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Organic Chemistry

Lecture Three

Hydrocarbon, Alkanes, formulation-Hydrocarbonssaturated

1. Hydrocarbon

Hydrocarbons are a class of organic chemical compounds composed only of the elements carbon I and hydrogen (H) in its structures. The molecular structure of hydrocarbon Carbon atoms can form four bonds in its molecular structures, while hydrogen has one bond, Figure 1.



Figure 1: Carbon-to-carbon bonds

There are two types of hydrocarbons:

a) Saturated hydrocarbon: for a saturated hydrocarbon molecule there is no double or triple carbon to-carbon bonds and will have a maximum number of hydrogen atoms by the chemical formula C_nH_{2n+2} ,

where: C symbol indicates carbone atom, n indicates numbers of Carbon atoms present. This mentioned formula applied for all saturated hydrocarbons.

b) The unsaturated molecule has double or triple bond in its structure, their types are:

- Alkene compounds which having double carbon-to-carbon bond. Its chemical formula CnH2n.
- The Alkyne unsaturated molecules have triple carbon-to-carbon bond with the chemical formula CnH2n-2 respectively.
- Also, Aromatic hydrocarbons are compounds containing Benzene ring in its structure, the benzene ring contains double carbon-to-carbon bond.

1.1. Classification of Hydrocarbons

Division of the Hydrocarbons Family depending on the activity of functional group, for that hydrocarbon are divided into two main groups:

1.1.1. Aliphatic Hydrocarbons

The aliphatic hydrocarbons saturated and unsaturated hydrocarbons may be present as saturated or unsaturated compounds:

a) Aliphatic Saturated Hydrocarbons, which contain:

- Alkanes (C_nH_{2n+2}), contain carbon-carbon single bond.
- Cycloalkanes (C_nH_{2n}), contain carbon-carbon single bond in a single ring.
- b) Aliphatic Unsaturated Hydrocarbons, which contain:
 - Alkenes (C_nH_{2n}) , contain carbon-carbon double bond.
 - Alkynes (C_nH_{2n-2}), contain carbon-carbon triple bond. Figure 2.



Figure 2: Classification of hydrocarbons

1.1.2. Aromatic Hydrocarbons

Aromatic compounds are organic compounds containing benzene ring and/or compounds that resemble benzene in chemical behavior. Aromatic compounds properties are those properties of benzene that distinguish it from aliphatic hydrocarbons. Benzene has the molecular formula C_6H_6 . See Figure 3.



Figure 3: Benzene structure

2. Alkanes

General formula for alkanes is C_nH_{2n+2} . In alkanes, the four sp³ orbitals of carbon repel each other into a tetrahedral arrangement with bond angles of 109.5° like in CH4. Each sp3 orbital in carbon overlaps with the 1s orbital of a hydrogen atom to form a C-H bond. Table 1 contain the first ten alkanes.

Name	Number of carbons	Molecular formula	Structural formula	Number of structural isomers
methane	1	CH ₄	CH ₄	1
ethane	2	C ₂ H ₆	CH ₃ CH ₃	1
propane	3	C_3H_8	CH ₃ CH ₂ CH ₃	1
butane	4	C_4H_{10}	CH ₃ CH ₂ CH ₂ CH ₃	2
pentane	5	C_5H_{12}	CH ₃ (CH ₂) ₃ CH ₃	3
hexane	6	C_6H_{14}	CH ₃ (CH ₂) ₄ CH ₃	5
heptane	7	C_7H_{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

Table 1: Names, Molecular formulas and Number of Isomers of the first ten Alkanes

2.1. Natural sources of alkanes

The three major sources of alkanes (and cycloalkanes) throughout the world are the fossil fuels: natural gas, petroleum, and coal.

a) Natural Gas

Natural gas consists of approximately 90–95% methane, 5–10% ethane, and a mixture of other relatively low-boiling alkanes—chiefly propane, butane, and 2-methylpropane.

b) Petroleum

Petroleum is a thick, viscous liquid mixture of literally thousands of compounds, most of them hydrocarbons, formed from the decomposition of marine plants and

animals. Petroleum and petroleum-derived products fuel automobiles, aircraft, and trains. They provide most of the greases and lubricants required for the machinery of our highly industrialized society. Furthermore, petroleum, along with natural gas, provides close to 90% of the organic raw materials used in the synthesis and manufacture of synthetic fibers, plastics, detergents, drugs, dyes, and a multitude of other products.

c) Coal

Coal can be used as araw material for the production of organic compounds. Synthesis gas is a mixture of carbon monoxide and hydrogen in varying proportions. Synthesis gas is prepared by passing steam over coal.

2.2. Classes of carbon and hydrogen in alkanes

A carbon atom classified as primary (1°) , secondary (2°) , tertiary (3°) , or quaternary (4°) , depending on the number of carbon atoms bonded to it:

- A primary (1°) carbon is one that is bonded to only one other carbon.
- A secondary (2°) carbon is one that is bonded to two other carbons.
- A tertiary (3°) carbon is one that is bonded to three other carbons.



Hydrogens are also referred to as 1° , 2° , or 3° according to the type of carbon they are bonded to.

2.3. Preparation of Alkanes

There are three ways to prepare alkanes:

1) Hydrogenation of alkenes



2) Reduction of alkyl halides, which contain two possible processes:

• Hydrolysis of Grignard reagent



Where *R*= any alkyl group

• Reduction by metal and acid

 $\mathbf{Rx} + \mathbf{Zn} + \mathbf{H}^{+} \longrightarrow \mathbf{RH} + \mathbf{Zn}^{++} + \mathbf{X}^{-}$

Example:



3) Coupling of alkyl halides with organometallic compounds



Where *R*= any alkyl group

2.4. Reactions of Alkanes

Saturated hydrocarbons undergo very few reactions, so they are called Paraffinic hydrocarbons. (Latin parum, little; affinis, affinity)

2.3.1. Combustion

 $C_nH_{2n+2} + excess O_2 \xrightarrow{\text{flame}} nCO_2 + (n+1)H_2O$ $\Delta H = \text{heat of combustion}$ Example:

$$n-C_5H_{12} + 8 O_2 \xrightarrow{\text{flame}} 5CO_2 + 6H_2O \qquad \Delta H = -845 \text{ kcal}$$

2.3.2. Halogenation

$$-C - H + X_2 \xrightarrow{250-400^\circ, \text{ or light}} -C - X + HX$$
Usually a
mixture

 Reactivity
 X_2 : $Cl_2 > Br_2$

 H: $3^\circ > 2^\circ > 1^\circ > CH_3$ --H

Examples:

CH₃ CH₃-C-CH₃ $\begin{array}{c} CH_{3} \\ \hline \\ \hline 250-400^{\circ} \end{array} \xrightarrow{} CH_{3} - CH - CH_{2}Cl \quad and \quad \end{array}$ CH₃ CH₃-CH-CH₃ Isobutyl chloride Isobutane tert-Butyl chloride $CH_3CH_3 \xrightarrow{Cl_2} CH_3CH_2 - Cl$ b.p. 13° Ethane Chloroethane Ethyl chloride $CH_3CH_2CH_2CH_3 \xrightarrow[light, 25]{CH_3}CH_3CH_2CH_2CH_2 -Cl$ and CH₃CH₂CHCH₃ *n*-Butane b.p. 78.5° ĊI 1-Chlorobutane b.p. 68° n-Butyl chloride 2-Chlorobutane 28% sec-Butyl chloride $\xrightarrow{\text{Br}_2}$ CH₃CH₂Br CH₃CH₃ Ethane



alkane $\xrightarrow{400-600^\circ; with or}_{without catalysts}$ $H_2 + smaller alkanes + alkenes$