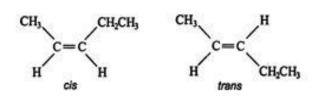
Lec. 3 Medical Chemistry Dr.Nada Hassan Alkenes & Alkynes

Molecular and Structural Formulas

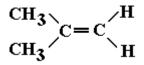
The alkenes are hydrocarbons that composed of carbon and hydrogen atoms with at least one double bond in the carbon chain. Alkenes with only one double bond have the general formula of C_nH_{2n} , where *n* equals any integer greater than one. The simplest alkene, ethene, has two carbon atoms and a molecular formula of C_2H_4 . The structural formula for ethene is $CH_2=CH_2$. In longer alkene chains, the additional carbon atoms are attached to each other by single covalent bonds. Each carbon atom is also attached to sufficient hydrogen atoms to produce a total of four single covalent bonds about itself. In chains with four or more carbon atoms, the double bond can be located in different positions, leading to the formation of **structural isomers.** For example, the alkene of molecular formula C_4H_8 has two isomers.

CH₃-CH₂-CH=CH₂ and CH₃-CH₂=CH₂-CH₃

In addition to structural isomers, alkenes also form geometric isomers (cis-trans isomers). Because rotation around a multiple bond is impossible without breaking it, groups attached to the double bonded carbon atoms always remain in the same relative positions. The *cis-trans* isomers differ from each other by the position of attached groups relative to double bond, one having similar groups on the same side is called *cis* and one having similar groups on opposite side called *trans*. An example of geometric isomerism is 2-pentene



The prefix *cis*- means on the same side and the prefix *trans* means across or on the opposite side .. The two groups attached to each carbon must be different for *cis- trans* isomerism to occur. If either carbon of the double bond of an alkene is bonded to identical atoms or groups, *cis-trance* isomers cannot exist. For example the following alkene has not optical isomerism



Alkenes are normally named using the IUPAC system. The rules for alkenes are similar to those used for alkanes. <u>The following rules</u> summarize alkenes naming.

1. Identify the longest continuous chain of carbon atoms that contains the carbon-carbon double bond. The parent name of the alkene comes from the IUPAC name for the alkane with the **same** number of carbon atoms, except the *ane* ending is changed to *ene* to signify the presence of a double bond. For example, if the longest continuous chain of carbon atoms containing a double bond has five carbon atoms, the compound is a pentene.

2. Number the carbon atoms of the longest continuous chain, starting at the end closest to the double bond.

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	CH ₃ -CH ₂ -CH=C 4 3 2 1	H_{2}	1-butene			
		Ŧ		6		
		C=CH ₂		CH ₃ -C	C=CH ₂	
	CH ₃ -CH ₂ -CH ₂	2 1	CH	3-CH2-CH2	4	
	5 4 3		1	2 3		
	pentene – corre	ect		<u>hexene</u> – n	ot correct	

3- The position of double bond(C=C) is indicated by placing the lower of the pair of numbers assigned to the double bonded carbon atomes in the front of the name of alkaen

CH₃- CH₂- CH₂ - CH = CH CH₃ 2-hexene 1 2 3 4 5 6 CH₃-CH=CH₂ propene (no need to say 1- prpene)

4. The location and name of any substituent molecule or group is indicated. For example,

 $\begin{array}{c|c} CH_3 & CH_3 \\ | & | \\ CH_3-CH_2-CH-CH_2-CH=CCH_3 \\ 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ \hline 2,5-dimethyl-2-heptene \end{array}$

Lec. 3 Medical Chemistry Dr.Nada Hassan Reactions of alkenes

Alkenes are relatively stable compounds, but are more reactive than alkanes due to the presence of a carbon–carbon double bond. The majority of the reactions of alkenes involve the rupture of this double bond, forming new single bonds.

<u>1-Hydrogenation</u>

Hydrogenation of alkenes produces the corresponding alkanes. The reaction is carried out under pressure at a temperature of 200 °C in the presence of a metallic catalyst Common industrial catalysts are based on Pt, Ni or Pd. The simplest example of this reaction is the catalytic hydrogenation of ethylene (ethane) to yield ethane:

$CH_2 = CH_2 + H_2 \rightarrow CH_3 - CH_3$

2- Hydration

Hydration, the addition of water across the double bond of alkenes, yields alcohol. The reaction is catalyzed by strong acids such as sulfuric acid. This reaction is carried out on an industrial scale to make ethanol.

$\begin{array}{c} H_2 SO_4 \\ CH_2 = CH_2 + H_2 O & \longrightarrow & CH_3 \text{-} CH_2 OH \end{array}$

<u>3- Halogenation</u>

In halogenation, the addition of elemental Br_2 or Cl_2 to alkenes yields <u>vicinal</u> dibromo- and dichloroalkanes (1,2-dihalides), respectively. The decoloration of a solution of bromine in water with dichloroethylene as catalyst is an analytical test for the presence of alkenes:

 $CH_2 = CH_2 + Br_2 \longrightarrow BrCH_2 - CH_2Br.$

4- Hydrohalogenation

Hydrohalogenation is the addition of hydrohalic such as HCl or HI to alkenes to yield the corresponding alkanhalides.

CH_3 - $CH=CH_2 + HI \longrightarrow CH_3$ -CHI- CH_3

If the two carbon atoms at the double bond are linked to a different number of hydrogen atoms, the halogen is found preferentially at the carbon with fewer hydrogen substituents (Markovnikov's Rule).

$CH_3\text{-}CH=CH_2+HBr \longrightarrow CH_3\text{-}CHBr\text{-}CH_3$

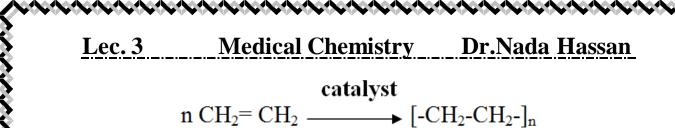
5- Oxidation

Alkenes are oxidized with a large number of oxidizing agents. In the presence of oxygen, alkenes burn with a bright flame to produce CO_2 and water:

 $CH_2 = CH_2 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$

6- polymerization

Polymerization is a process by which an organic compound reacts with itself to form a high molecular weight compound composed of repeating units of the original compound. The polymerization of ethylene produces polyethylene:

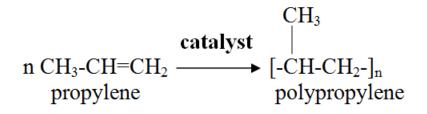


The starting alkene (in mentioned example is ethylene) is called **a monomer**, the large molecule formed as the final product is called **a polymer.** It is important to relize that a polymer is made up is many units of the monomer joined together.

polyethelene

Number of alkenes can be made to polymerize for example:

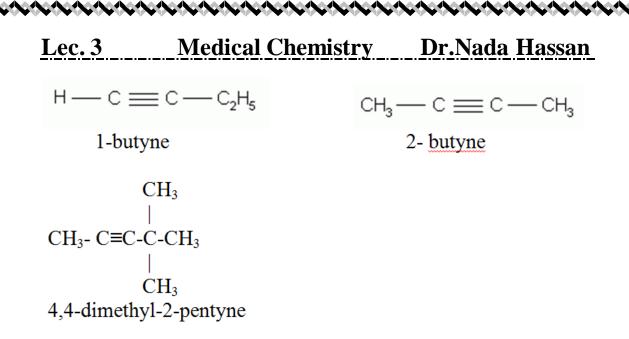
ethylene



<u>Alkynes</u>

Alkynes are unsaturated hydrocarbons that have at least one triple covalent bond between two carbon atoms. The general formula of the alkynes with one triple carbon-carbon bond is C_nH_{2n-2} . The simplest alkyne is acetylene (ethyne) CH=CH.

The IUPAC rules for naming alkynes are the same as those for alkenes except that the ending is –yne. The following examples illustrate the rules:



Most of the reactions of alkynes are similar to those of alkenes. The same reagents that add to carbon-carbon double bond also add to carbon-carbon triple bond. But it is possible to add two molecules of reagent to each alkyne.

<u>1-Halogenation</u>

 $\begin{array}{c} CH_3\text{-}CH_2\text{-}C \equiv CH + Br_2 \longrightarrow CH_3\text{-}CH_2\text{-}CBr = CHBr\\ CH_2\text{-}CBr = CHBr + Br_2 \longrightarrow CH_3\text{-}CH_2\text{-}CBr_2\text{-}CHBr_2 \end{array}$

1-butyne \longrightarrow 1,2-dibromo-1-butyne \longrightarrow 1,1,2,2-tetrabromobutane

2- Hydrogenation

<u>3- Hydrohalogenation – Markovnikov Rule</u>

 $CH_3-C \equiv CH + HC1 \rightarrow CH_3-CC1 = CH_2 + HC1 \rightarrow CH_3-CC1_2-CH_3$

Lec. 3 Medical Chemistry Dr.Nada Hassan <u>4- Hydration.</u>

One difference between the acid catalyzed hydration of alkenes and that of alkynes. Alkynes form alcohol (se above). Alkynes form compounds containing a C=O bond.

 $\begin{array}{c} OH & O\\ CH_3-C \equiv CH + H_2O \xrightarrow{H_2SO_4} CH_3-C = CH_2 \xrightarrow{rearrangement} H_3-C - CH_3 \end{array}$

Q.1 What is an alkyl group?

a- name and draw the structure of alkyl group derived from

Butane.

b- name the following alkyl groups:

 $(CH_3)_2$ - CH- , CH_3 - CH₂CH₃-

Q.2 Draw a structural formula for each of following names:

a)	2- methyl-1-butene	b) dimethylacetylene

c) diisopropylacetylene d) cis-2-butene

e) 4-ethyl-3-isopropyl-1-heptyne f) 2-methyl-2-pentene

g) 2,3-dimethyl-1-butene

i) 5-methyl-1-hexenel) 2-ethyl-1-hexene

j) 3-ethyl-2-pentenek) 4m) cyclopentene

h) cyclohexene

k) 4-methyl-2-hexene

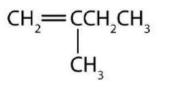
3. Name each compound according to the IUPAC system.

a.

b.

c.

4. Name each compound according to the IUPAC system.



b.

a.

CH₃ | CH₃CCH=CCH₂CH₃ | | CH₃ CH₃

c.

3. Classify each compound as saturated or unsaturated. Identify each as an alkane, an alkene, or an alkyne.

b. CH₃CH₂C≡CCH₃

a.

C.

 $CH_3CH = CCH_2CH_2CH_2CH_3$ | CH_3

Q.3 Write the equation for the reaction of 2-methyl-2-pentene with each of following reagent:

a- Br_2 b- H_2O , H_2SO_4 c- HCl d- H_2 , Pt

Q.4 Classify the following compounds as alkanes, alkenes or alkynes:

a-
$$C_3H_6$$
 b- C_5H_8 c- C_9H_{20} d- C_3H_8

Q.5 Which of following alkenes can exist as *cis-trans* isomers:

a) 2,3-dimethyl-2-butene b) 2-methyl-2-butene

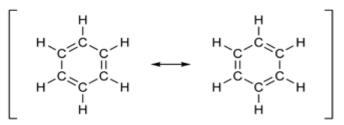
c) 1-hexene d) 2-methyl-1-butene

Lec. 3 Medical Chemistry Dr.Nada Hassan Aromatic compounds

All aromatic compounds are based on benzene, C_6H_6 , which has a ring of six carbon atoms with alternate double and single bonds structure, each carbon atom having one hydrogen atom attached



Kekule suggested that the position of double and single bonds could change producing two structures that represent benzene:



Some chemists replace these structures for benzene and its derivatives with a ring having a circle in the center

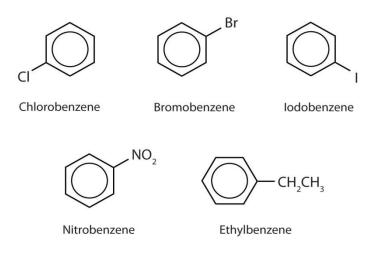


Others prefer to represent benzene by drawing just one of the alternating double and single bonds structures

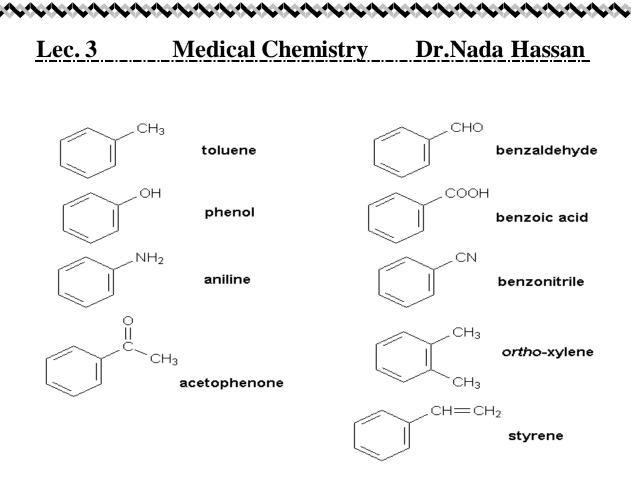
Lec. 3Medical ChemistryDr.Nada HassanTHE NAMES OF AROMATIC COMPOUNDS

<u>The phenyl group.</u> Remember that you get a methyl group, CH_3 by removing a hydrogen from, methane, CH_4 . You get a phenyl group, C_6H_5 , by removing a hydrogen from a benzene ring, C_6H_6 . Like a methyl or an ethyl group, a phenyl group is always attached to something else.

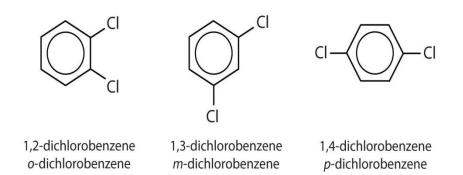
These compounds are named in the usual way with the group that replaces a hydrogen atom named as a substituent group: Cl as chloro, Br as bromo, I as iodo, NO_2 as nitro, and CH_3CH_2 as ethyl.



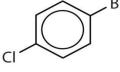
Some are more frequently denoted by common names. For example, methylbenzene is always known as toluene; hydroxybenzene, as phenol. The most important of these compounds are the following:



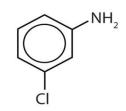
When there is more than one group attached to the benzene ring, the name must not only tell what group are present, but also where they are located. There are three possible disubstituted benzenes. We can distinguish the three possible isomers in two ways. The first is by use prefixes *ortho-, meta-,* and *para-*, which are abbreviated *o,m*, and *p*. The second is to number the carbon of the benzene ring. For example:



If the two groups are different and one of the groups is the kind that gives a special name to the molecule, then it is named as derivative of that special compound. For example:



1-Bromo-4-chlorobenzene *p*-Bromochlorobenzene



3-Chloroaniline *m*-Chloroaniline



2-Bromophenol o-Bromophenol



3-Bromotoluene *m*-Bromotoluene