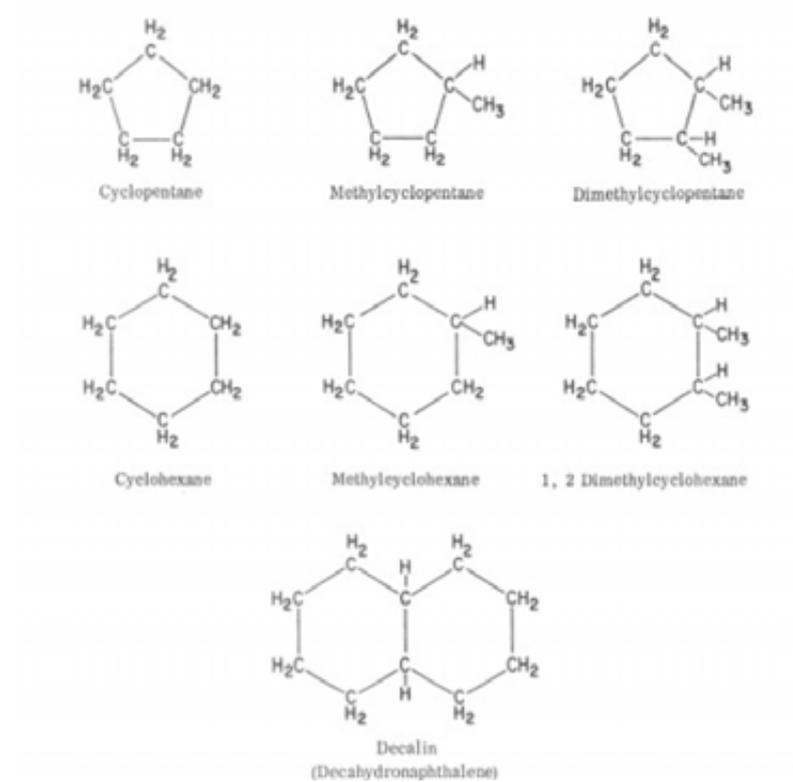


Figure 2: Naphthene compounds

✚ General formula C_nH_{2n} for one ring compounds

Aromatics

The aromatic series of hydrocarbons is chemically and physically very different from the paraffins and cycloparaffins (naphthenes). Aromatic hydrocarbons contain a benzene ring which is unsaturated but very stable and frequently behaves as a saturated compound. Some typical aromatic compounds are shown in (Figure 3).

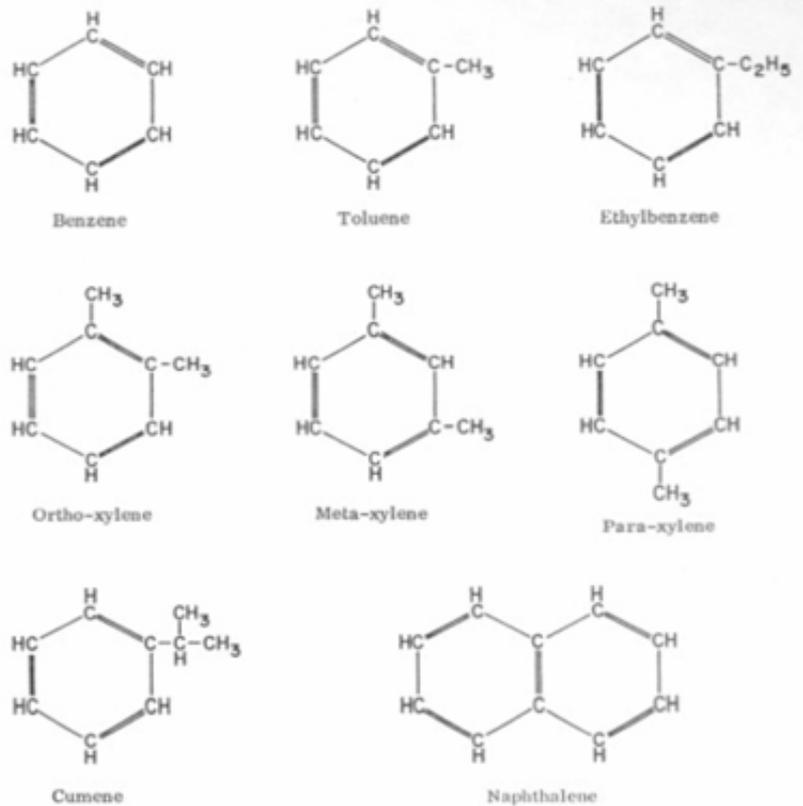


Figure 3: Aromatic compounds

Olefins

Olefins do not naturally occur in crude oils. However, they are formed during its processing. They are very similar to paraffins, but they exhibit double bonds, usually one per molecule (Figure 4), although some di-olefins (two double bonds in the same molecule, (Figure 5) can be found.

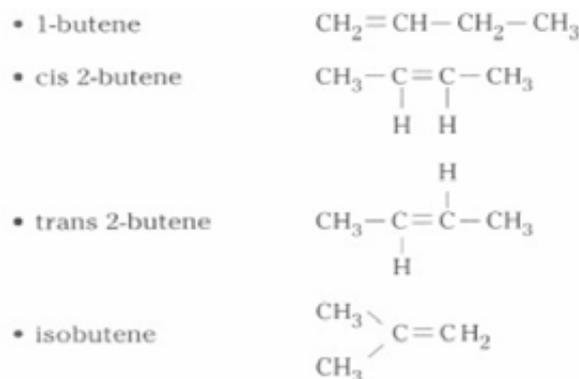


Figure 4: Olefin compounds

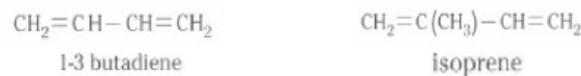


Figure 5: Di-olefin compounds

Heteroatom compounds

- ✚ Sulfur compounds might be present in inorganic and organic forms. In crude oils sulfur concentration can range from 0.1 to more than 8 weight percent. Such as dibenzylthiophene (2 benzene rings separated by 1 S atom) – is most difficult to release the Sulfur
- ✚ Oxygen compounds are responsible for petroleum acidity in particular.
 - Carboxylic (OH-C=O bonded to a benzene ring)
 - Phenolic (OH bonded to a benzene ring)
- ✚ Nitrogen compounds
 - carbazole (2 benzene rings separated by 1 N atom) – neutral
 - Quinoline (2 benzene rings with 1 N atom on 1 ring) - basic

Metal Compounds

- o Porphyrins contain Ni, V, or Fe