



**Zagazig University
Faculty of Science
Chemistry Department**



Basic Principles of Organic Chemistry

Chem – 101

***For
First Year Students***

Stuff Members of Chemistry Department

Classification and Nomenclature of Organic Compounds

Introduction

One great advantage of the structural theory is that it enables us to organise the vast number of organic compounds into structure-based families. The compounds that fall into a particular family are characterized by the presence, as a part of their overall structure, of certain arrangement of atoms called functional groups.

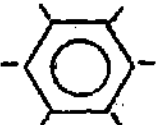
A functional group may be defined as an atom or group of atoms which determines the chemical behaviour of an organic compound.

Methane, CH_4 , for example, a very simple molecule, belongs to the family of molecules called *alkanes*. Molecules of alkanes contain only C-C and C-H single bonds. Ethane (C_2H_6), propane (C_3H_8) and butane (C_4H_{10})....etc. are also alkanes. All of these compounds show the same reactions that methane does.

Acetaldehyde (CH_3CHO), as another example, is a simple member of broad class of organic compounds known as *aldehydes*, which contain the functional group (-CHO). The understanding of the chemistry of acetaldehyde will give a general understanding of the chemistry of most aldehydes.

Our study will consider, in limited detail, representative members from some of the most important families encountered in a study of organic chemistry.

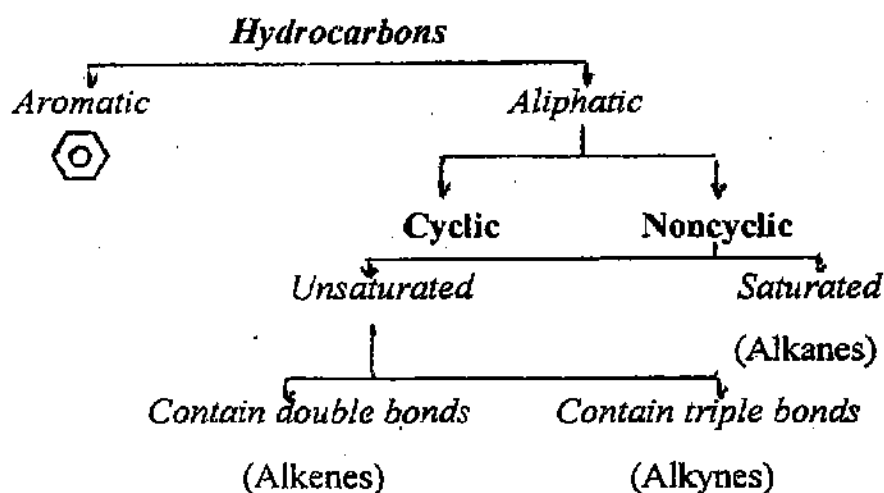
TABLE 1
Common Classes of Organic Compounds
and Important Functional Groups

General Formula	Name	Functional Groups
R-H	Alkanes	None
RCH=CH ₂	Alkenes	>C=C< double bond
R-C≡C-H	Alkynes	-C≡C- triple bond
R-OH	Alcohols	-OH hydroxy group
R-O-R'	Ethers	-O- ether group
R-NH ₂	Amines	-NH ₂ amino group
R-SH	Thiols	-SH sulphdryl group
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{H} \end{array}$	Aldehydes	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{H} \end{array}$ aldehyde group
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{R} \end{array}$	Ketones	$\begin{array}{c} \text{O} \\ \\ -\text{C}- \end{array}$ ketonic group
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OH} \end{array}$	Carboxylic acids	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{OH} \end{array}$ carboxyl grp.
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OR}' \end{array}$	Esters	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{O}- \end{array}$ ester group
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{NH}_2 \end{array}$	Amides	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{NH}_2 \end{array}$ amide group
ArH	Arens	

Naming Compounds Containing One Functional Group

HYDROCARBONS

Hydrocarbons as the name indicates, contain only hydrogen in addition to carbon. Hydrocarbons are divided into more than one group depending upon the mode of attachment between C and H in the internal structure of the molecule, this can be represented as follows:

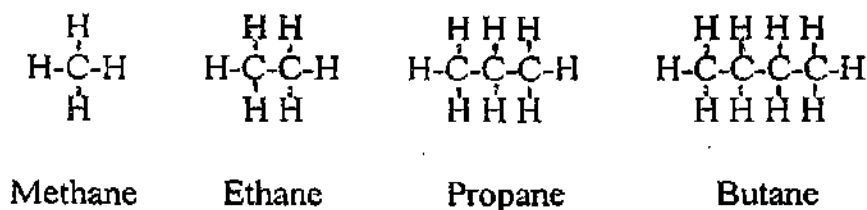


(1) Non-cyclic aliphatic hydrocarbons **ALKANES** (Paraffins)

General formula $R-H$

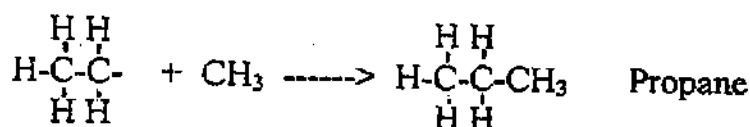
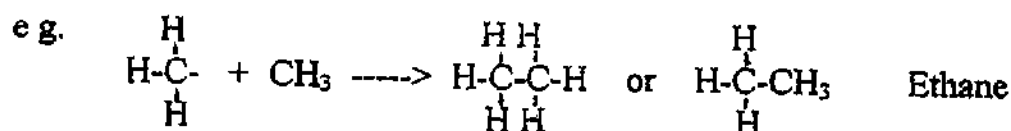
Functional group C-H and C-C bond

The first member of the series is *methane* which contains one carbon atom attached to 4 hydrogen atoms, its formula is CH_4 .

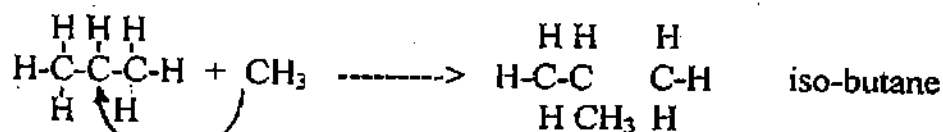
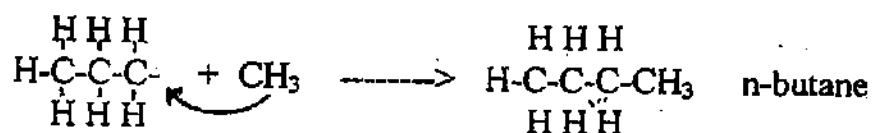


The next member is ethane (C_2H_6), apparently, carbon is trivalent, but it maintain the tetravalency of carbon, the two carbon atoms are linked together by a single covalent bond. The followers are propane (C_3H_8), butane (C_4H_{10}), pentane (C_5H_{12}) etc.

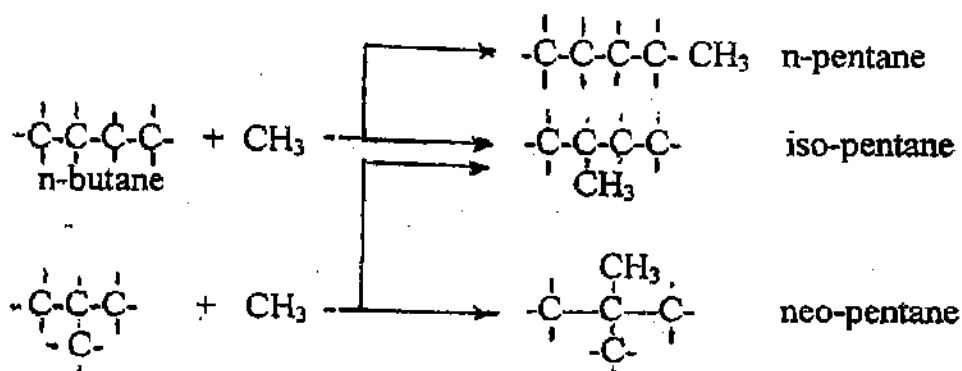
Any member of the series can be derived by inserting (CH_2) into the formula of the preceding member. In another words, a hydrogen atoms is removed from the molecule and replaced by a (CH_3), methyl group to obtain the next member.



When a hydrogen atom from *propane* is replaced by CH_3 there are two possibilities such as:



In case of butane, as seen above, both n-butane and iso-butane have the same formula (C_4H_{10}), but they differ in the mode of arrangement of carbon atoms in the chain. They are said to be *isomer* (see below). Pentane could be derived from butane in 3 isomers as follows:



Nomenclature of Alkanes

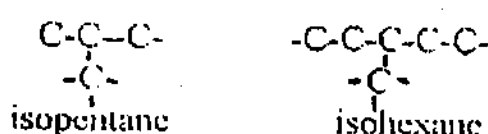
The oldest names for organic compounds are now called "*Common or Trivial Names*". The formal system of nomenclature that is used today is one proposed by International Union of Pure and Applied Chemistry (IUPAC).

The IUPAC system for naming alkanes is quite simple and the principals involved are used in naming compounds in other families as well. The names for several of the unbranched alkanes are listed in table 2 :

TABLE 2

No. of Carbons	Name	Structure
1	Methane	CH_4
2	Ethane	CH_3CH_3
3	Propane	$\text{CH}_3\text{CH}_2\text{CH}_3$
4	Butane	$\text{CH}_3(\text{CH}_2)_2\text{CH}_3$
5	Pentane	$\text{CH}_3(\text{CH}_2)_3\text{CH}_3$
6	Hexane	$\text{CH}_3(\text{CH}_2)_4\text{CH}_3$
7	Heptane	$\text{CH}_3(\text{CH}_2)_5\text{CH}_3$
8	Octane	$\text{CH}_3(\text{CH}_2)_6\text{CH}_3$
9	Nonane	$\text{CH}_3(\text{CH}_2)_7\text{CH}_3$
10	Decane	$\text{CH}_3(\text{CH}_2)_8\text{CH}_3$
20	Eicosane	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$

The ending of all the names of alkanes is *-ANE*. When all the carbon atoms in the molecule form a continuous chain (there is no branching) the hydrocarbon is called a normal (-n) alkanes. The prefix *-iso* has been used for lower hydrocarbons, where all the carbon atoms, except one, form a straight chain and the one carbon atom is attached to the carbon atom next to the terminal. e.g.



The alkyl groups (Radical):

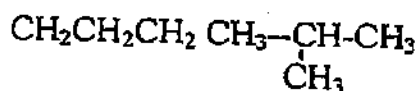
When one hydrogen atom from an alkane is substituted by another atom (or group of atoms), the remainder part of the molecule is called alkyl radicals, which are named by substituting *YL* for the suffix *ANE* of the alkane as follows:

Alkane		Alkyl Radical	
Name	Formula	Name	Formula
Methane	CH ₄	Methyl	CH ₃ -
Ethane	CH ₃ -CH ₃	Ethyl	CH ₃ CH ₂ -
Propane	CH ₃ CH ₂ CH ₃	Propyl	CH ₃ CH ₂ CH ₂ -
Butane	CH ₃ CH ₂ CH ₂ CH ₃	Butyl	CH ₃ CH ₂ CH ₂ CH ₂ -

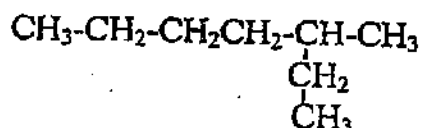
Nomenclature of Branched-Chain Alkanes

According to the *IUPAC* system, the following rules are applied for the nomenclature of branched-chain alkanes:

1- Locate the longest continuous chain of carbon atoms, this chain determines the base name of the alkane.

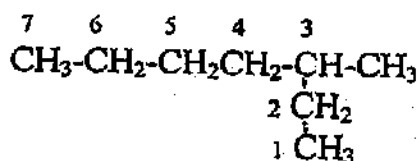
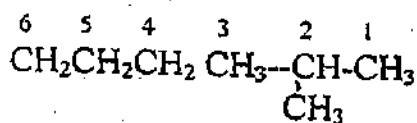


Base name hexane (6 C)



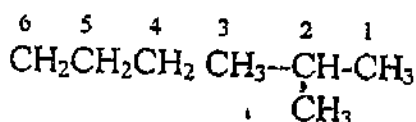
Base name heptane (7 C)

2- Number the longest chain beginning with the end of the chain nearest the branching. Applying this rule we number the two alkanes in step (1) in the following way

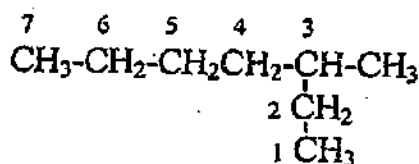


3- Use the numbers obtained by application of rule (2) to designate the location of the substituent groups. The base name is placed last, and the substituent group preceded by the number designating its location on the chain, is placed first. Numbers are separated from words by a dash

The above two examples are named as:

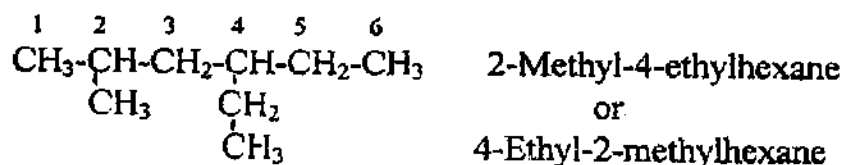


2-Methyl hexane

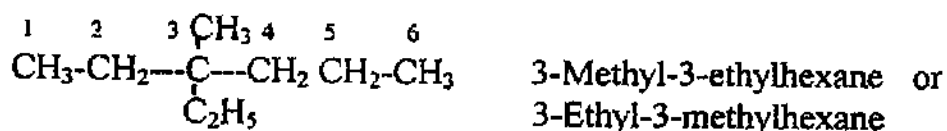


3-Methyl heptane

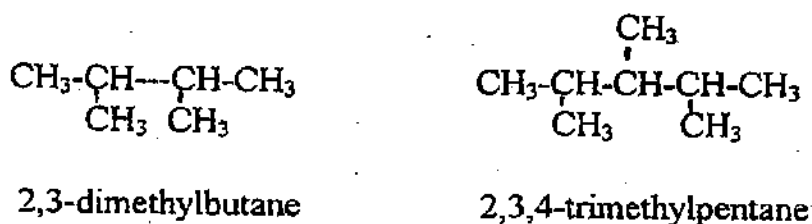
4- When two or more substituents are present, give each substituent a number corresponding to its location on the longest chain. For examples, we designate the compound below as 2-methyl-4-ethylhexane.



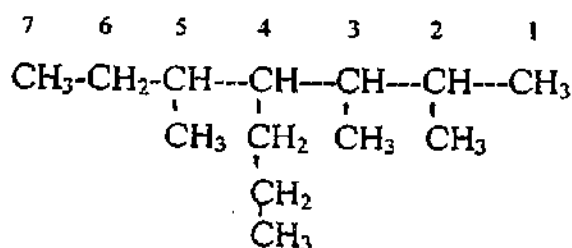
5- When two or more substituents are present on the same carbon atom, use that number twice



6- When two or more substituents are identical indicate this by the use of prefixes di-, tri-, tetra- and so on. Comes (,) are used to separate numbers from each other.

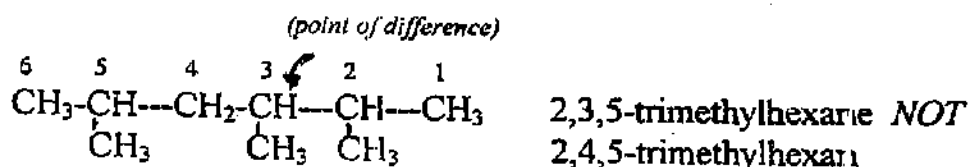


7- When two chains of equal length compete for selection as the base chain, choose the chain with the greater number of substitutions



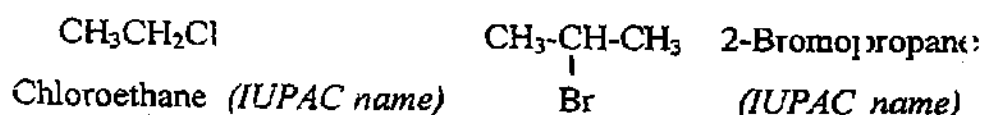
2,3,5-trimethyl-4-propylheptane *NOT* 2,3-dimethyl-4-sec.butylpentane

8- When branching first occurs at an equal distance from either end of the longest chain, choose the name that gives the lowest number at the first point of difference.

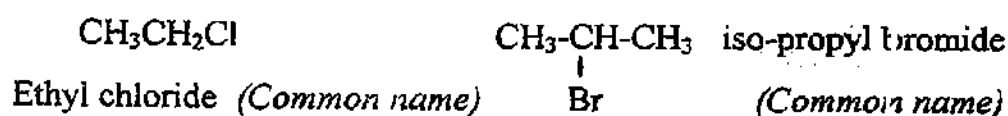


Nomenclature of Alkyl Halides

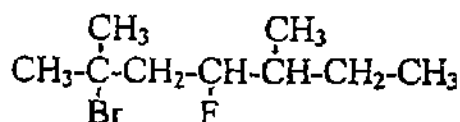
Those are the halogenated derivatives of alkanes. They have the general formula (RX), where R= alkyl radical, and X= halogen. According to IUPAC system they are named as Haloalkanes e.g.



Common names for any simple haloalkanes are still widely used however, in this common nomenclature system haloalkanes are named as if they were Alkyl halides:



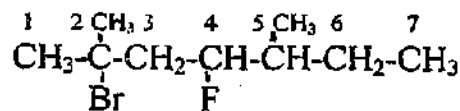
Example Provide IUPAC name for the following compound:



Solution:

(i) Number of carbons in longest chain = 7 carbons, therefore, basic name of alkane is heptane

(ii) Numbering the parent chain:

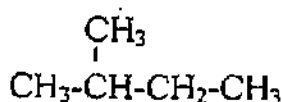


∴ IUPAC name of the compound: **2-bromo-4-fluoro-2,5-dimethylheptane**

Solved Problems

Example 1. Name the following structure. Say why the prefix number is

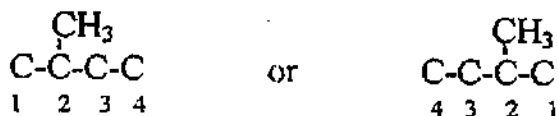
not needed in this name.



Solution:

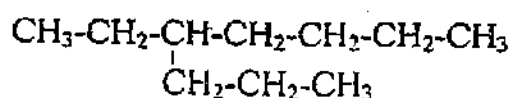
(i) Longest chain: 4 carbons. ∴ Parent alkane (base name): **butane**

(ii) Number the chain near to the branch (CH_3):



(iii) The prefix number is not needed because there is only one methylbutane as evident from (ii). The only other place to attach the CH_3 group would be the carbon 1 or 4 but this compound is pentane (5 carbons in a continuous chain) and not methylbutane.

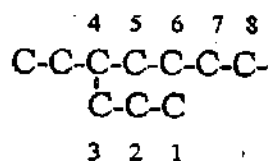
Example 2. Name the following branched alkane,



Solution:

(i) The longest chain : eight carbons ∴ The parent alkane **isooctane**

(ii) Number from end closer to branch



(iii) Alkyl group : ethyl at carbon 4 $\therefore$ Name of alkyl group 4-ethyl

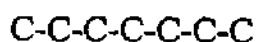
(iv) Name of branched alkane : **4-ethyloctane**

Example 3 Write the structure of the compound whose IUPAC name is

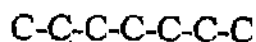
5-ethyl-2-dimethylheptane

Solution:

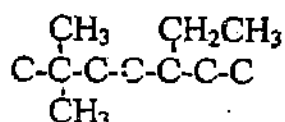
(i) Write the parent chain (heptane : 7 carbons)



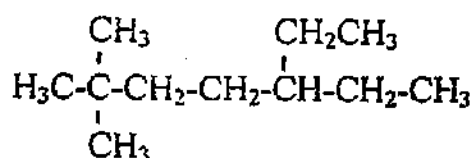
(ii) Number the carbons



(iii) Attach ethyl(CH_3CH_2) to carbon 5 and two methyls (CH_3) to carbon 2



(iv) Add hydrogen so that each carbon has four bonds :

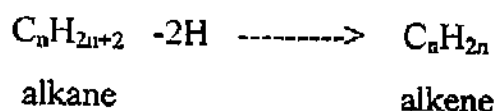


ALKENES (Olefins)

General Formula $RCH=CH_2$, $RCH=CHR$, $R_2C=CH_2$, $R_2C=CR_2$

Functional group $C=C$

The members of this class of hydrocarbons contain two hydrogen atoms less than the corresponding members of the alkanes series. The general formula of this series is then:



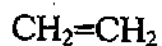
Nomenclature of Alkenes

Many older names of alkenes are still in common use. Ethylene, the simplest olefin (alkene) has the structure $CH_2=CH_2$. In the following Table we find a series of olefinic compounds according to *Common name*.

C_2H_4	$H_2C=CH_2$	Ethylene
C_3H_6	$H_2C=CH-CH_3$	Propylene
C_4H_8	$H_2C=CH-CH_2-CH_3$	n-Butylene
C_5H_{10}	$H_2C=CH-CH_2-CH_2-CH_3$	n-Pentylene
C_6H_{12}	$H_2C=CH-CH_2-CH_2-CH_2-CH_3$	n-Hexylene
C_7H_{14}	$H_2C=CH-CH_2-CH_2-CH_2-CH_2-CH_3$	n-Heptylene

According to *IUPAC* system the name of alkene is similar to that of alkane having the same number of carbon atoms by adding the prefix *-ENE* instead of *-ANE*. e.g. C_2H_4 ethylene or ethene, C_3H_6 propylene or proene.

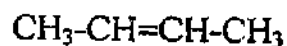
In some cases the alkenes are named as ethylene substituted derivatives as follows:



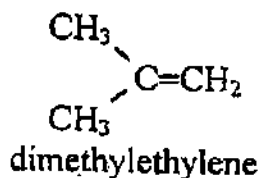
ethylene



methylethylene



dimethylethylene



dimethylethylene

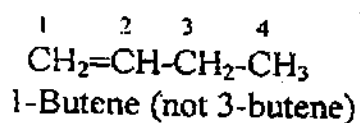


methyl-ethyl-ethylene

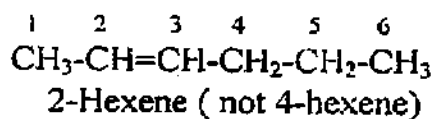
The *IUPAC* rules for naming alkenes are similar in many aspects to those for naming alkanes.

1- We determine the base name by selecting the longest chain that contains the double bond and changing the ending at the name of the alkane of identical length from ANE TO ENE as seen above. Thus, if this longest chain contains 5 carbon atoms, the base name of the alkene is pentene and so on

2- We number the chain so as include both carbons of the double bonds, and we began numbering at the end nearest the double bond. We designate the location of the double bond by using the number of the first atom of the double bond as prefix. e.g.

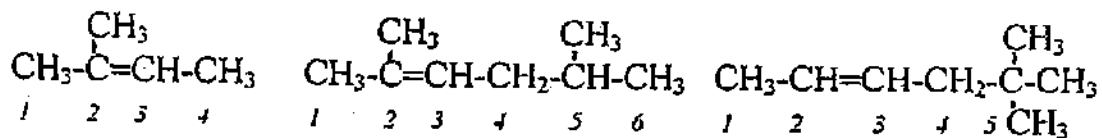


1-Butene (not 3-butene)

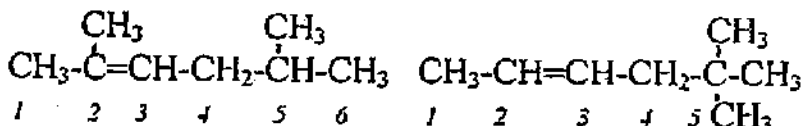


2-Hexene (not 4-hexene)

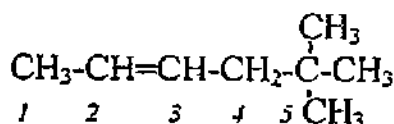
3- We indicate the location of the substituent groups by the number of carbon atom which they are attached.



2-methyl-2-butene



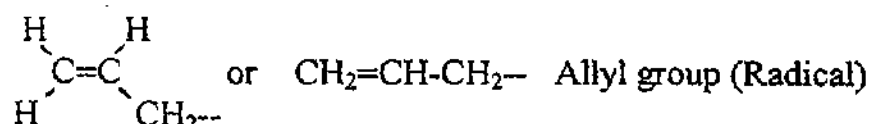
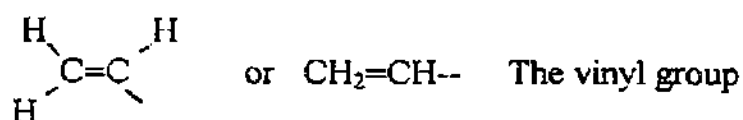
2,5-dimethyl-2-hexene



5,5-dimethyl-2-hexene

4- Two alkene groups are often named as though they were substituents.

These groups are the *vinyl group* & the *allyl group*.



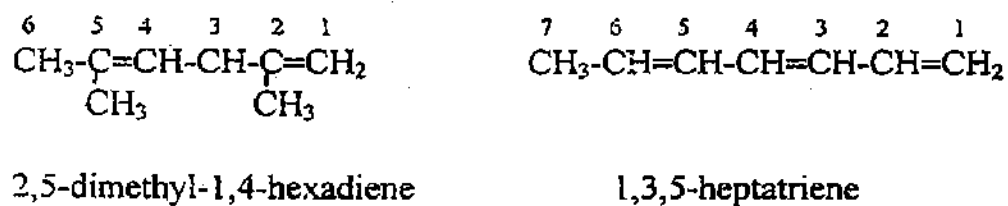
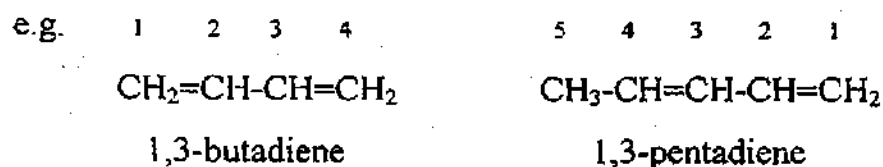
e.g. $\text{CH}_2=\text{CHBr}$ $\text{CH}_2=\text{CH}-\text{CH}_2\text{Br}$
 Bromoethene or vinyl bromide 3-Bromopropene or allyl bromide

5-For alkenes containing two or more double bonds, such as :

2 double bonds -----> diene

3 double bonds -----> triene

4 double bonds -----> tetraene



Alkenyl groups

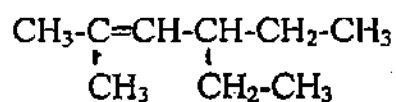
The groups derived by removing a hydrogen atom from an alkene molecule, are called *alkenyl group*. The IUPAC name of an individual such group is obtained by dropping -e of the corresponding alkene and adding the suffix -yl. The numbering of the group-chain starts with the carbon attached

directly to the parent chain. A few alkenyl groups have trivial names which are commonly used. The IUPAC and common (trivial) names of some alkenyl groups are listed in the table:

Structure	IUPAC Name	Common Name
$\text{CH}_2=\text{CH}-$ 3 2 1	Ethenyl	Vinyl
$\text{CH}_2=\text{CH}-\text{CH}_2-$ $\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_2=\text{C}- \end{array}$ 2 1	2-propenyl	Allyl
$\text{CH}_3-\text{CH}=\text{CH}-\text{CH}_2-$ 4 3 2 1	1-methylethenyl	Isopropenyl
$\text{CH}_2=\text{CH}-\text{CH}_2-\text{CH}_2-$ 4 3 2 1	2-butenyl	
	3-butenyl	

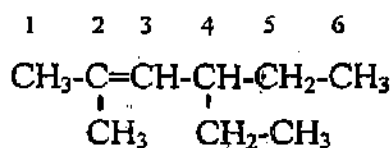
Solved Problems

Example 1. Name the alkene



Solution:

- (i) Longest chain containing C=C is 6 carbons
- (ii) Parent name (base name) : hexene
- (iii) Number the chain from the left to right and prefix locator of double bond.

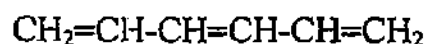


This gives the basic name : 2-hexene

(iv) Name the substituent groups : CH_3 and CH_2-CH_3 with locator numbers indicated before them.

(v) $\therefore$ Complete IUPAC name of the alkene is **4-ethyl-2-methylhexene**.

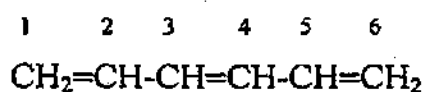
Example 2. Name the compound



Solution:

(i) The six-carbon chain has three double bonds. The basic name is **hexatriene**.

(ii) Number the carbons of the chain and assign locator numbers to double bonds.



As evident, the locator numbers of double bonds are : 1,3,5.

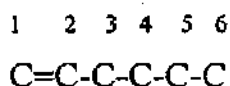
(iii) Prefixing the locator numbers of the basic name, the complete IUPAC name is **1,3,5-hexatriene**.

Example 3. Write the structure for 5-methyl-1-hexene

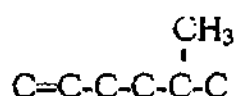
Solution:

(i) Parent name hexene show the presence of a 6-carbon chain.

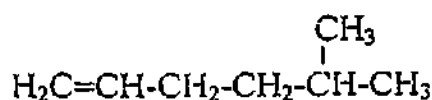
(ii) Position of double bond on the chain being 1, we have



(iii) Attach methyl (CH₃) group to carbon 5 :



(iv) Supply requisite hydrogens to get the complete structure



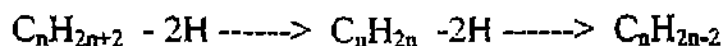
ALKYNES (Acetylenes)

General formula $\text{R}-\text{C}\equiv\text{CH}$, $\text{R}-\text{C}\equiv\text{C}-\text{R}$

Functional group $-\text{C}\equiv\text{C}-$

This class of hydrocarbons contain two hydrogen atoms less than the alkenes. Those two hydrogen are detected from the two carbons already joined by the double bond. This deficiency is represented by consisting of 6 electrons (forming a triple bonds) shared between two carbon atoms.

Thus, the general formula of this class is:

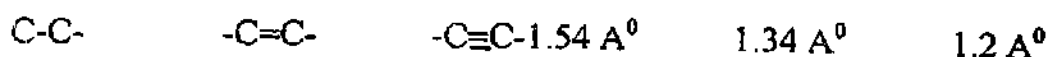


alkane

alkene

alkyne

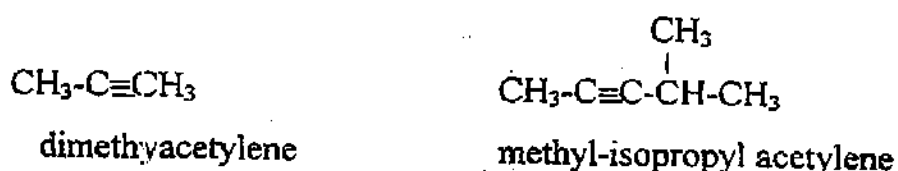
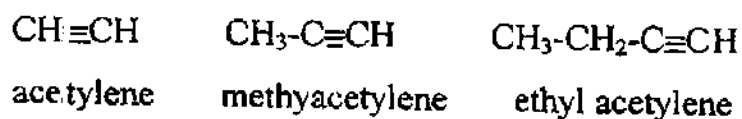
The six shared electrons hold the two carbon atoms more closely than in the case of the double bond, and the distance between the two carbon atoms becomes shorter.



Nomenclature of Alkynes

Common names :

acetylene, is sometimes called methylacetylene. The disubstituted acetylene, 2-butyne, is called dimethyl acetylene. The following examples illustrate the older system of nomenclature :



The name acetylene is not only used for the compound ($\text{CH}\equiv\text{CH}$), but it is also used as a general name for all of the alkynes. We could say for example, that propyne, 1-butyne and 2-butyne are alkynes. we could also say that they all acetylenes.

IUPAC system :

Alkynes are named in such the same way as alkenes. One names unbranched alkynes, for example, by replacing the -ANE of the name of

the corresponding alkane with the adding -YNE. The chain is numbered in order to give the carbon atoms of the triple bond the lowest possible numbers. The lower number of the carbon of the triple bond is used to designate the location of the triple bond. The IUPAC name of several unbranched alkynes are shown below :

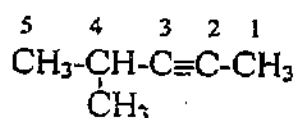
$\text{CH}\equiv\text{CH}$	ethyne or acetylene
$\text{CH}_3\text{C}\equiv\text{CH}$	propyne
$\text{CH}_3\text{-CH}_2\text{-C}\equiv\text{CH}$	1-butyne
$\text{CH}_3\text{-C}\equiv\text{C-CH}_3$	2-butyne
$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-C}\equiv\text{CH}_3$	1-pentyne
$\text{CH}_3\text{-CH}_2\text{-C}\equiv\text{C-CH}_3$	2-pentyne etc.

The location of substituent groups of branched alkynes and substituted alkynes are also indicated with numbers as follows:

$\begin{array}{ccccccc} & 3 & 2 & 1 & & & \\ \text{Cl-CH}_2\text{-C}\equiv\text{CH} & & & & & & \end{array}$	$\begin{array}{ccccccc} & 4 & 3 & 2 & 1 & & \\ \text{CH}_3\text{-C}\equiv\text{C-CH}_2\text{Cl} & & & & & & \end{array}$
3-chloropropyne	1-chloro-2-butyne
$\begin{array}{ccccccc} 6 & 5 & 4 & 3 & 2 & 1 & \\ \text{CH}_3\text{-CH-CH}_2\text{-CH}_2\text{-C}\equiv\text{CH} & & & & & & \\ & & & & & & \\ \text{CH}_3 & & & & & & \end{array}$	$\begin{array}{ccccccc} & 5 & & \text{CH}_3 & & 2 & 1 \\ \text{CH}_3\text{-C-CH}_2\text{-C}\equiv\text{CH} & & & & & & \\ & & & & & & \\ \text{CH}_3 & & & & & & \end{array}$
5-methyl-1-hexyne	4,4-dimethyl-1-pentyne

Solved Problems

Example 1. Assign IUPAC name for the following branched alkyne:



Solution:

(i) Longest chain containing triple bond = 5 carbons

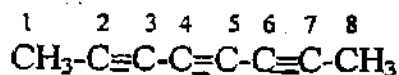
∴ Basic name is **pentyne**

(ii) Number the chain; prefix triple-bond locator number with basic name : 2-pentyne

(iii) Name the substituent : 4-methyl

(iv) IUPAC name of the hydrocarbon : **4-methyl-2-pentyne**

Example 2. Provide systematic name for :



Solution:

(i) Continuous chain 8 carbons. Number of triple bonds = 3, (**octatriyne**)

(ii) Prefix locator number of triple bonds on the chain membered as above.

Thus systematic name is : **2,4,6-Octatriyne**

CYCLIC ALIPHATIC HYDROCARBONS

Cycloalkanes

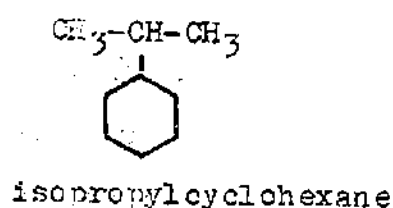
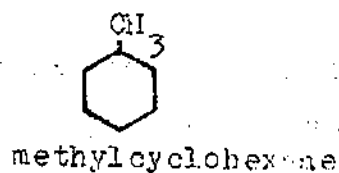
Cycloalkanes are alkanes in which the carbon atoms are arranged in a *ring*. Alkanes have the general formula C_nH_{2n+2} , cycloalkanes have two fewer hydrogen atoms, and the general formula of cycloalkanes is C_nH_{2n} .

They are named as alkanes by the addition of the word “*cyclo*” before the name of the alkane having the same number of carbon atoms thus

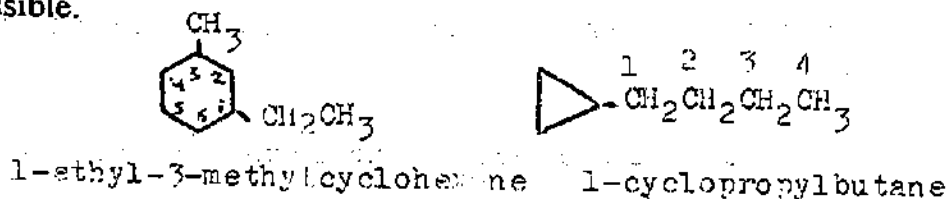
Substituted Cycloalkanes.

These are named according to the following rules:

1. The name of the alkyl side-chain is prefixed to the name of the parent cycloalkane.

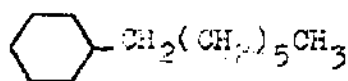


2. When more than one side-chain is present, we number the ring beginning with one side-chain so that the next side-chain gets the lower number possible.



3. If the alkane chain has a greater number of carbons than the ring, we designate the ring as substituent, (See above).

Example 1. Give the name of the following substituted cycloalkanes:

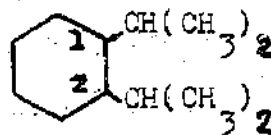
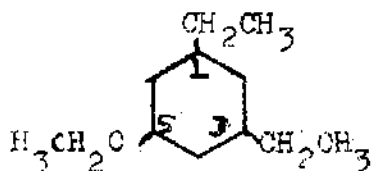


Solution:

(a) The side-chain has 7 carbons, while the ring has 6. Therefore, it will be named as a substituted alkane.

(b) There are two methyl substituents in positions 1 and 3 on a four-carbon ring. Therefore, it will be 1,3-dimethylcyclobutane.

Example 2. Name the following compounds



Solution:

(a) There are three ethyl groups (C_2H_5) on the cyclohexane ring in 1,3,5 positions. Thus its name is **1,3,5-triethylcyclohexane**.

(b) There are two isopropyl, $(CH_3)_2CH$, substituents in 1,2 positions. Thus its full name is **1,2-diisopropylcyclohexane**.

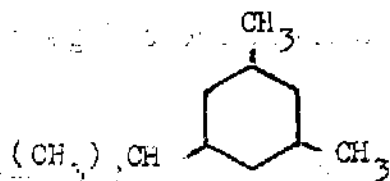
Example 3. Write the structure of 5-isopropyl-1,3-dimethylcyclohexane.

Solution:

(a) Since it is cyclohexane, the ring structure may be written as :



(b) Attaching isopropyl, $(CH_3)_2CH$, in position 5 and methyl (CH_3) in positions 1,3 we get the desired structure.

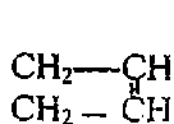


Cycloalkenes

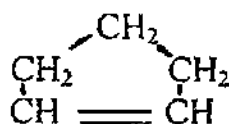
Cycloalkenes are derived from cycloalkanes by the loss of two atom from the two adjacent carbon atoms to form double bond.

Nomenclature

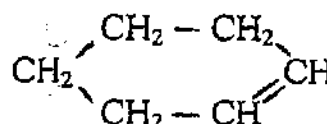
Simple cycloalkenes are named as the parent alkenes ending with *ene* instead of *ane* and the addition of the word "cyclo" before the name



cyclobutene

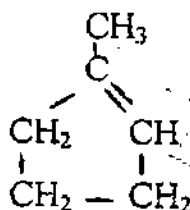


cyclopentene

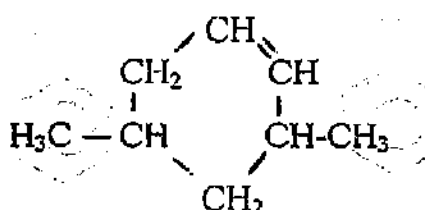


cyclohexene

Substituted cycloalkenes are numbered in the way that gives the carbon atoms of the double bond the 1- and 2-positions and that also gives the substituent group lowest numbers at the first point of deference.



1-methylcyclopentene



3,5-dimethylcyclohexene

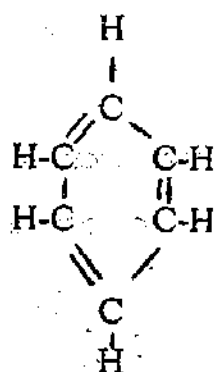
AROMATIC HYDROCARBONS

Benzene

Family : Arens. General formula : ArH. Functional group : Aromatic ring.

Kekule formula of Benzene

Kekule proposed a structure for benzene in which the 6-carbon atoms are in a ring, that they bounded to each other by alternative single and double bonds, and that one hydrogen atom is attached to each carbon.



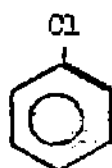
Kekulé formula for benzene



Nomenclature of benzene derivatives

1- Two systems are used in naming monosubstituted benzene, those are:

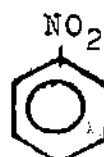
- a) In compounds of one type, benzene is the base name and the substituent is simply indicated by a prefix, e.g.



Chlorobenzene



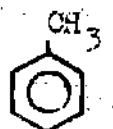
Bromobenzene



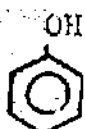
Nitrobenzene

For compounds of the other type, the substituent and the benzene ring taken together form a new base name.

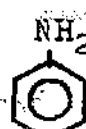
- Methylbenzene is always called toluene.
- Hydroxybenzene is always called phenol.
- Aminobenzene is always called aniline.



Toluene

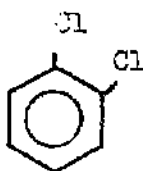


Phenol

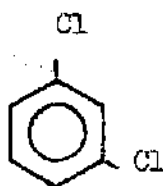


Aniline

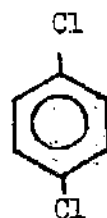
2- When two substituents are present, their relative positions are indicated by the use of ortho, meta and para (o-, m and p-). This is shown for dibromobenzene as example, as follows:



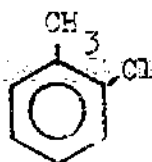
o-dichlorobenzene



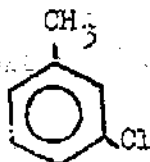
m-dichlorobenzene



p-dichlorobenzene



o-chlorotoluene

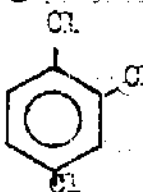


m-chlorotoluene

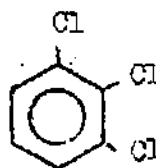


p-chlorotoluene

- 3- If more than two groups are present on the benzene ring their positions must be indicated by the use of numbers, the benzene ring is numbered so as to give the lowest possible numbers to the substituents as follows:



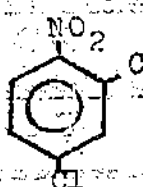
1,2,4-trichlorobenzene



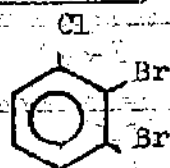
1,2,3-trichlorobenzene

NOT 1,3,4-trichlorobenzene

- 4- When more than two substituents are present, and the substituents are different, they are usually listed in alphabetical order, e.g.

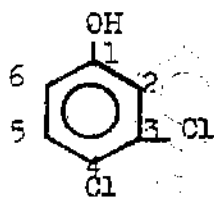


2,4-dichloro-1-nitrobenzene

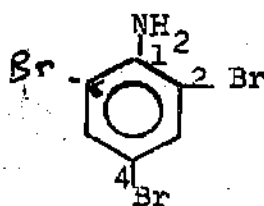


2,3-dibromo-1-chlorobenzene

- 5- When a substituent is one that when taken together with benzene ring gives a new base name, that substituent is assumed to be in position -1 and the new base name is used. e.g.



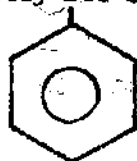
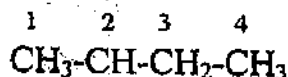
3,4-dichlorophenol



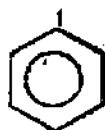
2,4,6-tribromoaniline

6- When the benzene ring itself is a substituent it is called phenyl group.

e.g.



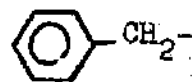
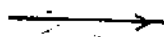
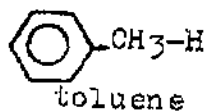
2-phenylbutane



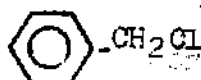
or C₆H₅--

phenyl group.

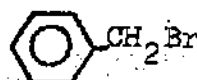
7- The name benzyl radical is reserved for the group derived from toluene in which one of the hydrogens of the methyl group is replaced.



benzyl group



benzyl chloride



benzyl bromide

ALCOHOLS, PHENOLS & ETHERS

Family	Alcohols	Phenols	Ethers
General formula	R-OH	Ar-OH	R-O-R
Functional group	-C-OH	-C-OH	-C-O-C-

Structure:

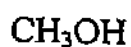
Those are the compounds containing C, H and oxygen in their internal structure.

ALCOHOLS

General formula $C_nH_{2n+1}OH$

Are compounds in which a hydroxyl ($-OH$) group is attached to the saturated carbon. If this ($-OH$) group is attached to unsaturated carbon atom of a double bond ($C=C$) the compound is said to be an enol.

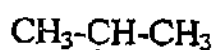
The saturated carbon may be a carbon of a simple alkyl group:



Methanol



Ethanol



2-Propanol

The carbon may be a saturated carbon of an alkenyl or alkynyl group



2-propenol



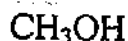
2-propynol

The carbon may be a saturated carbon that is attached to an aromatic ring

Alcohols are classified, according to the type of the carbon atom to which the hydroxyl group is attached, to the following types:

• Primary alcohols

In this type of alcohols, the carbon atom that carries the ($-OH$) group must at least carry *two hydrogen atoms*.



Methanol

1ry alcohol

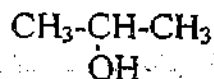


Ethanol

1ry alcohol

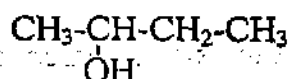
• Secondary alcohols

In this case, the carbon atom that carries the (-OH) group is attached to *one* hydrogen only.



2-propanol

2ry alcohol

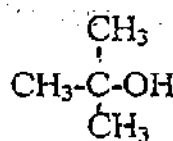


2-butanol

2ry alcohol

• Tertiary alcohols

In this type of alcohols, the carbon atom that carries the (-OH) group has *no* hydrogen atoms.



tert-butyl alcohol

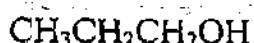
3ry alcohol

Nomenclature of alcohols

i- Simple alcohols are often called by their common names. This is shown as follows:



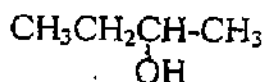
ethyl alcohol



n-propyl alcohol



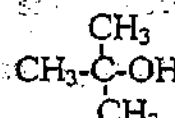
n-butyl alcohol



sec-butyl alcohol



iso-butyl alcohol

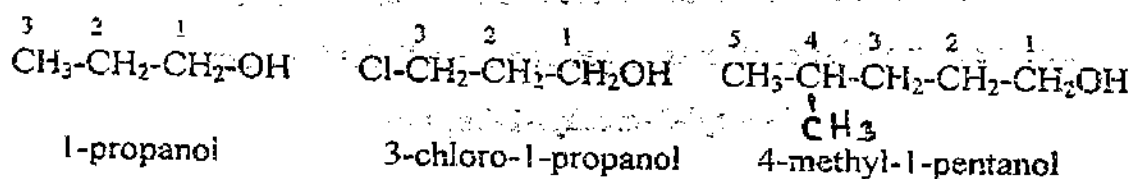


tert-butyl alcohol

[Common name of alcohols (name of alkyl radical + alcohol)]

ii- The IUPAC rules for naming alcohols:

1. Select the longest carbon chain to which the hydroxyl (-OH) group is directly attached. Change the name of the alkane corresponding to this chain by dropping the final (-e) and adding (-ol). This gives the base name.
2. Number the longest continuous carbon chain so as to give the carbon carrying the hydroxyl group the lowest possible number. Indicate the position of the hydroxyl group by using this number; indicate the position of other substituents (or multiple bonds) by using the numbers corresponding to their position along the carbon chain. e.g.



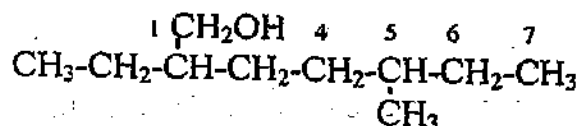
iii- Alcohols containing two hydroxyl groups are commonly called glycols. In the IUPAC system they are named diols.

The following examples show the difference between the 2-system for nomenclature of dihydroxy compounds:

Compounds	$\begin{array}{c} \text{CH}_2-\text{CH}_2 \\ \quad \\ \text{OH} \quad \text{OH} \end{array}$	$\begin{array}{c} \text{CH}_3-\text{CH}-\text{CH}_2 \\ \quad \\ \text{OH} \quad \text{OH} \end{array}$	$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \quad \quad \\ \text{OH} \quad \quad \text{OH} \end{array}$
Common name	Ethylene glycol	Propylene glycol	Trimethylene glycol
IUPAC name	1,2-Ethanediol	1,2-Propanediol	1,3-Propanediol

Solved Problems

Example 1. Provide IUPAC name for the following alcohol :

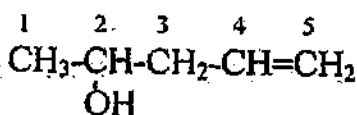


Solution:

- (i) The longest chain bearing OH = 7 carbons $\therefore$ Basic name : **heptanol**
- (ii) Number the chain as above and write names of substituent alkyl groups
2-ethyl and 5-methyl
- (iii) Provide position number of OH to the basic name: **1 heptanol**
- (iv) Prefix the name of substituents to get complete IUPAC name:

2-ethyl-5-methyl-1-heptanol

Example 2. Assign systematic name to the following compound:



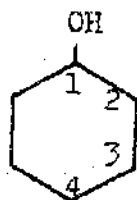
Solution:

- (i) The longest chain bearing oh = 5 carbons $\therefore$ Basic name : **pentenol**
- (ii) Number the chain and prefix position number of double bond **4-pentenol**
- (iii) Insert position number of OH : **4-penten-2-ol**

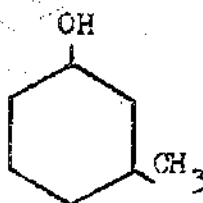
Example 3. Give the structure for 3-methyl-1-cyclohexanol.

Solution:

- (i) Since OH has position number 1, the structure of the basic alcohol is

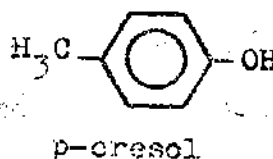


(ii) Providing substituent methyl ($-\text{CH}_3$) at position 3 :

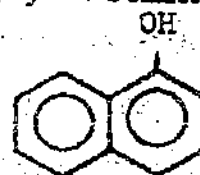


PHENOLS

Compounds that have a hydroxyl group attached directly to the benzene ring are called phenols.



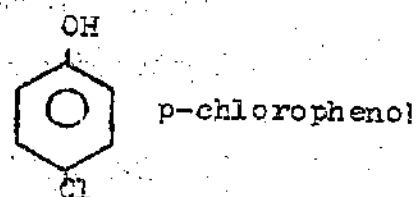
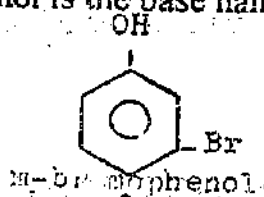
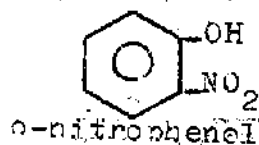
Compounds that have a hydroxyl group attached to a polycyclic benzenoid ring are similar to phenols, but they are called naphthols.



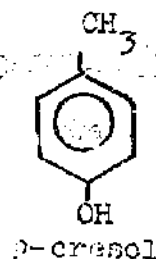
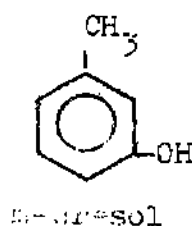
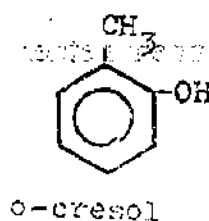
a-naphthol

Nomenclature of phenols

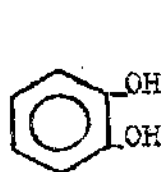
1- In many compounds, phenol is the base name:



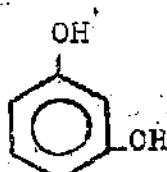
2- The methylphenols, however, are called cresols:



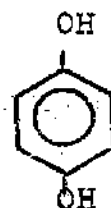
3- The dihydroxybenzenes have special names:



catechol



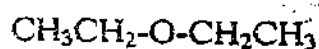
resorcinol



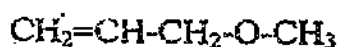
hydroquinone

ETHERS

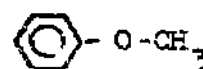
Ethers differ from alcohols and phenols in that the oxygen atom of an ether is bonded to two carbon atoms. The hydrocarbon groups may be alkyl, alkenyl, alkynyl, or aryl e.g.



diethyl ether



methyl allyl ether



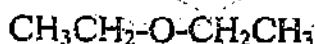
methyl phenyl ether

Nomenclature of ethers

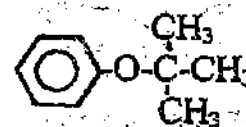
1- Ethers are frequently given common name and to do so it is quite easy. One simply names both groups that are attached to the oxygen. When two different alkyl radicals are present, the smaller one is mentioned first. Moreover, a n-group precedes the branched group having the same number of carbons.



methyl ethyl ether



diethyl ether



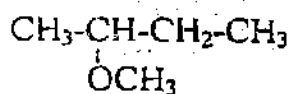
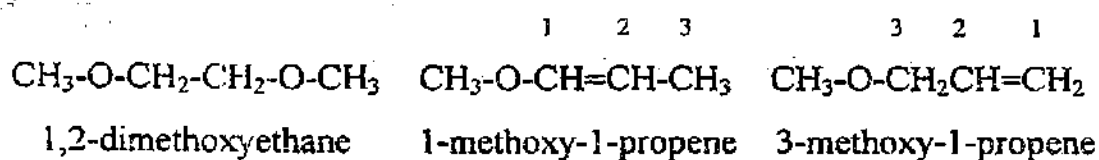
tert-butyl phenyl ether



divinyl ether

2- IUPAC names

In the IUPAC system, ethers are named as Alkoxy-Alkanes, Alkoxy Alkenes, and Alkoxy-Arenes :

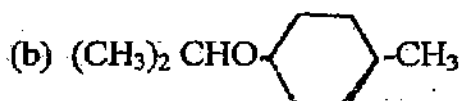
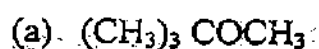


2-methoxypentane



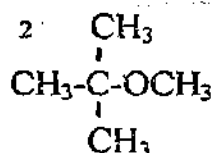
p-methoxy toluene

Example Assign both IUPAC and common names to the following ethers :



Solution:

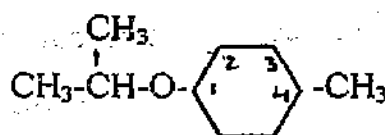
(a) The structure of ether may be written as below and the name assigned



IUPAC name : 1-methoxy-1,1-dimethylethane

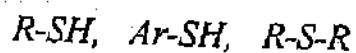
Common name : tert-butyl methyl ether

(b) The structure of the ether may be written as below and name assigned



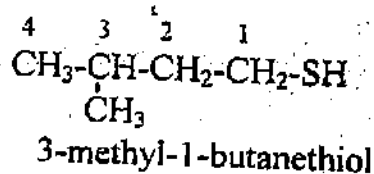
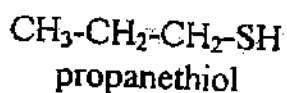
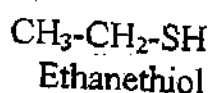
- (i) Basic alkane : 4-methylcyclohexane
- (ii) Substituent alkoxy group : isopropoxy
- (iii) Complete IUPAC Name : 1-isopropoxy-4-methylcyclohexane
- (iv) Common Name : isopropyl methyl ether.

Thioalcohols(thiols), Thiophenols, Thioethers

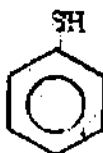


Sulphur is directly below oxygen in group VI of the periodic table and, so we might expect there are sulphur counterparts of the oxygen compounds that we have studied.

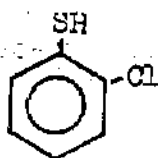
- 1- The sulphur counterpart of the alcohol is called Thiol or mercaptan. The following examples show the nomenclature of thiols:



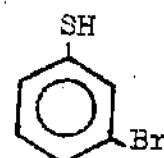
- 2- Thiophenols: are named as phenols but ending with thiophenol:



Thiophenol

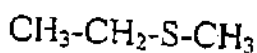


o-chlorothiophenol

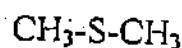


m-bromothiophenol

- 3- Thioethers: are also named like ethers, but ending with thioether:

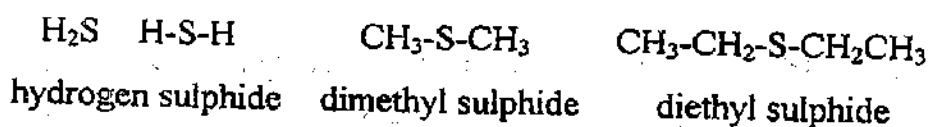


methyl ethyl thioether



dimethyl thioether

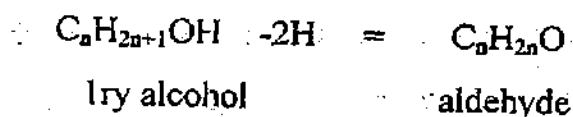
Thioethers, may also be named as substituted hydrogen sulphide:



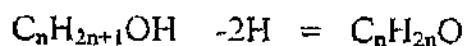
ALDEHYDES & KETONES

	<u>Aldehydes</u>	<u>Ketones</u>
General formula	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{H}$	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{R}$
Functional group	$-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{H}$	$-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{C}-$

When primary alcohol are oxidised they give compounds which contain two hydrogen atoms less than the original compounds i.e. they are dehydrogenated. These products are named ALDEHYDES (from Alcohol dehydrogenated). They contain the functional group written as (-CHO). The general formula is then:



On the other hand, oxidation of secondary alcohols gives the second members of the carbonyl compounds which are called KETONES. These also contain two hydrogens less than the corresponding alcohol and have the general formula:

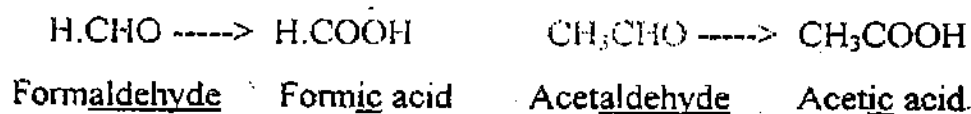


2ry alcohol ketone

It is clear that both aldehydes and ketones have the same molecular formula. The carbonyl group ($C=O$) is then common to both aldehydes and ketones. In the first class it carries one hydrogen, while in ketones it is joined to two alkyl groups.

Nomenclature: * Aldehydes

1- In the common names, the aldehydes are names after the acid they form on oxidation, by the omission of the term of acidity (*-IC*) and placing the terminal *aldehyde*.



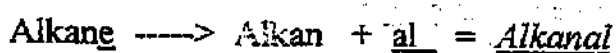
HCHO	Formaldehyde	CH ₃ (CH ₂) ₃ CHO	Valeraldehyde
CH ₃ CHO	Acetaldehyde	CH ₃ (CH ₂) ₄ CHO	Caproaldehyde
CH ₃ CH ₂ CHO	Propionaldehyde	CH ₃ (CH ₂) ₅ CHO	Heptylaldehyde
CH ₃ (CH ₂) ₂ CHO	Butraldehyde		

The positions of substituents and side chain are indicated by the Greek letters α , β , γ , δ , ... beginning from the carbon atom directly linked to the (**-CHO**) group.



α, β -dibromo- γ -methylvaleraldehyde

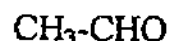
2- According to the IUPAC system, aldehydes are considered as alkanes in which one carbon atom is changed to (-CHO) group. This is indicated By adding the ending (-AL) to the name alkane (after dropping the final e). The longest chain is taken as the parent hydrocarbon and the positions of substituents are indicated by numbers, so as the aldehyde group takes the first number (No. 1):



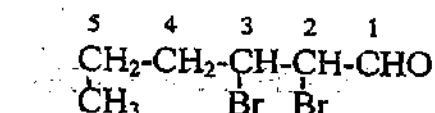
e.g.



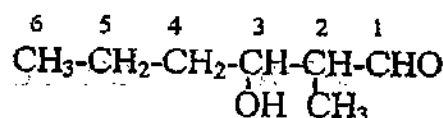
propanal



ethanal

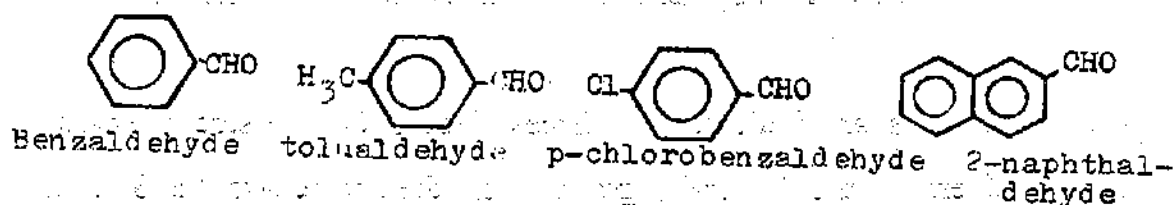


2,3-dibromo-5-methylpentanal



3-hydroxy-2-methylhexanal

3- When the carbonyl group is attached to an aromatic ring, we name the compound as *benzaldehyde*, *tolualdehyde*, *naphthaldehyde*, and so on.

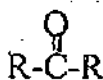


Name of some aldehydes

Structure	IUPAC	Common name
HCHO	Methanal	Formaldehyde
CH ₃ CHO	Ethanal	Acetaldehyde
CH ₃ CH ₂ CHO	Propanal	propionaldehyde
CH ₃ (CH ₂) ₂ CHO	Butanal	n-butyraldehyde
(CH ₃) ₂ CHCHO	2-methylpropanal	isobutyraldehyde
CH ₃ CH=CHCHO	2-butenal	crotonaldehyde

Ketones

1- Ketones are named according to the alkyl groups attached to the carbonyl group and ending with the word ketones (common names). When the two alkyl groups are similar, the ketones is said to be simple, and if they are different, the ketone is mixed.



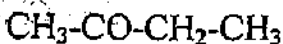
simple ketone



mixed ketone



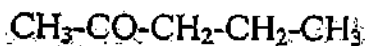
Acetone(dimethyl ketone)



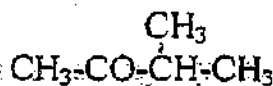
methyl ethyl ketone



diethyl ketone

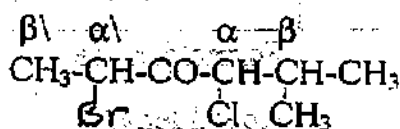
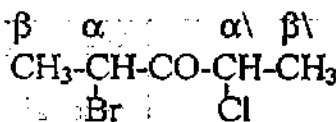


methyl n-propyl ketone



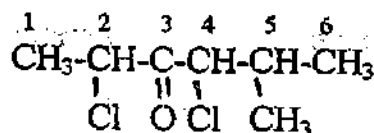
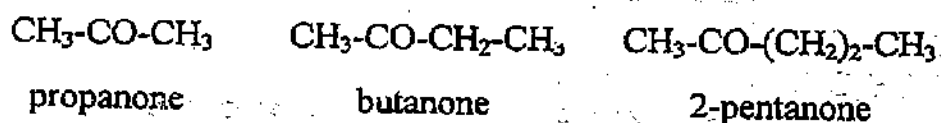
methyl iso-propyl ketone

The substituents are indicated by Greek letters. On one side, the carbon atom adjacent to the (C=O) group is (α), the one next to it is β , ..., the chain of the other side is lettered α , β .

 α, α -dibromo-ethyl-iso-butyl ketone α -bromo- α -chloro-diethyl ketone

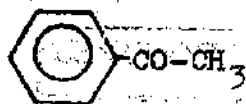
(Notice that bromo- precedes chloro- alphabetically)

2- According to the IUPAC system, *ketones are considered as derivatives of alkanes* in which one carbon atom is transformed into *carbonyl group*. This is indicated by adding the ending (-ONE) to the name of the alkane (without the E). The longest continuous chain with the carbonyl group is chosen as the base name and it is so numbered so as to give the carbonyl group the smallest number possible.



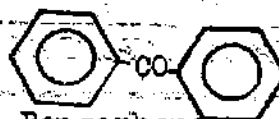
2,4-dichloro-5-methyl hexan-3-one

3- Some aromatic ketones have *special names*



Acetophenone

Comm. methyl phenyl ketone



Benzophenone

Comm. diphenyl ketone

4- When the (-CO-R) groups are named as substituents, they are called Acyl groups.



p-Acetylbenzoic acid

Name of some ketones

Structure	IUPAC	Common name
$\text{CH}_3\text{-CO-CH}_3$	Propanone	Acetone
$\text{CH}_3\text{CH}_2\text{-CO-CH}_3$ 5 4 3 2 1	Butanone	methyl ethyl ketone
$\text{CH}_3\text{CH}_2\text{CH}_2\text{-CO-CH}_3$ 1 2 3 4 5	2-pentanone	methyl n-propyl ketone
$\text{CH}_3\text{CH}_2\text{-CO-CH}_2\text{CH}_3$	3-pentanone	diethyl ketone
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{-C(=O)-CH}_3$ 6 5 4 3 2 1	2-hexanone	methyl n-butyl ketone

CARBOXYLIC ACIDS & THEIR DERIVATIVES

General formula $R\text{-CO-OH}$, Functional group -CO-OH

The characteristic functional group of this series is the carboxylic group (CO-OH) which results from the combination of a carbonyl and hydroxyl group. The carboxylic group is univalent, so it is a terminal group.

Acids are classified into mono-, di- ... and poly-carboxylic acids, according to whether they contain one, two, ... or more carboxylic acid groups, in the molecule, respectively.

The saturated monocarboxylic aliphatic acids have been named as Fatty acids, because some of the lighter members, e.g. palmitic and stearic acids, occur in fats.

Carboxylic acids contain one oxygen in excess than aldehydes, so their general formula is $C_nH_{2n}O_2$, and functional group $C_nH_{2n+1}.COOH = R.COOH$.

The carboxylic group is one of the most widely occurring functional groups in chemistry and biochemistry. Not only are carboxylic acids themselves important, but the carboxyl group is the parent group of a large family of related compounds all of these carboxylic acid derivatives contain the acyl group ($R-CO-$). As result, they are often called Acyl compounds.

The following table shows the carboxylic acid derivatives:

Name	Structure
Acyl (or acid) chloride	$R-CO-Cl$
Acid anhydride	$R-CO-O-CO-R$
Ester	$R-CO-O-R'$
Amides	$R-CO-NH_2$ $R-CO-NHR'$ $R-CO-NR_2$

Nomenclature

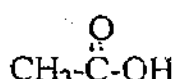
- Monocarboxylic acids:

1- The **IUPAC** names for carboxylic acids are obtained by dropping the final **(-E)** of the name of the alkane corresponding to the longest chain in the acid and by adding **(-OIC ACID)** as follows:

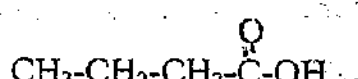
Alkane $\rightarrow$ Alkan + oic acid $\rightarrow$ Alkanoic acid



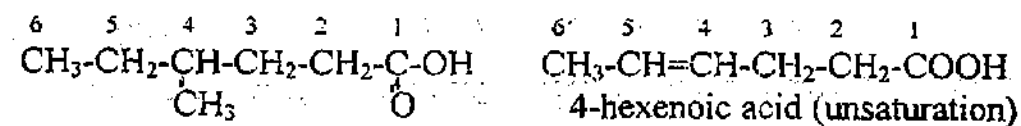
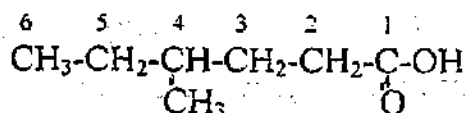
Methanoic acid



Ethanoic acid



Butanoic acid



4-hexenoic acid (unsaturation)

4-methylhexanoic acid

2- Many carboxylic acids have common name that are derived from Latin or Greek words that indicate on their natural sources. This is shown in the following table:

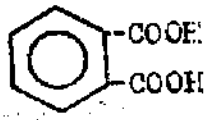
Structure	IUPAC Name	Common Name
H.COOH	Methanoic acid	Formic acid
CH ₃ .COOH	Ethanoic acid	Acetic acid
CH ₃ .CH ₂ .COOH	Propanoic acid	Propionic acid
CH ₃ .(CH ₂) ₂ .COOH	Butanoic acid	Butyric acid
CH ₃ .(CH ₂) ₃ .COOH	Pentanoic acid	Valeric acid
CH ₃ .(CH ₂) ₄ .COOH	Hexanoic acid	Caproic acid

3- Carboxylic acids have also been named as derivatives of acetic acid (notice that formic acid contains no carbon attached to carboxyl group)

• Dicarboxylic Acids:

Dicarboxylic acids are named as Alkanedioic acid in the *IUPAC* system.

Most dicarboxylic acids have common names as shown below:

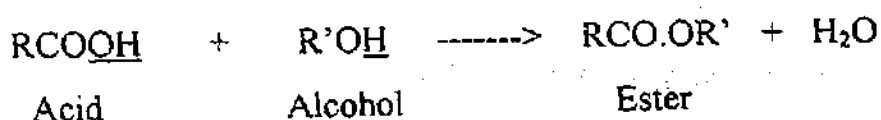
	$\begin{array}{c} \text{COOH} \\ \\ \text{COOH} \end{array}$	$\begin{array}{c} \text{CH}_2\text{COOH} \\ \\ \text{CH}_2\text{COOH} \end{array}$	
Common	Oxalic acid	Succinic acid	Phthalic acid
<i>IUPAC</i>	Ethanedioic acid	Butanedioic acid	

	$\begin{array}{c} \text{COOH} \\ \diagup \quad \diagdown \\ \text{CH}_2 \\ \diagdown \quad \diagup \\ \text{COOH} \end{array}$	$\begin{array}{c} \text{CH}_2\text{COOH} \\ \diagup \quad \diagdown \\ \text{CH}_2 \\ \diagdown \quad \diagup \\ \text{CH}_2\text{COOH} \end{array}$
Common	Malonic acid	Glutaric acid
<i>IUPAC</i>	Propanedioic acid	Pentanedioic acid

ESTERS

General formula : R-CO-OR' **Functional group :** $-\text{CO-O-C}-$

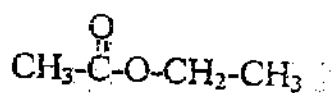
Esters are the group of organic compounds obtained by the interaction between carboxylic acids and alcohols by the loss of one molecule of water



They have usually pleasant odors. The odor of some ester resemble those of fruits and these esters are used in manufacturing synthetic flavors.

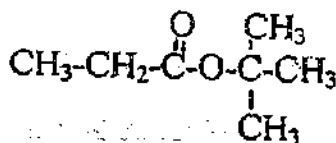
Nomenclature:

The names of esters are derived from the names of alcohol portion (the alkyl portion) and the acid portion (with the ending **-ATE** or **-OATE**). The portion of the named derived from the alcohol comes first:



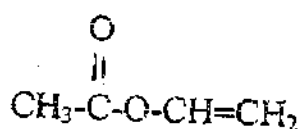
Ethyl acetate (common)

Ethyl ethanoate (IUPAC)



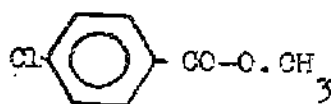
tert-butyl propionate (common)

tert-butyl propanoate (IUPAC)



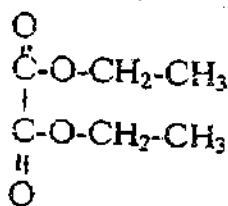
Vinyl acetate (common)

Vinyl ethanoate (IUPAC)



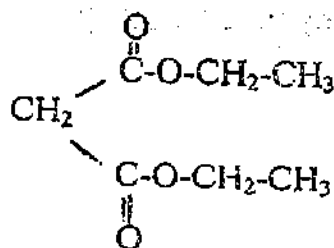
Methyl-p-chlorobenzoate

(common and IUPAC)



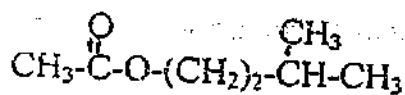
Diethyl oxalate (common)

Diethyl ethanedioate (IUPAC)

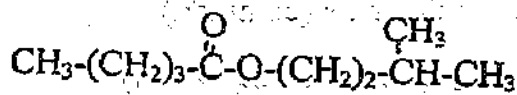


Diethyl malonate (common)

Diethyl propanedioate (IUPAC)



Isopentyl acetate (banana flavor)



Isopentyl pentanoate (apple flavor)

CARBOXYLIC ACID ANHYDRIDES

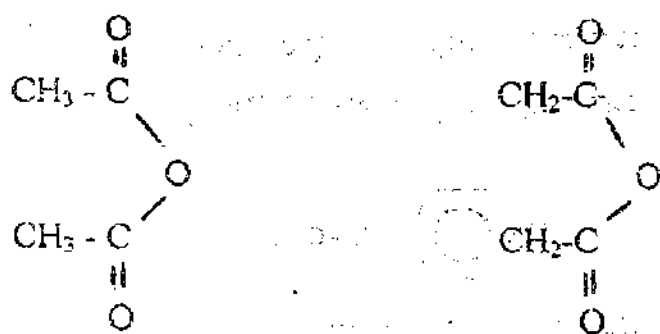
General formula $R-CO-O-CO-R$ Functional group $\begin{array}{c} \text{O} \quad \text{O} \\ \parallel \quad \parallel \\ -C-O-C- \end{array}$

Monocarboxylic acid (2 mols) $\longrightarrow$ anhydride + H_2O

Dicarboxylic acid (1 mol) $\longrightarrow$ anhydride + H_2O

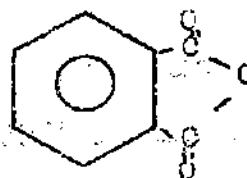
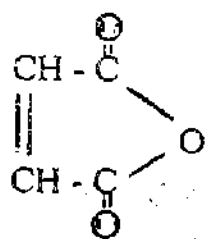
Nomenclature

Most anhydrides are named by dropping the word acid from the name of the carboxylic acid and then adding the word anhydride.



Acetic anhydride (common) Succinic anhydride (common)

E thanedioic anhydride (IUPAC) Butanedioic anhydride (IUPAC)



Maleic anhydride (common)

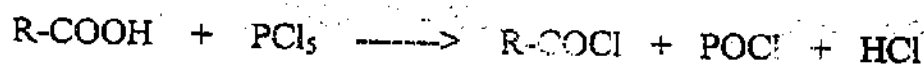
Phthalic anhydride

2-Butenedioic anhydride (IUPAC)

ACYL CHLORIDES

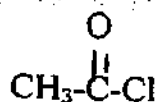
General formula **R-CO-Cl** *Functional group* **-CO-Cl**

Those are obtained usually by the interaction of the corresponding carboxylic acids and PCl_5 .



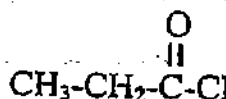
Nomenclature:

The acyl chlorides are often called acid chlorides. They are named by dropping (-IC) from the name of the acid then adding (-YL CHLORIDE).



Acetyl chloride (common)

Ethanoyl chloride (IUPAC)



Propionyl chloride (common)

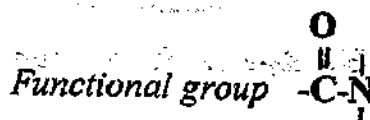
Propanoyl chloride (IUPAC)



Benzoyl chloride

AMIDES

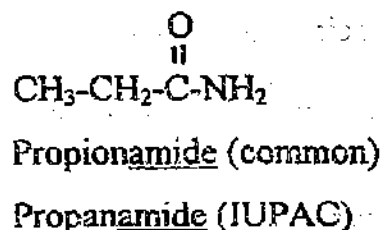
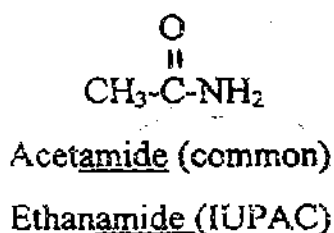
General formula **R-CO-NH₂**, **R-CO-NHR'**, **R-CO-NR₂'**



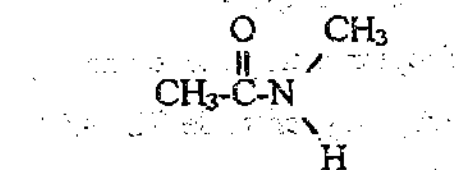
Amides are the acyl or acyl-alkyl derivatives of ammonia.

Nomenclature:

1- Amides that have no substituents on nitrogen are named by dropping (-IC) from the common name of the acid or (-OIC) from the IUPAC name and adding (-AMIDE) as follows:

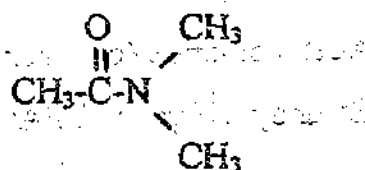


2- Substituents on the nitrogen atom of amides are named as **alkyl groups** and the named substituent is prefaced by (N-) in case of mono-substituent and (N,N-) in case of disubstituents :



N-Methylacetamide (common)

N-Methylethanamide (IUPAC)



N,N-Dimethylacetamide (common)

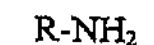
N,N-Dimethylethanamide (IUPAC)

AMINES

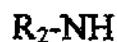
General formula R-NH_2 , $\text{R}_2\text{-NH}$, $\text{R}_3\text{-N}$ Functional group $\begin{array}{c} \text{ } \\ | \\ \text{-C-N-} \\ | \end{array}$

Amines are considered to be the alkylated derivatives of ammonia (NH_3). When one alkyl substituent is only attached to the nitrogen atom, the compound is then called primary amine. When two substituents are presented the compound is said to be secondary amine. When complete

substitution takes place (i.e. three substituents are present) the compound is called tertiary amine.



1ry amine



2ry amine



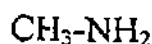
3ry amine

Nomenclature:

1- Common Name:

Primary Amine

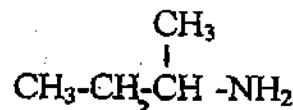
In common nomenclature most primary amines are named by specifying the organic group attached to nitrogen and then adding the ending (-AMINE).



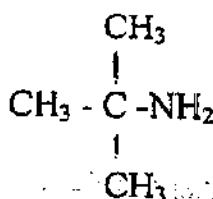
Methylamine



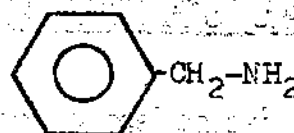
Ethylamine



Isobutylamine



tert-butylamine



Benzylamine

Most secondary and tertiary amines are named in the same general way; we either designate the organic groups individually if they are different, or use the prefixes di- or tri- if they are the same as follows:

Secondary amines



Methylethylamine



Diethylamine

Chapter 2

ISOMERISM IN ORGANIC COMPOUNDS

Isomerism is the phenomenon of exhibiting two or more compounds with same molecular formula but different physical and chemical properties.

Isomers are the compounds showing different physical and chemical properties but same molecular formula.

The isomerism in organic compounds can be classified broadly into:

- **Structural isomerism (constitutional isomerism)**
- **Stereo isomerism**

STRUCTURAL ISOMERISM

The structural isomerism or constitutional isomerism arises when atoms within a molecule are arranged in different orders. The structural isomers have the same molecular formula but different structural formulae.

The structural isomers usually show different physical and chemical properties.

The structural isomerism is further divided into:

- **Chain isomerism**
- **Positional isomerism**
- **Functional isomerism**

- Metamerism
- Tautomerism

CHAIN ISOMERISM

The **chain isomerism** arises due to different arrangements of carbon atoms leading to linear and branched chains. The **chain isomers** have same molecular formula but different types of chains i.e., linear and branched.

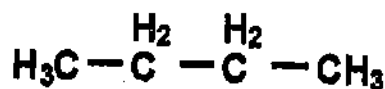
The chain isomers have almost similar chemical properties but different physical properties. For example, the branched chain isomers have lower boiling points than that of their linear counterparts. It is because, the linear ones have more surface area of contact and hence the intermolecular forces of attraction are maximum.

E.g. Two chain isomers possible with the molecular formula, C_4H_{10} .

i.e.,
n-butane: a linear chain isomer.

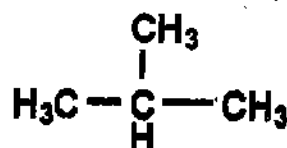
isobutane (or 2-methylpropane): a branched isomer

linear



butane

branched



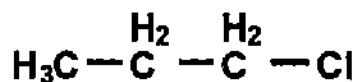
isobutane
or 2-methylpropane

POSITIONAL ISOMERISM

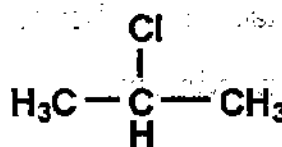
The **positional isomerism** arises due to different positions of side chains, substituents, functional groups, double bonds, triple bonds etc., on the parent chain.

E.g.

1) Propyl chloride and isopropyl chloride are the positional isomers with the molecular formula, C_3H_7Cl . These isomers arise due to difference in the position of the chloro group on the main chain.

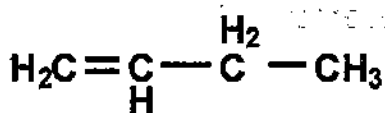


propyl chloride
or **1-chloropropane**



isopropyl chloride
or **2-chloropropane**

2) In the following positional isomers i.e., but-1-ene and but-2-ene the position of double is different but they have the same molecular formula, C_4H_8 .

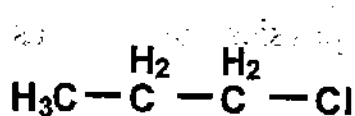


but-1-ene

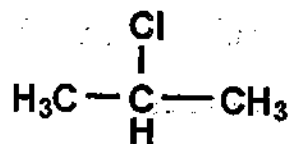


but-2-ene

3) The functional group, -OH is at different positions on the main chain of the following alcohols. They have the same molecular formula, C_3H_7OH .

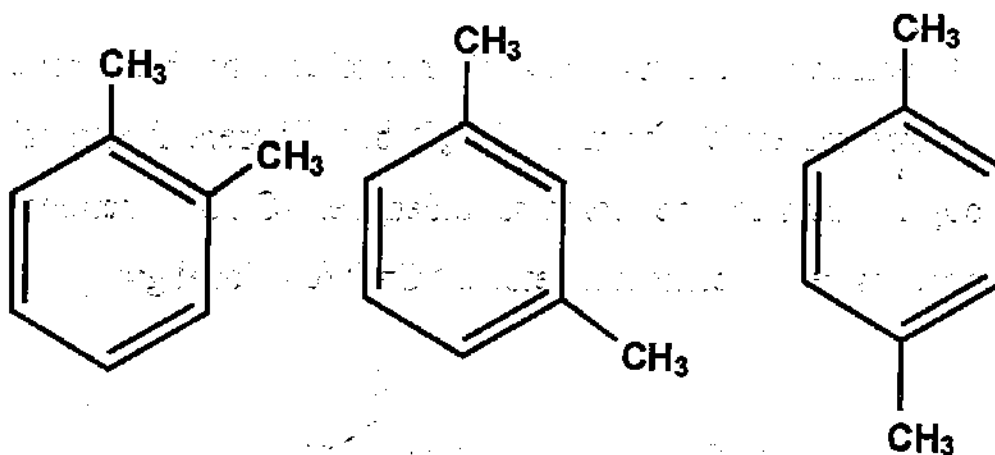


propyl alcohol
or propane-1-ol



isopropyl alcohol
or propane-2-ol

4) In the following positional isomers i.e., ortho xylene, meta xylene and para xylene, the relative positions of methyl groups on the benzene ring are different



ortho xylene or 1,2-dimethylbenzene meta xylene or 1,3-dimethylbenzene para xylene or 1,4-dimethylbenzene

FUNCTIONAL ISOMERISM

The **functional isomerism** arises due to presence of different functional groups. The **functional isomers** have the same molecular formula but possess different functional groups.

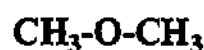
The functional isomers show different physical as well as chemical properties.

E.g.

1) The dimethyl ether is the functional isomer of ethyl alcohol. Both have the same molecular formula, C_2H_6O . However they have different functional groups.



ethyl alcohol

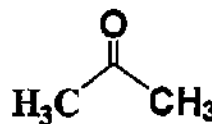


dimethyl ether

2) Acetaldehyde is a functional isomer of acetone. They have the same molecular formula, C_3H_6O but different functional groups. Acetaldehyde contains aldehyde, $-CHO$ functional group, whereas acetone has ketone, $>C=O$ functional group.



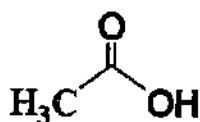
acetaldehyde
or propanal



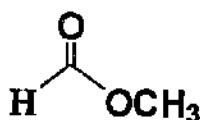
acetone
or propan-2-one

3) Both Acetic acid and methyl formate are also functional isomers. They have the same molecular formula, $C_2H_4O_2$.

Acetic acid is a carboxylic acid with -COOH group whereas methyl formate is an ester with -COOCH_3 group.



acetic acid



methyl formate

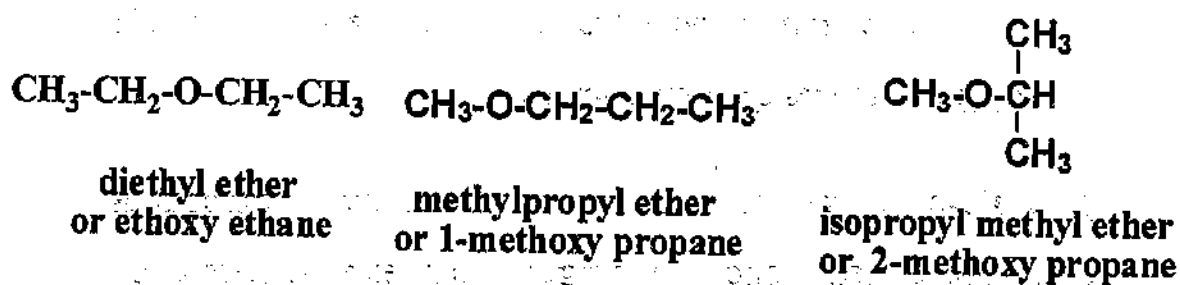
METAMERISM

The **metamerism** arises when different alkyl groups are attached to same functional group.

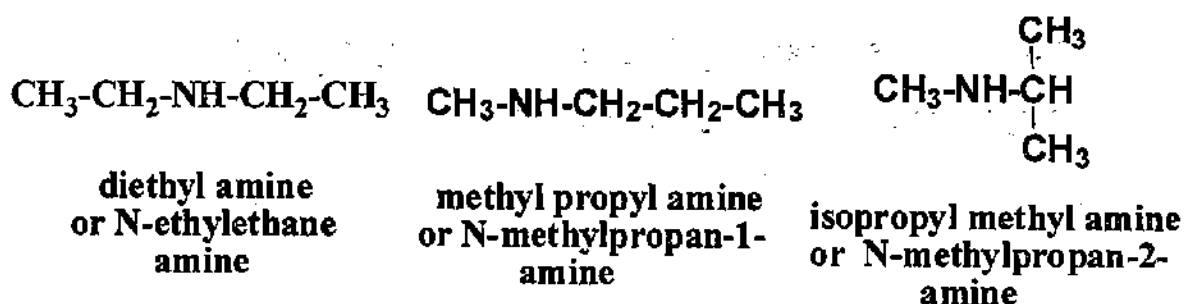
E.g.

1) The following metamers contain the ether functional group.

However they differ by the nature of alkyl groups attached to the oxygen atom.



2) The metamerism is also possible in amines as shown below.



TAUTOMERISM

Tautomerism refers to the dynamic equilibrium between two compounds with same molecular formula. It is also called as desmotropism or kryptotropism or prototropy or allelotropism.

It is most often a special case of functional group isomerism. In general, the **tautomers** have different functional groups and exist in dynamic equilibrium with each other due to a rapid interconversion from one form to another.

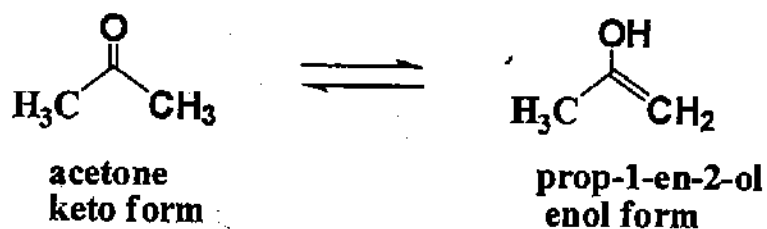
It is very important to note that the tautomers are not the resonance structures of same compound.

1) **Keto-enol tautomerism:** The carbonyl compounds containing at least one α -hydrogen atom exhibit keto-enol tautomerism. The carbonyl group can be converted to enol form due to transfer of one of the α -hydrogen onto the oxygen atom.

Note: An alcoholic group on C=C is called enol. It is an alkene alcohol.

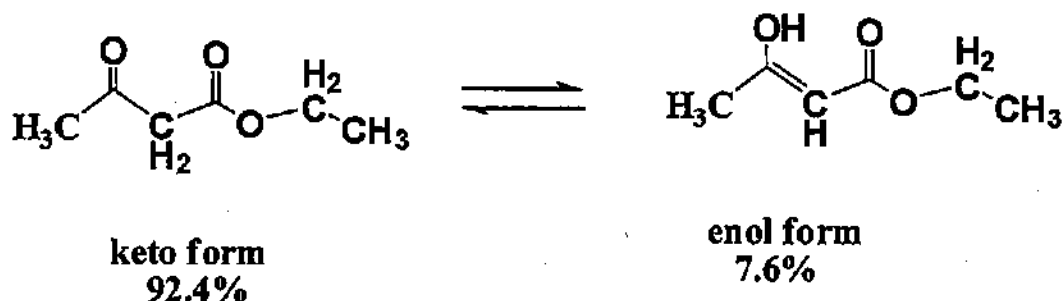
The % composition of keto enol tautomeric mixture depends on the relative stabilities of these two forms. In general the keto form is the low energy form and is more stable than the enol form. However the enol form is also stable in certain cases due to other stability factors.

The dynamic equilibrium between a keto form and an enol form exhibited by acetone is shown below. The tautomers are formed due to complete transfer of hydrogen. However the relatively stable keto form exists in higher percentage (about 99%).

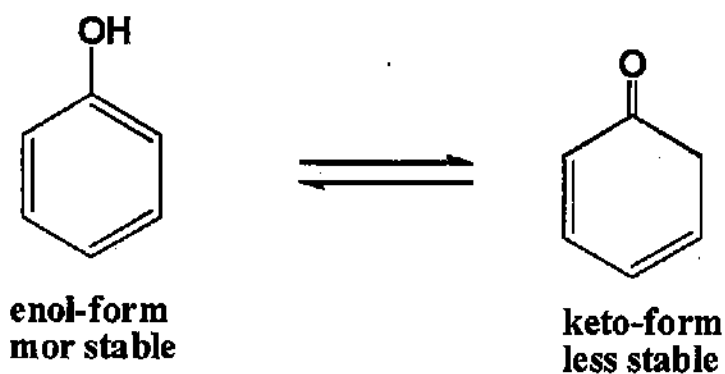


However enol form is also appreciably stable in case of 1,3-dicarbonyl compounds like acetoacetic ester (ethyl aceto acetic ester) as depicted below.

keto-enol form tautomerism in acetic acid ester

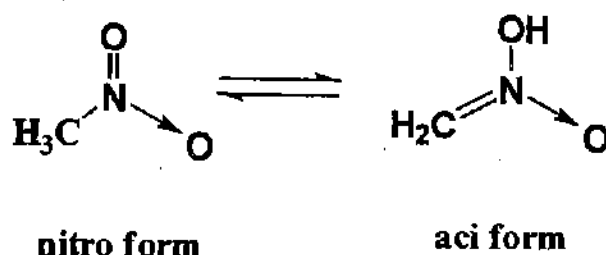


The enol form is more stable than the keto form in case of phenols due to resonance stabilization of aromatic ring.



2) **The nitro-aci tautomerism:** It is exhibited by nitro compounds containing atleast one α -hydrogen. In this case also, the hydrogen atom is transferred completely from one atom to another during the conversion of nitro form to aci form and vice versa.

e.g. The nitro-aci tautomerism exhibited by nitromethane is shown below.



STEREoisomerism in Organic Compounds

The isomerism which arises due to different spatial arrangements of atoms or groups is called stereo isomerism. It is broadly divided into:

- Geometrical isomerism

The stereo isomers have same structural formula i.e., same connectivity order between atoms. However the atoms or groups are arranged differently in space.

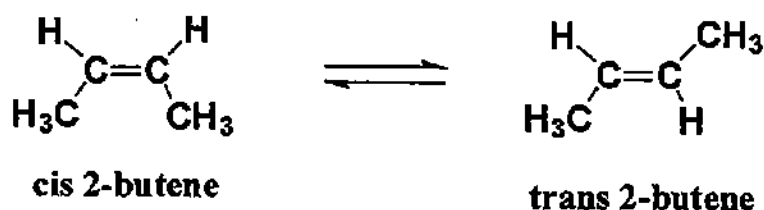
GEOMETRICAL ISOMERISM

The geometrical isomerism arises when atoms or groups are arranged differently in space due to restricted rotation of a bond or bonds in a molecule.

E.g.

1) Two different spatial arrangements of methyl groups about a double bond in 2-butene give rise to the following geometrical isomers.

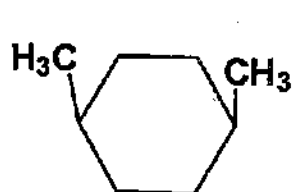
i.e., cis-2-butene and trans-2-butene



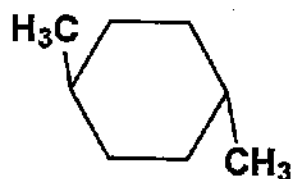
Above two forms are not inter convertible due to restricted rotation of double bond.

In the cis isomer, the two methyl groups are arranged on the same side of a double bond. Whereas in the trans isomer, they are on the opposite side.

2) There are two geometrical isomers (cis & trans) possible in case of 1,4-dimethylcyclohexane as shown below:



cis 1,4dimethylcyclohexane



trans 1,4dimethylcyclohexane

In the above geometrical isomers, the methyl groups are arranged differently about the plane of the cyclohexane ring. These isomers are not inter convertible since it is not possible to rotate the bonds in the cyclohexane ring.

* The geometrical isomers often show different physical and chemical properties. The difference in their physical properties is more significant when there is more difference in their polarity.

* Usually the dipole moment of cis-isomers is greater than that of trans isomers. Hence the cis isomers usually have more solubility in polar solvents.

* In general, the trans isomers are more stable than cis isomers.

ORBITAL PICTURE OF BONDING: ORBITAL COMBINATIONS, HYBRIDIZATION THEORY, & MOLECULAR ORBITALS

LEARNING OBJECTIVES

To introduce the basic principles of molecular orbital theory and electronic geometry of molecules.

ORBITAL COMBINATIONS

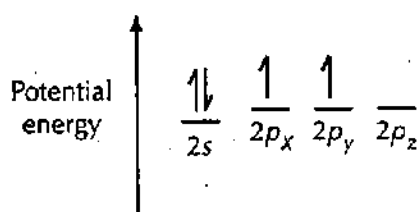
Atomic orbitals can be combined and reshaped—much like dough—to make other orbitals of different shapes and properties. There are two basic types of orbitals that can result from such processes. They are:

1. HYBRID ORBITALS. They result from combinations of orbitals **within** a given atom, either prior to or as bonding with another atom takes place.

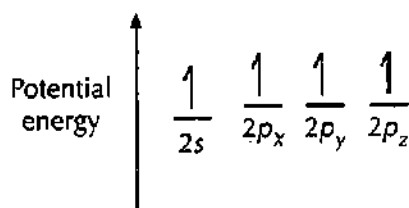
2. MOLECULAR ORBITALS. They result from combinations of orbitals **between** atoms as bonding takes place to form molecules.

ORBITAL HYBRIDIZATION THEORY

If we look at the valence shell configuration of carbon, we find two paired electrons in the $2s$ orbital, and two unpaired electrons in the $2p_x$ and $2p_y$ orbitals, one in each:



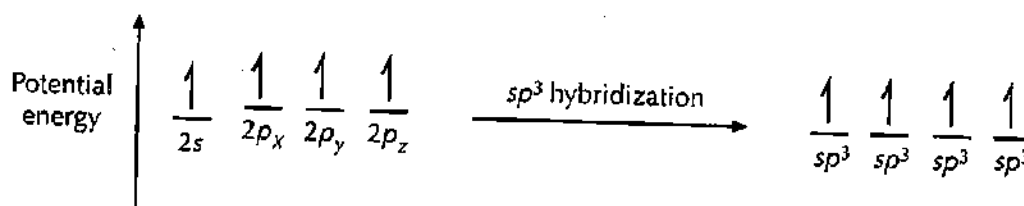
In order to fulfill the octet rule, carbon must use its 4 valence electrons when bonding to other atoms. However, only unpaired electrons can bond. That means that **the two paired electrons occupying the $2s$ orbital must become unpaired before they can bond**. Since the energy gap between the $2s$ and $2p$ orbitals is very small, one of the $2s$ electrons can be promoted to the empty $2p$ orbital, leading to the following situation:



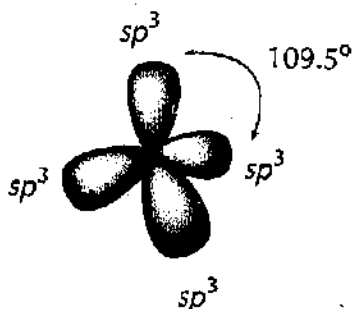
Now the four electrons appear to be ready for bonding, but there is a problem. The $2p$ orbitals are known to be at right angles to each other. If bonding occurs in this state, the 3 equivalent p electrons would form 3 equivalent bonds oriented at 90° to each other, and the s electron would form a bond of a different type and orientation from the other three. No such compound exists. The simplest hydrocarbon—methane (CH_4)—is known to have tetrahedral geometry, where the four C–H bonds are all equivalent and positioned at 109.5° angles to each other. In addition, there are some carbon compounds where the bond angles are 120° or even 180° . **The shapes and relative positions of the valence orbitals in atomic carbon do not explain the shapes and relative positions of the bonds in carbon compounds.**

HYBRIDIZATION THEORY ATTEMPTS TO EXPLAIN THE ACTUAL SHAPES OF MOLECULES BY INVOKING THE FORMATION OF HYBRID ORBITALS DURING, OR PRIOR TO, THE BONDING PROCESS.

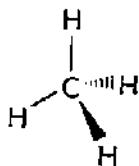
Going back to the carbon model with four unpaired electrons in the valence shell, we can take it as a point of departure for formation of hybrid orbitals. The first step is to take either 2, 3, or all four of those orbitals and equalize their energies. Let's say that we take all four of them and form 4 equivalent new orbitals. These orbitals are now of the same energy, which is intermediate between those of the original 2s and 2p orbitals. At the same time, we cannot name the new orbitals s or p, for they're neither. We have to find a new name that reflects the fact that they were created from **one s orbital and three p orbitals**. We will call them **sp³ orbitals**. The process that leads to their formation is called **sp³ hybridization**.



All four sp³ orbitals that result from this process are **equivalent**. That means that they have **the same size, shape, and energy**. According to VSEPR (valence shell electron pair repulsion) theory, such orbitals will orient themselves in 3-D space **to be as far apart from each other as possible**. The resulting shape is then a tetrahedron, where the carbon nucleus is at the center and the orbitals point to the corners of the tetrahedron. The ideal angle between orbitals is then 109.5 degrees.



When an sp³ hybridized carbon bonds to hydrogen, it forms methane, whose geometry is known to be tetrahedral.



A 3-D representation of methane. The single lines represent bonds that are positioned on the plane of the paper. The solid wedge represents a bond coming out of the plane of the paper towards the front. The broken wedge represents a bond going behind the plane of the paper towards the back.

HYDROCARBONS

Hydrocarbons are substances containing only carbon and hydrogen. Hydrocarbons are classified into the following major categories: **alkanes**, **alkenes**, **alkynes**, and **aromatic hydrocarbons**. In the following pages we will do an overview of the basic characteristics of the first three, but will postpone the study of aromatics until later.

ALKANES AND sp^3 HYBRIDIZATION OF CARBON

Alkanes are hydrocarbons where all the carbon atoms are sp^3 -hybridized, all bonds are single bonds, and all carbons are tetrahedral. Methane is the simplest alkane, followed by ethane, propane, butane, etc. The carbon chain constitutes the basic skeleton of alkanes. Carbon chains with four or more atoms can be linear or branched. Some examples are shown below including Lewis, molecular, and condensed formulas. Refer to chapter 2 of the Wade textbook for additional examples.

Linear alkanes

$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$	$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \end{array}$	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array}$
methane	ethane	propane	butane
CH_4	C_2H_6	C_3H_8	C_4H_{10}
CH_4	CH_3CH_3	$\text{CH}_3\text{CH}_2\text{CH}_3$	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$
CH_4	CH_3-CH_3	$\text{CH}_3-\text{CH}_2-\text{CH}_3$	$\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}_3$

Some examples of branched alkanes are shown below. Notice that sometimes Lewis formulas become cumbersome and difficult to write without cluttering. Condensed formulas are more convenient to use in such situations.

Branched alkanes

$\begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C}-\text{C}-\text{CH}_3 \\ \\ \text{H} \end{array}$	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{CH}-\text{CH}_2-\text{CH}_3 \end{array}$	$\begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C}-\text{C}-\text{CH}_3 \\ \\ \text{CH}_3 \end{array}$
isobutane	isopentane	neopentane
C_4H_{10}	C_5H_{12}	C_5H_{12}
$(\text{CH}_3)_3\text{CH}$	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$	$(\text{CH}_3)_4\text{C}$

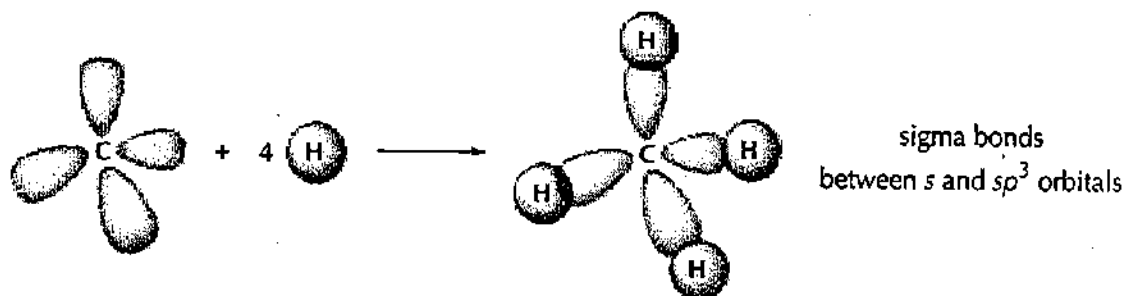
As can be seen from the above examples, all alkanes have the general formula $\text{C}_n\text{H}_{2n+2}$ where n is the total number of carbon atoms. This holds regardless of whether the alkane is linear or branched.

SIGMA BONDING

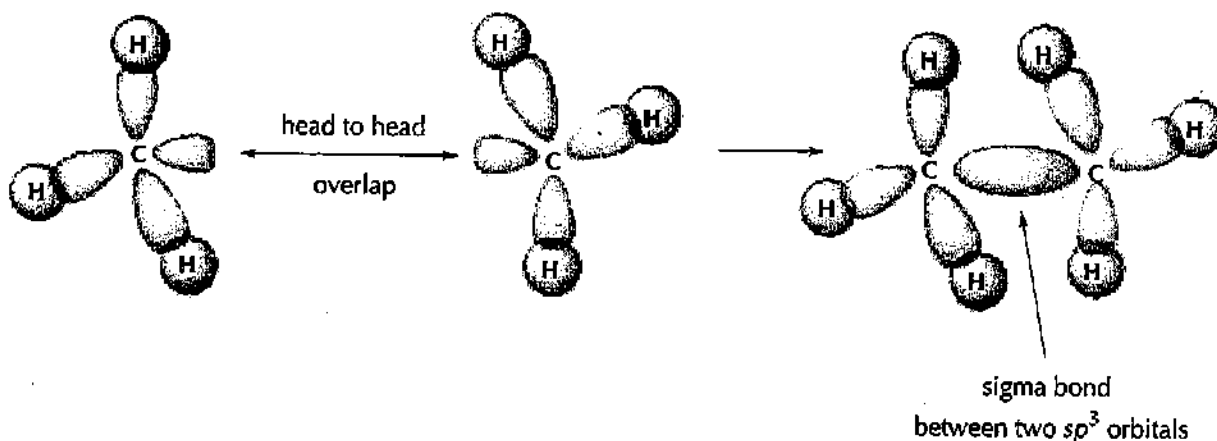
When atomic orbitals (pure or hybrid) of different atoms overlap to form covalent bonds, they may approach each other in two major ways: **head to head**, or **sideways**. Only head to head overlap is possible with *s*-orbitals because they are spherical. Hybrid orbitals also undergo mostly head to head overlap when forming covalent bonds. *p*-orbitals, on the other hand, can approach each other either sideways or head to head. For now, however, we are concerned only with head to head overlap because that's the only type that occurs in alkanes. We'll discuss sideways overlap later in connection with alkenes and alkynes, that is, hydrocarbons that have double and triple bonds respectively.

When orbitals approach each other in a head to head fashion, the resulting covalent bonds are called sigma bonds.

As illustrations, consider the bonds that have already been studied. The bond between two hydrogen atoms is an example of sigma bonding. The bonds between the sp^3 orbitals of hybridized carbon and the *s* orbitals of hydrogen in methane are also example of sigma bonds.



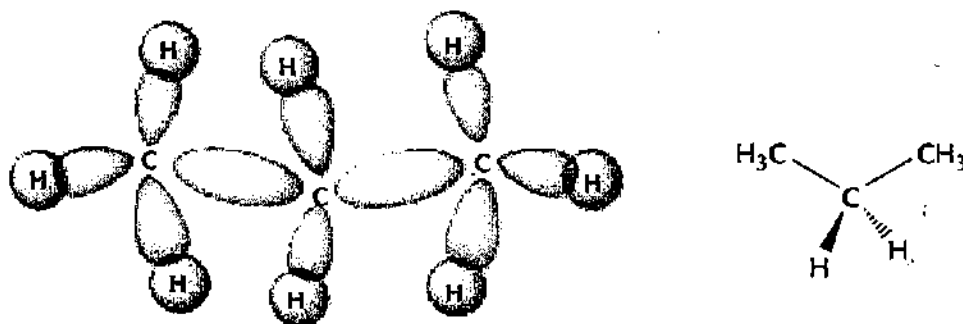
Two sp^3 carbons can also overlap to form a C-C sigma bond where two sp^3 orbitals overlap head to head, such as in the formation of the ethane molecule:



It can be easily seen that the only type of covalent bonds present in alkanes are sigma bonds, also loosely known as single bonds.

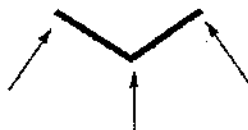
LINE-ANGLE FORMULAS

In alkanes of 3 carbon atoms or more, the main carbon chain acquires a zig-zag structure due to the 109.5° angle between C–C bonds, such as in propane:



Two representations of propane, where the zig-zag structure of the carbon chain becomes apparent

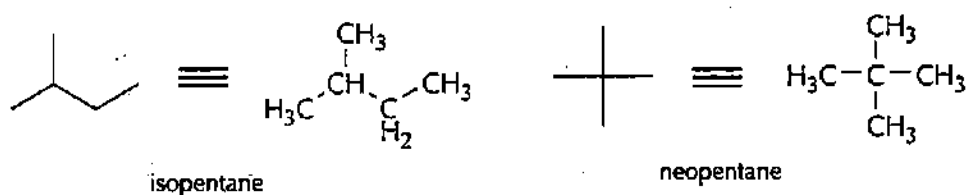
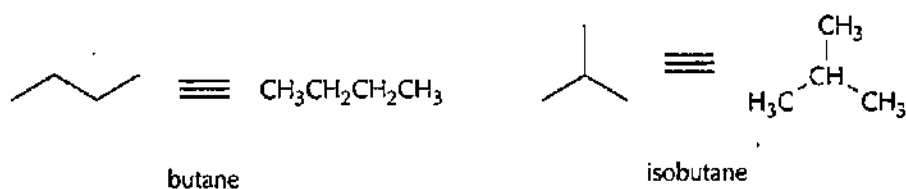
Writing Lewis formulas, or even condensed formulas, for alkanes of many carbon atoms can quickly become cumbersome. A short hand notation that uses zig-zag lines has been developed. The resulting representations are known as **line-angle formulas**. The beginning and the end of the zig-zag line, as well as any breaks in direction represent carbon atoms.



Line angle representation for propane equivalent to $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_3$ or $\text{CH}_3\text{CH}_2\text{CH}_3$

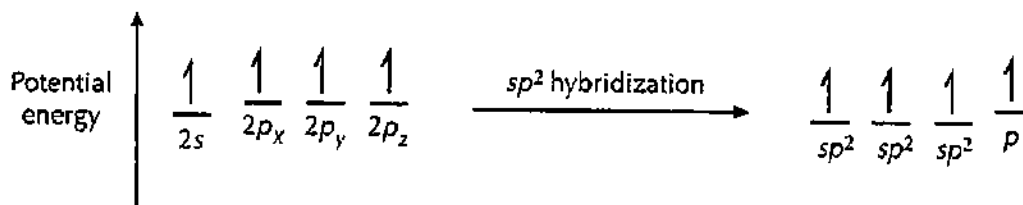
The arrows point to the positions of the carbon atoms.

Every carbon atom has to form 4 bonds. **The bonds that are not shown are assumed to be bonds to hydrogen.** Other examples are:

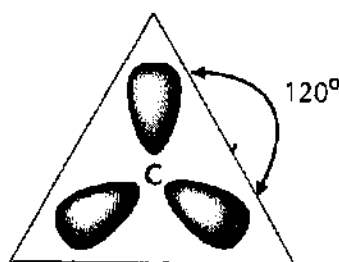


ALKENES AND sp^2 HYBRIDIZATION OF CARBON

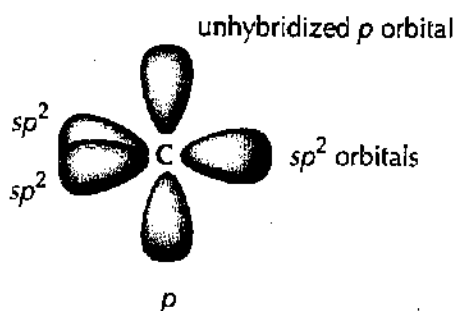
We will now reproduce the sp^3 hybridization process for carbon, but instead of taking one s and three p orbitals to make four equivalent sp^3 orbitals, this time we'll take only **one s and two p orbitals to make three equivalent sp^2 orbitals, leaving one p orbital untouched**. The process is shown below.



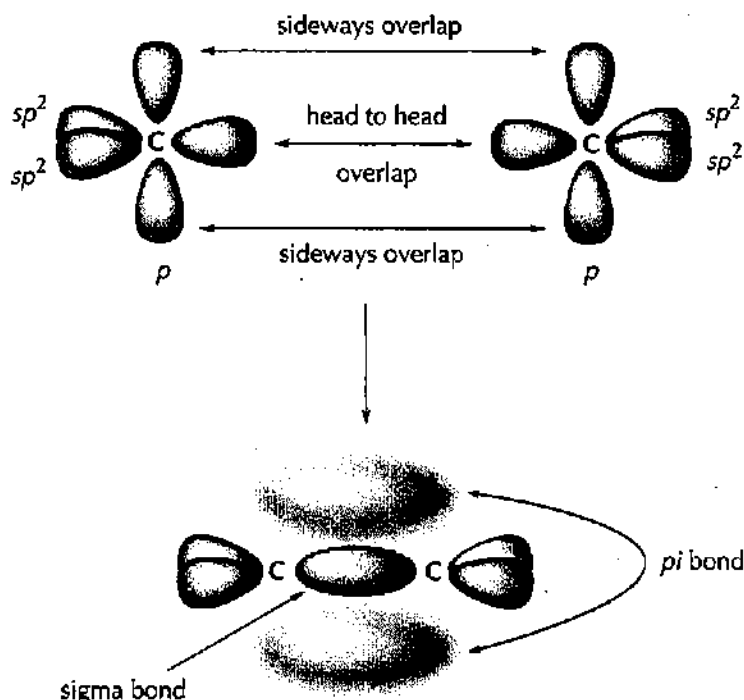
As shown, the three resulting sp^2 orbitals are equivalent in energy, but the remaining p orbital has not been affected. It still retains its original energy and shape. Again, according to VSEPR theory, equivalent orbitals will arrange themselves in 3-D space to be as far apart from each other as possible. Therefore, the three equivalent sp^2 orbitals will arrange themselves in a **trigonal planar** configuration. That is to say, the carbon nucleus will be at the center of an equilateral triangle, and the three sp^2 orbitals will point to the corners of that triangle. **The ideal angle between sp^2 orbitals is therefore 120°** . A top view of this arrangement is shown below.



In this top view, the **unhybridized p orbital** cannot be seen because it also arranges itself to be as far apart from the sp^2 orbitals as possible. That is to say, it is **positioned at right angles to those orbitals**, with one lobe coming out of the plane of the page and the other going behind the page. To see this arrangement clearly, we must switch to a **side view** of the orbital system.



When two sp^2 hybridized carbon atoms approach each other to bond, two sp^2 orbitals approach each other head to head, and two p orbitals approach each other sideways. The bond formed by the sp^2 orbitals is a sigma bond, and the bond formed by the p orbitals is called a **pi bond**. The process is shown below.

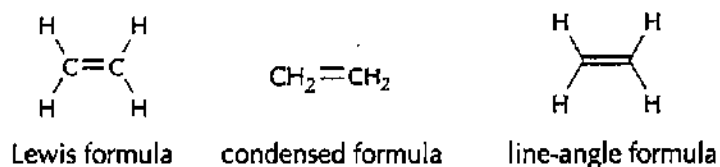


The illustration above tries to convey a basic feature of the π bond as compared to the sigma bond. The sigma bond is short and strong. As a rule, **head to head overlap is the most efficient way to bond and results in relatively strong and stable bonds**. The π bond, on the other hand, is relatively long and diffuse. **Sideways overlap is less efficient than head to head overlap and results in formation of weaker bonds**.

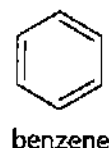
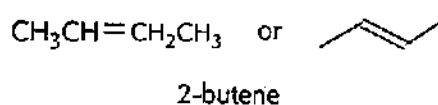
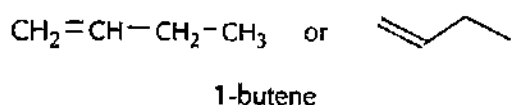
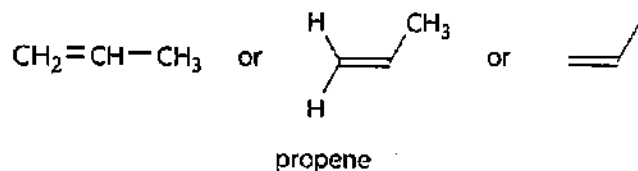
This has some implications in the properties and chemical reactivity of sigma and π bonds. The electrons in the sigma bond (or sigma electrons) are more tightly bound to the nucleus and don't move too much. In other words, they are more **LOCALIZED**. The electrons in the π bond (or π electrons) are less tightly bound by the nucleus, and therefore **they are relatively mobile**. Under certain conditions, they have the capability to become **DELOCALIZED**, that is to say, they can move in the molecular skeleton from one atom to another, or even become spread over several atoms, according to principles we'll study later.

At the same time, in chemical reactions where electrons are to be traded, **the π electrons are more readily available because they are more exposed and less tightly bound by the nucleus**. It is relatively easy to break a π bond compared to the sigma bond. The principles of all this chemistry will be discussed later in the course.

ALKENES ARE HYDROCARBONS THAT CONTAIN AT LEAST ONE π BOND AS PART OF THEIR MOLECULAR STRUCTURE. By this definition, the simplest possible alkene must contain two carbon atoms. It is called **ethene**. Below is a Lewis and a line-angle representation of ethene, which is sometimes informally called **ethylene**. Notice that although C-H bonds are not usually shown in line-angle formulas, sometimes they are included for enhanced clarity. In this case a pure line-angle formula for ethene would look awkward because it would resemble an equal sign (=).



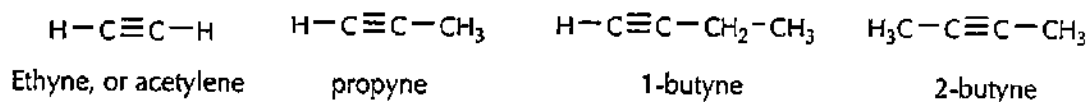
Notice that a Lewis representation does not differentiate between the sigma and the pi bonds in the so-called "double bond." It simply shows the two together as two equal dashes. The orbital picture better represents the actual nature of the two types of bonds. Additional examples are shown below. For a full discussion of the structure of alkenes refer to chapter 7 of the Wade textbook.



Observe that the general formula for open chain monoalkenes—that is, alkenes that do not form cyclic structures and which contain only one pi bond—is C_nH_{2n} where n is the total number of carbon atoms.

ALKYNES AND sp HYBRIDIZATION OF CARBON

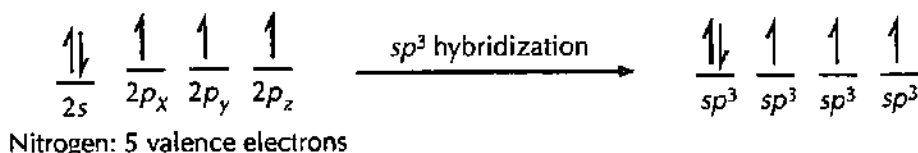
The process for understanding the sp hybridization process for carbon is basically an extension of the other two types (sp^3 and sp^2). You should try to work out this scheme on your own and see if your predictions agree with those presented in the textbook. sp hybridization gives rise to the formation of hydrocarbons known as alkynes. Alkynes contain at least one triple bond, and have linear geometry around the carbons comprising the triple bond. Therefore, the ideal angle between the sp hybrid orbitals is 180° . Some examples of alkynes are shown below. For additional information refer to chapter 9 of the Wade textbook.



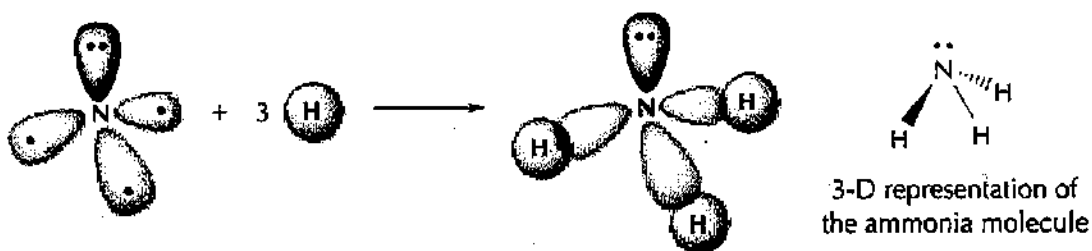
Observe that the general formula for open chain monoalkynes is $\text{C}_n\text{H}_{2n-2}$ where n is the total number of carbon atoms.

ORBITAL HYBRIDIZATION IN NITROGEN AND OXYGEN

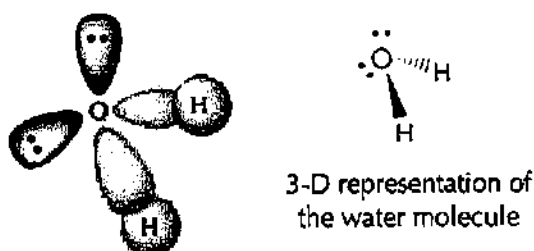
The hybridization schemes for nitrogen and oxygen follow the same guidelines as for carbon. For example, sp^3 hybridization for nitrogen results in formation of four equivalent sp^3 orbitals, except that this time only three of them contain unpaired electrons, and one of them contains paired electrons. A similar situation holds true for oxygen, which ends up with two of the sp^3 orbitals occupied with unpaired electrons, and the other two with paired electrons.



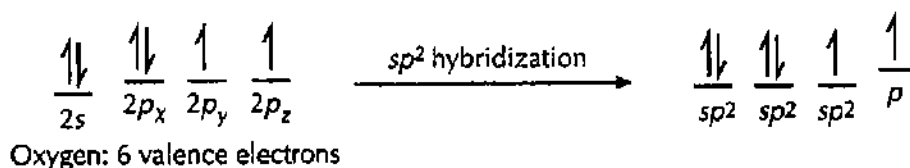
The four sp^3 orbitals again orient themselves in 3-D space to be as far apart from each other as possible, but the ideal 109.5° angle becomes distorted because the orbital with two electrons repels the others more strongly than they repel themselves. However the geometry of this arrangement is still fundamentally tetrahedral. When this sp^3 hybridized nitrogen bonds to hydrogen, the three unpaired electrons are used for bonding, and the remaining pair remains as nonbonding electrons.



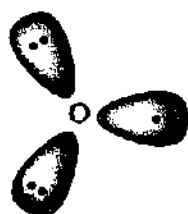
A similar analysis for oxygen should lead to formation of two sp^3 orbitals with unpaired electrons, and two with paired electrons. Thus, when sp^3 oxygen bonds with hydrogen it forms water, which has a distorted tetrahedral angle, and two pairs of nonbonding electrons in the structure.



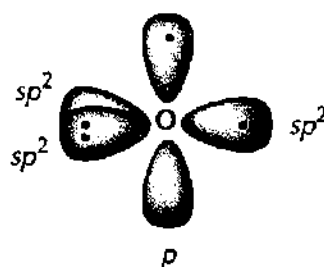
Now, what happens when nitrogen or oxygen become sp^2 hybridized? The exact same thing that happened with carbon, with some minor changes. Let's go through the process with oxygen to illustrate how it bonds to carbon to make a class of substances known as carbonyl compounds.



Three equivalent sp^2 orbitals have formed, two of them containing paired electrons, and one containing a single unpaired electron. The unhybridized p orbital remains, with an unpaired electron in it. Again, VSEPR theory dictates that the three equivalent sp^2 orbitals will acquire a trigonal planar arrangement, while the unhybridized p orbital will remain at right angles to the sp^2 orbitals.

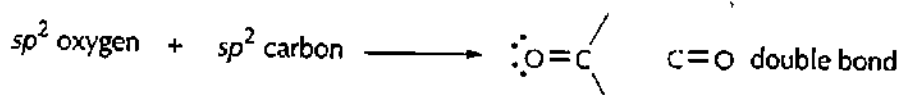
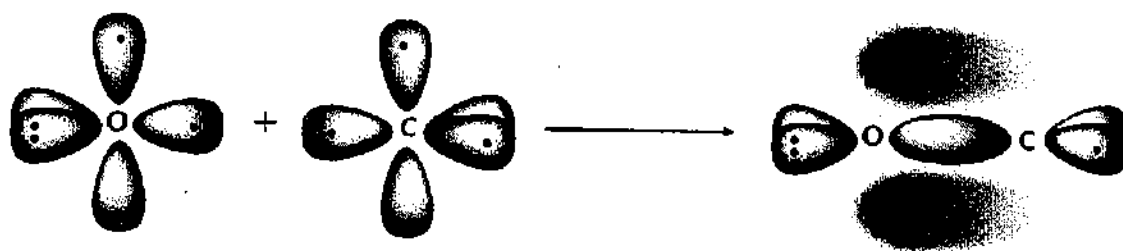


sp^2 oxygen, top view

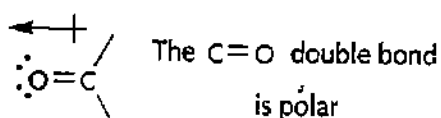


sp^2 oxygen, side view

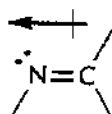
When an sp^2 oxygen approaches an sp^2 carbon for bonding, the process is analogous to that followed by two sp^2 carbons that bond to form a "double bond." Only those orbitals containing unpaired electrons can bond. In this case, the sp^2 orbitals from oxygen and carbon that contain unpaired electrons will overlap head to head to form a sigma bond. At the same time, the p orbitals will overlap sideways to form a pi bond. Thus, we have the effective formation of a $C=O$ "double bond."



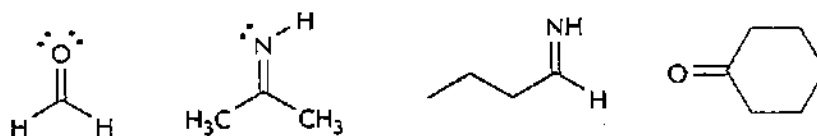
Notice that the π bond in the $C=O$ "double bond" appears distorted, indicating higher electron density around the oxygen than around the carbon. This is because the $C=O$ bond is polar. The more electronegative oxygen atom attracts bonding electrons towards itself more strongly than carbon.



A similar analysis for nitrogen leads to the picture and geometry of a $C=N$ double bond:



Some examples of compounds containing sp^2 carbon, nitrogen, and oxygen are shown below. Notice that Lewis and line-angle formulas frequently neglect showing the lone pairs of electrons. Unless there is a specific purpose for showing nonbonding electrons, they are usually omitted and assumed to be present.



By going through an analogous process for sp hybridization of nitrogen and oxygen we can arrive at the molecular structure of species containing carbon-nitrogen and carbon-oxygen triple bonds. Notice that an oxygen containing a triple bond must also carry a positive charge in observance of the rules of covalent bonding.

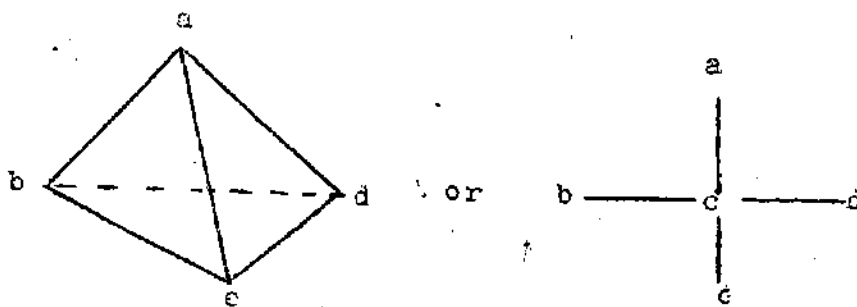


Also notice that when two sp or sp^2 atoms are bonded together to form a double or triple bond, they both must be of the same hybridization. There are some exceptions, but this is true in most common situations.

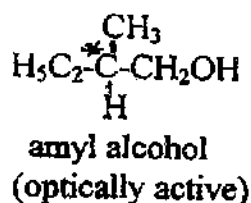
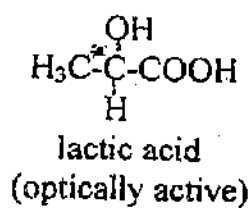
SUMMARY

The preceding discussion covers the most common cases of atom hybridization encountered in this course. The following summarizes the concepts associated with each type of hybridization.

sp^3 hybridization	4 orbitals	tetrahedral geometry	ideal angle: 109.5°	single bonds
sp^2 hybridization	3 orbitals	trigonal planar geometry	ideal angle: 120°	double bonds
sp hybridization	2 orbitals	linear geometry	ideal angle: 180°	triple bonds



An asymmetric carbon in formula is usually indicated by an asterisk (*) placed near it. All organic compounds containing one asymmetric carbon atom (lactic acid, amyl alcohol, etc.) are optically active

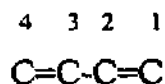


Questions

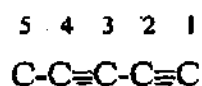
1. Explain what is meant by isomerism. Describe and illustrate the different types of isomerism known to you.
2. Dimethyl ether and ethyl alcohol; n-butane and isobutane are isomeric with one another. What type of isomerism do they exhibit? Explain.
3. Explain the necessary conditions for a molecule to show geometrical isomerism with example.
4. What is optical activity? Discuss briefly the isomeric structures of tartaric and lactic acid.
5. Indicate the types of isomerism exhibited by the following compounds.

$\text{H}(\text{D})\text{C}=\text{C}(\text{D})\text{H}$	$\text{C}_6\text{H}_5\text{CH}(\text{OH})\text{COOH}$
$\text{CH}_3-\text{CH}(\text{OH})-\text{CO}_2\text{H}$	$\text{HOOC}-\text{C}=\text{C}-\text{COOH}$
6. Which of the following compounds can exhibit cis-trans isomerism?

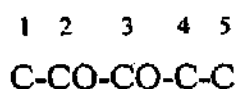
1-pentene	2-pentene	2-methyl-1-pentene
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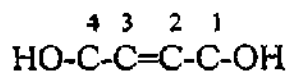
1,3-Butadiene



1,3-Pentadiyne



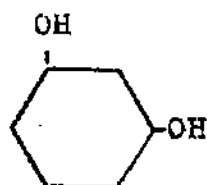
2,3-Pentadione



2-Butyn-1,4-diol



Divinylbenzene



1,3-Cyclohexanediol

QUESTIONS

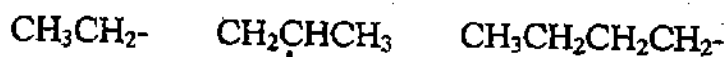
1. Indicate the functional groups in the following compounds:-



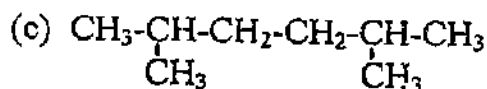
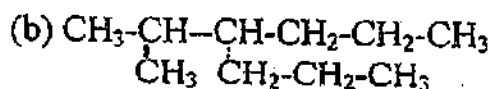
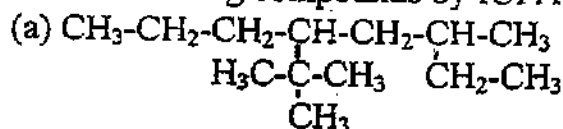
2. What do you understand by a family or class? Write the general formula and functional groups of the following classes of organic compounds:
ethers, thiols, aldehydes, ketones, amides, alcohols.

3. Define the terms: Alkanes, Cycloalkanes and Alkynes. Name a normal hydrocarbon of each type containing six carbons.

4. What are branched alkanes ? Give the IUPAC name of the following structures :



5. Name the following compounds by IUPAC nomenclature :



6. Draw the structure of the compounds:

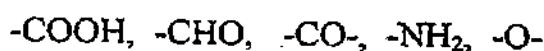
(a) 3-ethyl-4-propyloctane.

(b) 4-ethyl-2-methylhexane.

(c) 2,2-dimethylpentane.

(d) 3-ethyl-2,5-dimethylhexane.

7. What is meant by a Principal function ? Give the priority of the following functions :



8. Write the formulas of the following compounds:

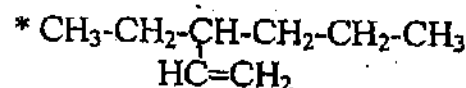
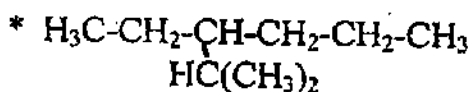
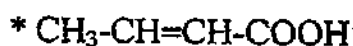
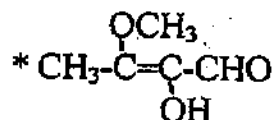
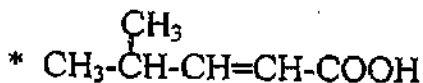
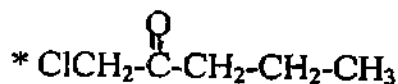
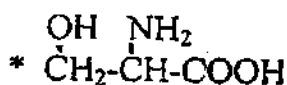
(a) 3-chloro-2-propene.

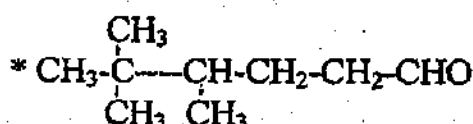
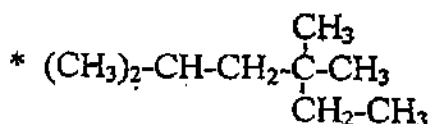
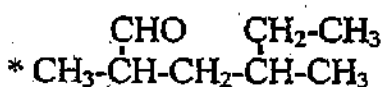
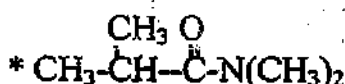
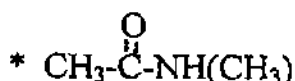
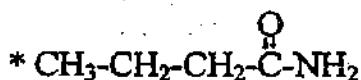
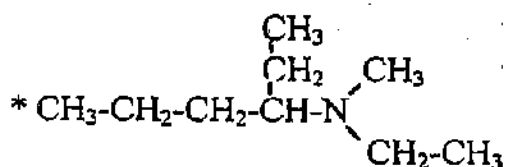
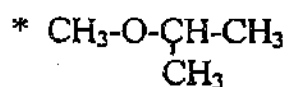
(b) 1-bromo-3-pentanone.

(c) 3,4-dimethylpentanol.

(d) 4-methyl-3-pentyne.

9. Write the IUPAC names for the following :





10. Write the structural formula of the following:

* 2,2-dimethyl-1,4-diethylheptane.

* Pentane-2,4-dione.

* 2,2-dimethyl-1-propanol.

* 4-methyl-1-pentene-2.

* Pent-2,4-dione.

* 3-methyl-2-chlorobutanoic acid

* Butane-2-sulphonic acid.

* 2,5,5-trimethyl-3-hexynoic acid

* 2,4,4-trimethyl-3-isopropyl-1-pentene.

* Methyl-2-chloro-3-cyano-3-hydroxypentanoate.

* 1-hexene-3-yn-5-ol.

* 2-nitro-1,3-propenediol.

* 1-amino-4-methylpentan-2-one

* Pent-3-en-1-oic acid.

* Hepta-1,5-dien-3-ol.

* Isopropyldimethylamine.

* Hex-1-en-4-yne.

* 2-methyl-pent-2-en-1-ol.

* Glycerol.

* Acetyl chloride.

* 4-cyano-3-methoxy-butanoic acid

* 3,5-octadiene.

* 4-chloro-2-isopropyl-3-methyl-cyclopentanone.

* 4-amino-2-ethyl-2-pentanal.

* 2-methyl-3-pentynoic acid

* But-2-yne-1,4-diol.

* Ethyl-3-methoxy-4-nitrobutanoate

* trans-2-pentene.

* cis-2-chlorobutene-2.

* cis-1,2-diphenylethene.

* cis-1,2-dibromocyclopropane.

* 3-methylcyclopentanone.

* 3-methylcyclohexene.

* 3-methyl-1-cyclohexyl-4-pentanol

* Cyclohexanecarboxamide.