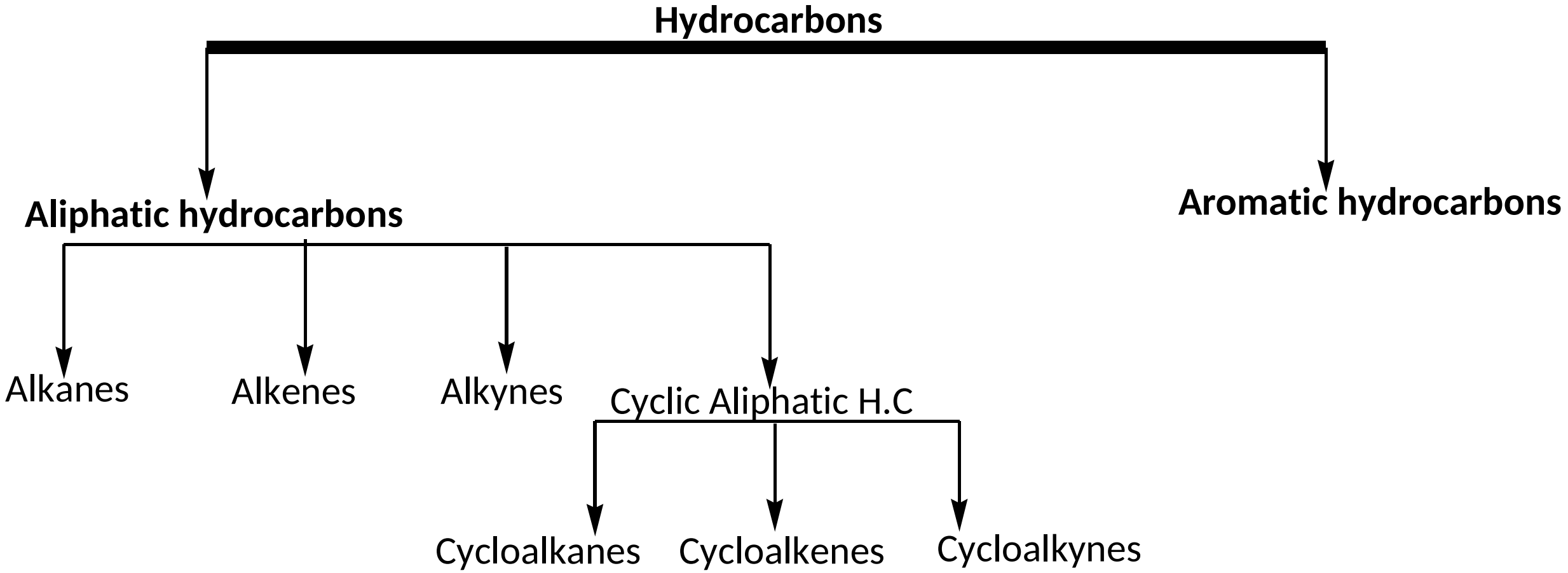
Chapter-9

Nomenclature of organic compounds
Introduction

- ✓ **Organic chemistry** is a branch of chemistry that studies the structure, properties and reactions of **organic compounds**, which contain carbon in covalent bonding and it is as the chemistry of the carbon atom
- ✓ Organic compounds are arranged into classes according to the particular functional groups that they contain and members of each class of compounds share common chemical and physical characteristics
- ✓ The names of organic compounds are assigned according to the class of the compound as determined by the functional groups
- ✓ Organic compounds contains only two elements, hydrogen and carbon, are known as **hydrocarbons**.

Hydrocarbons are classified in to two major parts:

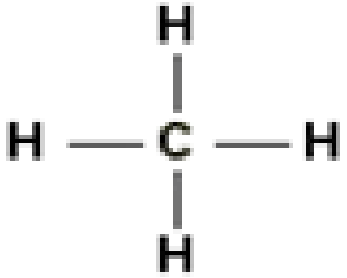


- The main **difference between aliphatic** and **aromatic hydrocarbons** is that **aliphatic hydrocarbons** have a high carbon-to-hydrogen ratio whereas **aromatic hydrocarbons** have a less carbon-to-hydrogen ratio

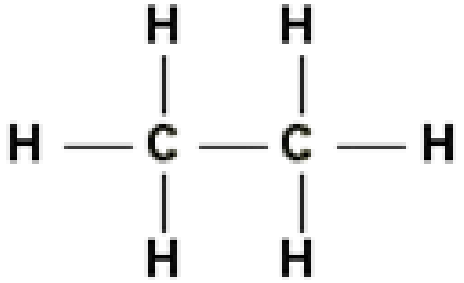
1. Alkanes (Saturated Hydrocarbons)

- Contain carbon-carbon single bond. They are tetrahedral in shape.
- alkanes have a general formula C_nH_{2n+2} (n = 1, 2, 3…), the simplest Alkane is methane.
- Each consecutive member differs only by one – CH_2 group._Thus they form a Homologous series

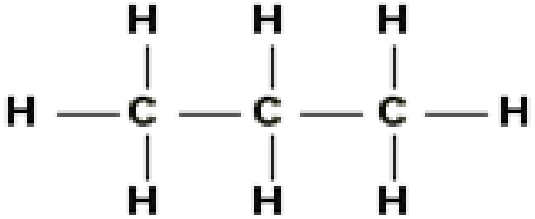
Example:-



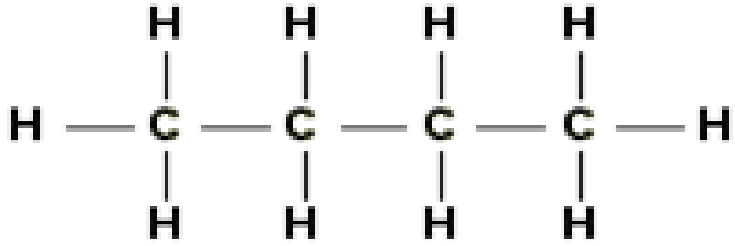
Methane (CH_4)



ethane (C_2H_6)



propane (C_3H_8)



Butane (C_4H_{10})

Nomenclature of Alkanes

- Long chain hydrocarbons can be named by the IUPAC rules.

Rule–1: Find the longest continuous chain atoms in the skeletal structure & name the compound as alkane with this number of carbon atoms.

Rule- 2 : Name the substituents on the chain, substituents derived from alkanes are named by replacing the-ane ending with–yl.

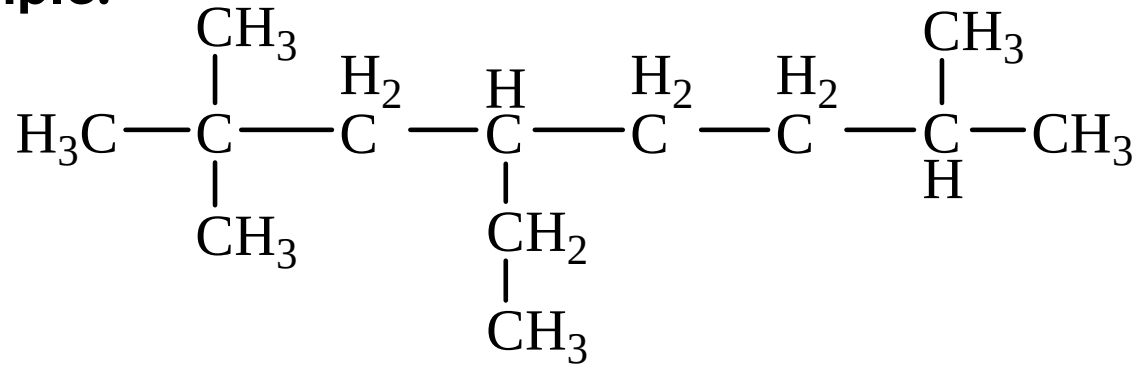
Example: The substituent derived from methane is methyl (CH_3-)

Rule- 3: Number the longest chain starting at the end nearest to the first substitute specify the number of carbon atoms on which the substituents are located

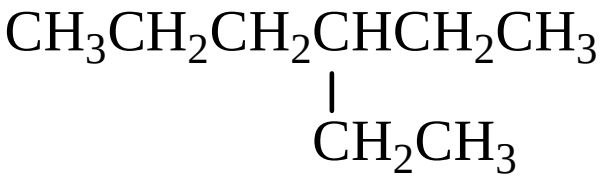
Rule- 4 : Use the prefixes di-,tri-, and tetra- to describe substituents that are found two, three of four times respectively on the same chain.

Rule- 5 : Arrange the names of the substituents in alphabetical order.

Example:-

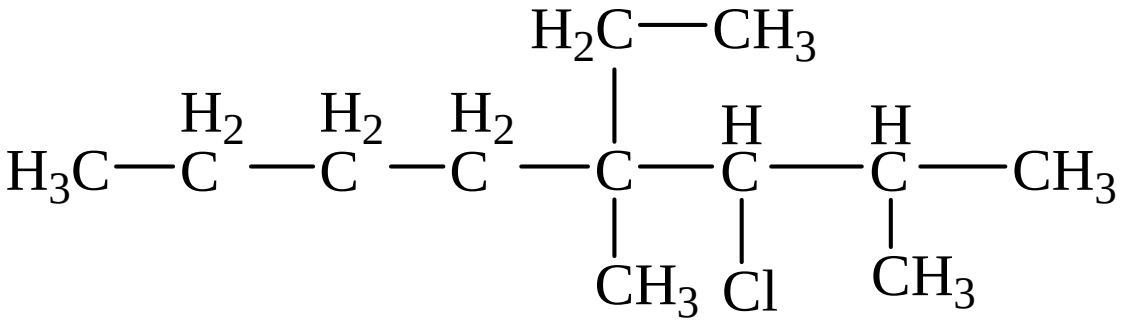


Is named as 4-ethyl- 2,2,7-trimethyl octane

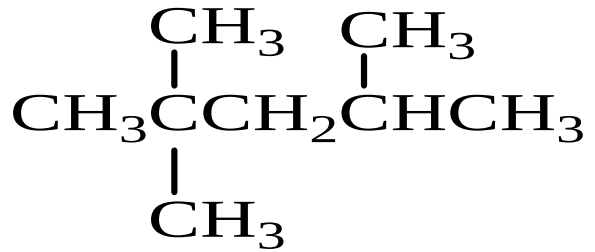


3-ethylhexane

? Write the IUPAC name of the following structure.

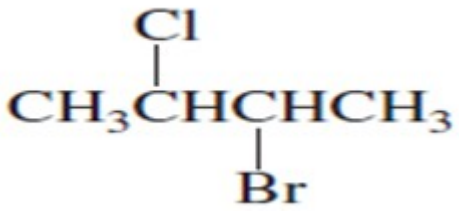


3-chloro-4-ethyl-2,4-dimethyloctane

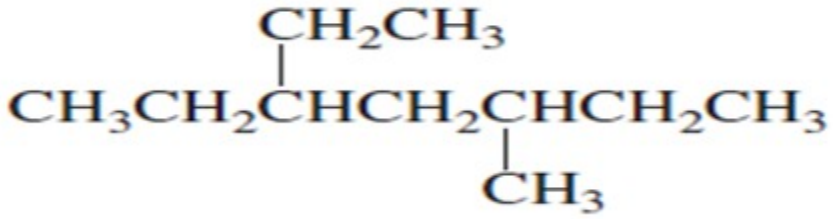


2,2,4-trimethyl pentane

- If the same substituent numbers are obtained in both directions, the first group cited receives the lower number. **Example:-**

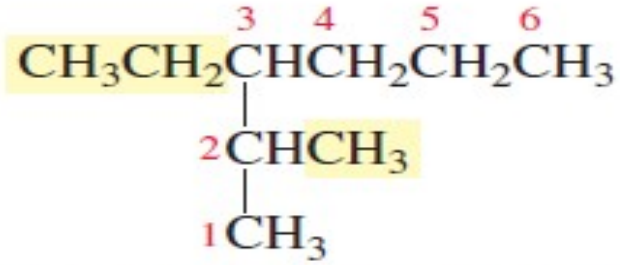


2-bromo-3-chlorobutane
not
3-bromo-2-chlorobutane

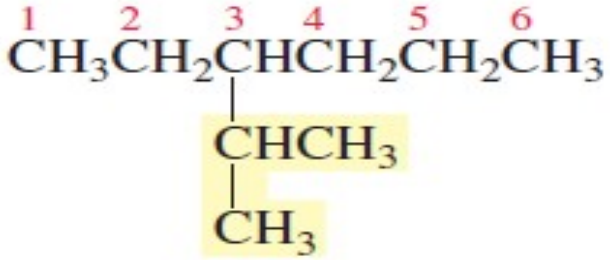


3-ethyl-5-methylheptane
not
5-ethyl-3-methylheptane

- If a compound has two or more chains of the same length, the parent hydrocarbon is the chain with the greatest number of substituents



3-ethyl-2-methylhexane (two substituents)



not
3-isopropylhexane (one substituent)

Properties of alkanes

Physical properties

- ✓ At standard conditions: CH_4 to C_4H_{10} – gases, C_5H_{12} to $C_{17}H_{36}$ -liquids and above $C_{17}H_{36}$ solids
- ✓ **Chemical properties of alkanes**
- ✓ Alkanes are also called **paraffins** which comes from Latin meaning lacking affinity. Therefore, alkanes have **low reactivity**
- ✓ They under go **substitution**, **elimination** and **oxidation** reaction but **inert towards addition** reaction due to their stability.

Isomerism in alkanes

- ✓ Saturated hydro carbons shows structural isomerism.
- ✓ The maximum number of structural isomers of alkane is determined by the general formula of $2^{n-4}+1$, where n is the number of carbon atoms.

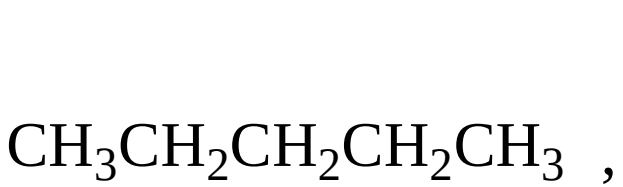
Example : How many isomers does pentane C_5H_{12} have ?

Solution : n=5

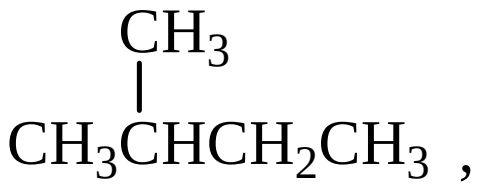
number of isomers = $2^{n-4}+1$

$= 2^{5-4}+1$

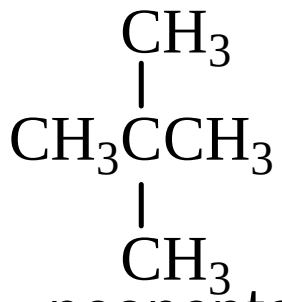
$= 3$



n- Pentane



Isopentane



neopentane

Preparations of alkanes

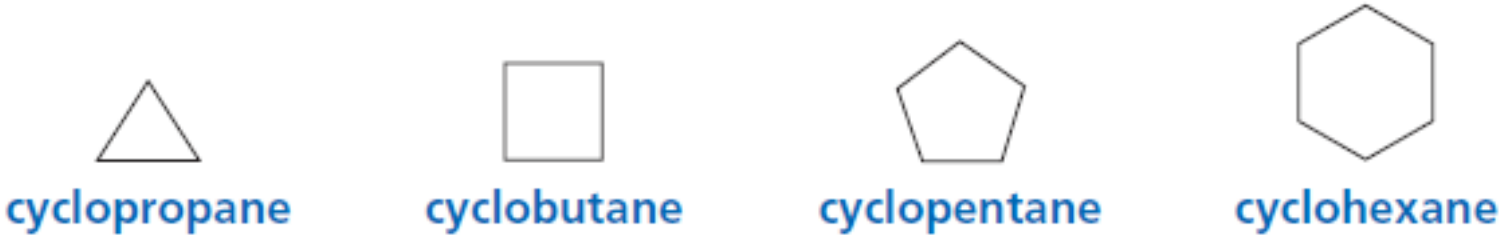
- Alkanes are prepared in the laboratory by decarboxylation of carboxylate salts.



i.e. $RCOONa + NaOH \xrightarrow{heat} R\text{-}H + Na_2CO_3$

carboxylate salt — alkane

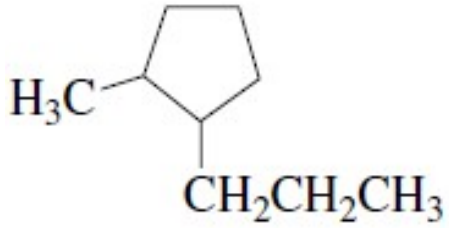
- ✓ **Cycloalkanes** are alkanes with their carbon atoms arranged in a ring. Because of the ring, a cycloalkane has two fewer hydrogens than an acyclic (noncyclic) alkane with the same number of carbons
- ✓ This means that the general molecular formula for a cycloalkane is $\mathbf{C_nH_{2n}}$
- ✓ Cycloalkanes are named by adding the prefix "cyclo" to the alkane name that signifies the number of carbon atoms in the ring



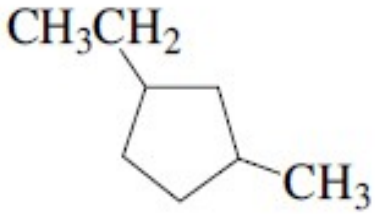
The rules for naming Cycloalkanes resemble the rules for naming acyclic alkanes:

- ➢ In the case of Cycloalkanes with an attached alkyl substituent, the ring is the parent hydrocarbon unless the substituent has more carbon atoms than the ring

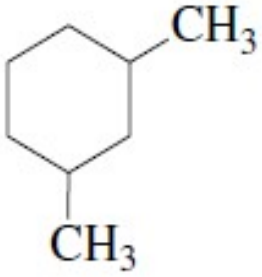
- If the ring has two different substituents, they are cited in alphabetical order and the number 1 position is given to the substituent cited first



1-methyl-2-propylcyclopentane

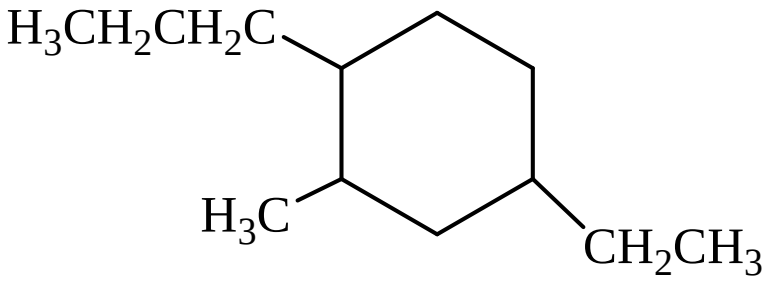


1-ethyl-3-methylcyclopentane

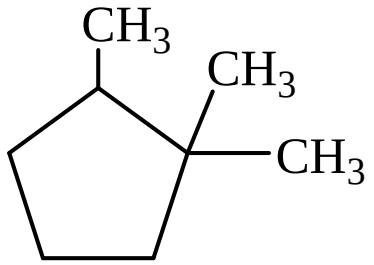


1,3-dimethylcyclohexane

- If there are more than two substituents on the ring, they are cited in alphabetical order
- The substituent given the number 1 position is the one that results in a second substituent getting as low a number as possible



4-ethyl-2-methyl-1-propylcyclohexane



1,1,2-trimethylcyclopentane

2. Nomenclature of unsaturated hydrocarbon

➢The unsaturated hydrocarbons consist of three families of homologous compounds that contain multiple bonds between carbon atoms

- **Alkenes** contain carbon-carbon double bonds
- **Alkynes** contain carbon-carbon triple bonds
- **Aromatic compounds** contain benzene rings

Alkenes:-*olefins* (oil forming).

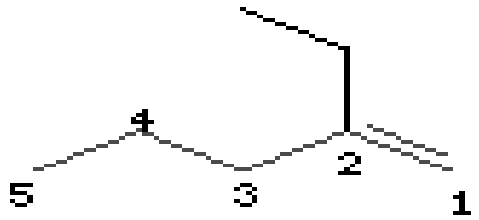
✓have the general formula $\mathbf{C_nH_{2n}}$,$(n>2)$ because, as a result of the carbon–carbon double bond, an alkene has two fewer hydrogens than an alkane with the same number of carbon atoms

✓the general molecular formula for a *cyclic alkene* must be C_nH_{2n-2}

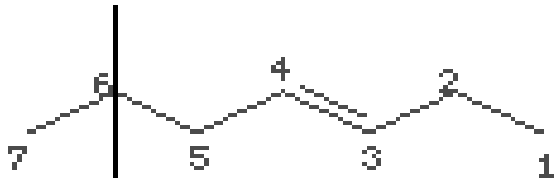
Nomenclature of alkenes

- Find the longest chain containing the double bond(Change the '**ane**' suffix of corresponding alkane in to **ene**).
- Number the chain, giving the double bond the lowest possible number

Example:-

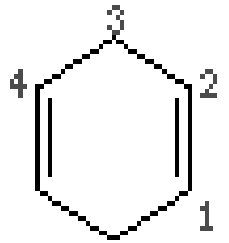


2-ethyl-1-pentene

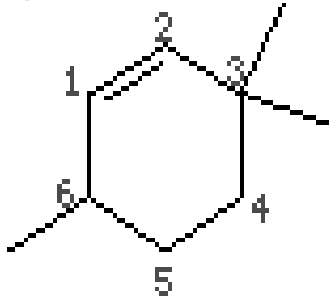


6,6-dimethyl-3-heptene

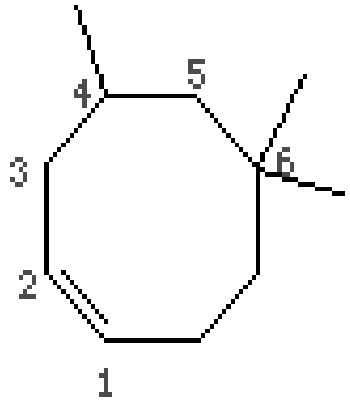
- For **cycloalkenes,** begin numbering at the double bond and proceed through the double bond in the direction to generate the lowest number



1,4-cyclohexadiene

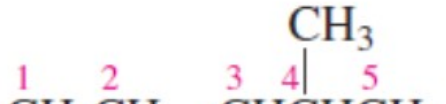


3,3,6-trimethylcyclohexene

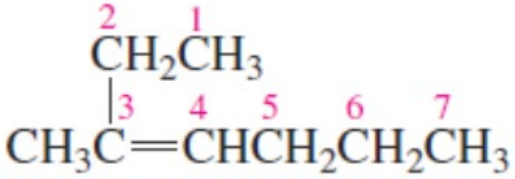


4,6,6-trimethylcyclooctene

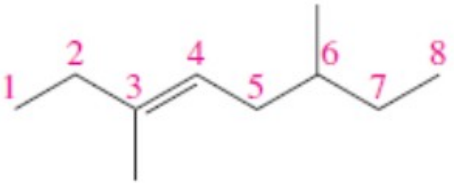
- The systematic (IUPAC) naming of acyclic or straight chain alkene



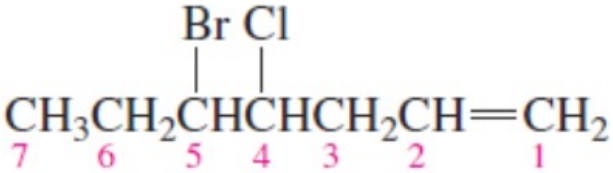
4-methyl-2-pentene



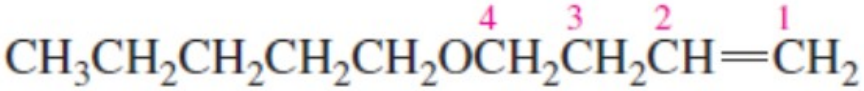
3-methyl-3-heptene



3,6-dimethyl-3-octene

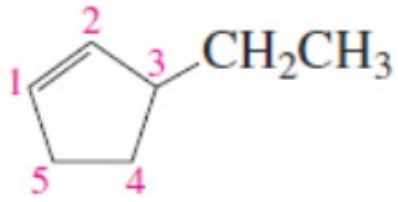


5-bromo-4-chloro-1-heptene

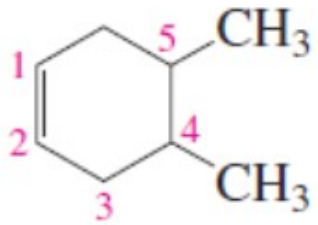


4-pentoxy-1-butene

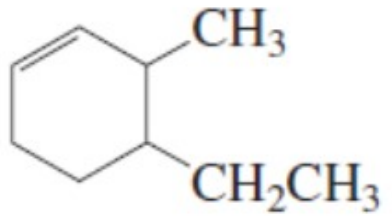
- ✓ In cyclic alkenes, a number is not needed to denote the position of the functional group, because the ring is always numbered so that the double bond is between carbons 1 and 2



3-ethylcyclopentene



4,5-dimethylcyclohexene



4-ethyl-3-methylcyclohexene

Physical Properties of Alkenes

- The first three alkenes are gases, the intermediate alkenes are liquids and higher members of the olefin series are wax like solids at room temperature.
- The alkenes are insoluble in water, but are soluble in organic solvents. The liquids
- solids have a density less than water.

Compound	Formula	MP deg.(℃)	BP deg.(℃)	Density (g/ml)
Ethylene	C_2H_4	-170	-102	0.6128
Propene	C_3H_6	-185	-47	0.6142
1-Butene	C_4H_8	-130	-6.5	0.6356

- Un like alkanes alkenes have geometric isomerism in addition to its position isomerism& constitutional isomerism.
  - ✓ **constitutional (structural) isomerism** is due to substituents.
  - ✓ **position isomerism** is due to the position of the double bond.

Alkenes Preparation

- There are two general methods. Both methods involve the dehydration of alcohol (i.e. the removal of a molecule of water from an alcohol).

$$CH_3CH_2OH \longrightarrow CH_2{=}CH_2 + H_2O$$

1. dehydration of the alcohol using concentrated sulphuric acid as the dehydrating agent (to be used in the laboratory)
2. by passing the vapour of the alcohol over hot alumina (used in the industrial scale preparation of alkenes).

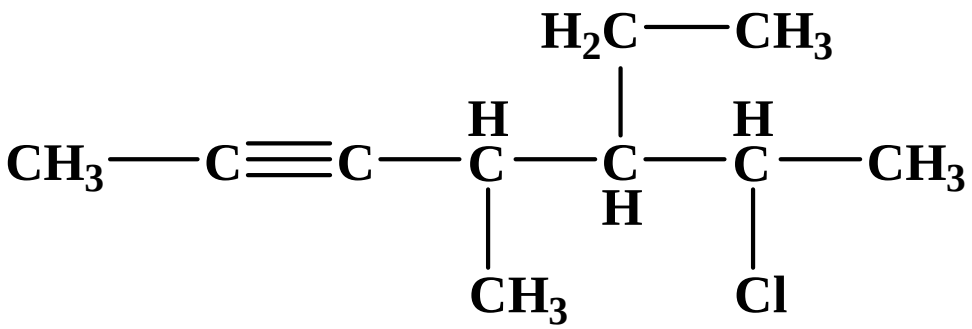
- Have a general form of R–C≡C–R . where R- is alkyl group
- Have the general formula of $\mathbf{C_nH_{2n-2}}$ where n= 2,3,4,.....

Example, C_5H_8- represents

$$H_3C—C\equiv C—CH_2CH_3$$

Nomenclature of Alkynes

- Drop the "ane" ending and add the "yne" ending.
- The rest of the rules are similar with alkanes and alkenes.



6-Chloro-5-ethyl-4-methyl-2-heptyne

Physical Properties of Alkynes

- Alkynes have physical properties that are essentially the same as those of the alkanes and alkenes.
- They are insoluble in water.
- They are quite soluble in the usual organic solvents of low polarity (e.g. ligroin, ether, benzene, carbon tetrachloride, etc.).
- They are less dense than water.
- Their boiling points show the usual increase with increasing carbon number.
- They are very nearly the same as the boiling points of alkanes or alkenes with the same carbon skeletons.

- Dehydrogenation of an alkane or alkene(Fig a)
- Dehalogenation of a tetrahaloalkane (Fig b)
- Dehydrohalogenation of a dihaloalkane (Fig c)

(a) $H_3C-\overset{H_2}{C}-CH_3 \xrightarrow{Pt} H_3C-\underset{H}{C}=CH_2 \xrightarrow{Pt} H_3C-C\equiv CH$

(b) $H_3C-\underset{Cl}{\overset{Cl}{C}}-\underset{Cl}{\overset{Cl}{CH}} + 2\,Zn \xrightarrow{CH_3COOH} H_3C-C\equiv CH + 2\,ZnCl_2$

(c) $H_3C-\underset{Cl}{\overset{H}{C}}-\underset{Cl}{CH_2} + 2\,KOH \xrightarrow{Heat} H_3C-C\equiv CH + 2\,KCl + 2\,H_2O$

❖Compounds like benzene, which have relatively few hydrogens in relation to the number of carbons, are typically found in oils produced by trees and other plants

❖Chemists called such compounds **aromatic** compounds because of their pleasing fragrances.

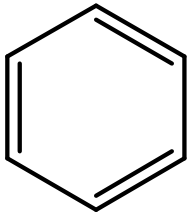
❖To be classified as aromatic, a compound must meet all of the following conditions simultaneously:

✓It is cyclic

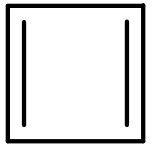
✓It is planar. In general presence of SP^2 hybridized carbon imparts planarity.

✓It exhibits continuous delocalization of π electrons (continuous delocalization is possible if p orbitals are available on each carbon for overlap.

✓It should follow Huckel's rule, also known as magic number, that is, it should have (4n + 2) π number of delocalized electrons where n is ***zero*** or a **whole number**.



Benzene
six pi eletrons (4n + 2)
Aromatic



Cyclobutadiene
4n pi electrons
anti aromatic

Source of aromatic hydrocarbons

❖Destructive distillation of coal at high temperature of 1000^{o}c results in the formation of coal gas, ammonia, and coal tar. Coal tar is rich in aromatic hydrocarbons.

❖Coal is formed naturally by the decomposition of plant matter over several millions of years.

❖Heating mineral coal in the absence of air, or oxygen is called destructive distillation of coal or coking of coal.

Properties of aromatic hydrocarbons

Benzene is colorless liquid with boiling point 80^{o}c.
It is immiscible with water
Due to high carbon it burns with sooty flame
It is used as solvent , however it exhibits carcinogenic properties

5.Alcohols

Alcohols are organic compounds in which a hydrogen of an alkane has been replaced by an OH group. They are classified as **primary**, **secondary**, or **tertiary**, depending on whether the OH group is bonded to a primary, secondary, or tertiary carbon

- Alcohols have a general form of R-OH ; where **R= alkyl group & -OH= functional group**

Alcohols – Nomenclature

1) **Prefix** : Take the alkane name that corresponds to the number of carbon atoms and remove the final ***e*** from the name.

(2) Position number : Count the number of carbon atoms from the nearest chain end to where the hydroxyl group, ***-OH***, is attached.

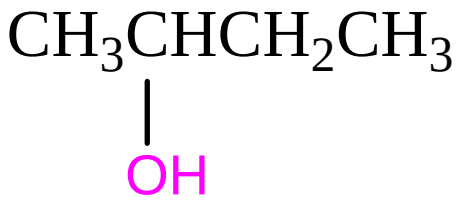
(3) **Suffix** : Finally the suffix ***ol*** is added to denote an alcoh***ol*.**

✓The **common name** of an alcohol consists of the name of the alkyl group to which the OH group is attached, followed bv the word “alcohol.”

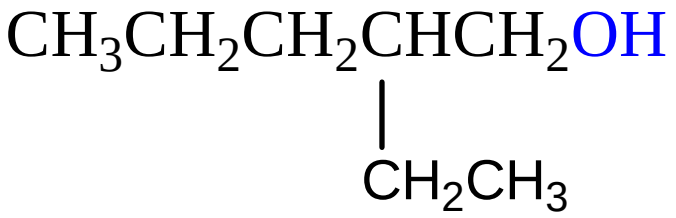
- **Example:-**



✓ The ***systematic name*** of an alcohol:



2-butanol or butan-2-ol



2-ethyl-1-pentanol or 2-ethylpentan-1-ol

Alcohols - Preparation of ethanol

(1) Fermentation

- procedure involves the action of zymase (***yeast***, an ***enzyme***) on an aqueous solution of ***sucrose*** (***a simple sugar***).
- The *by-products of the consumption of the sugar by the yeast* are ***carbon dioxide*** and ***ethanol***.



(2) Hydration of ethene

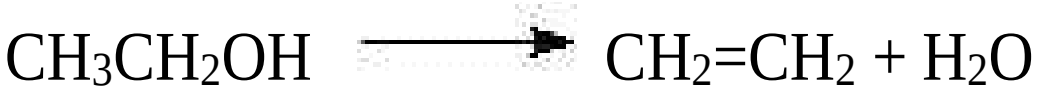
- water can be added to ethene to produce ethanol, with no other by-products



Reaction of alcohols

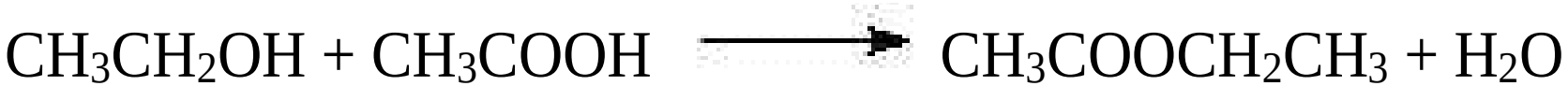
(1) Dehydration

- This process is the ***removal*** of the elements ***of water*** (2 H atoms and 1 ‘O’ atom) from ethanol leaving ***ethene***



(2) Esterification

- An ester is formed by reacting an ***alcohol*** with a ***carboxylic acid***.



6.Ethers

❖**Ethers** are compounds in which an ***oxygen is bonded to two alkyl substituents***. If the alkyl substituents are identical, the ether is a **symmetrical ether**.

❖If the substituents are different, the ether is an **unsymmetrical ether**

Example:-



➢ **Naming of ether:** two types of naming of ether common and systematic or IUPAC naming

✓ **Common name:**

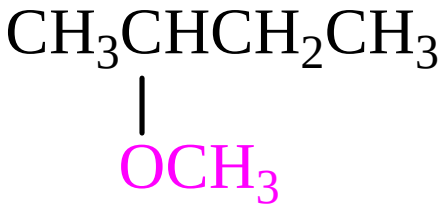
$CH_3CH_2OCH_3$

ethyl methyl ether

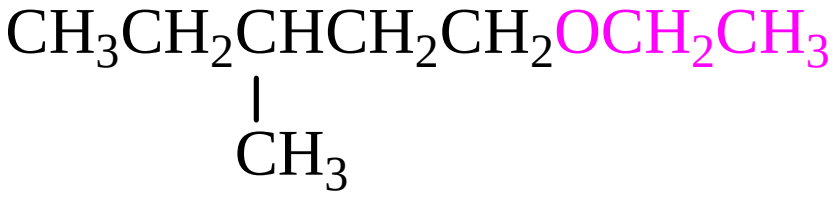
$CH_3CH_2OCH_2CH_3$

diethyl ether

- The IUPAC system names an ether as an alkane with an **RO substituent**. The substituents are named by replacing the "**yl**" ending in the name of the alkyl substituent with "oxy"

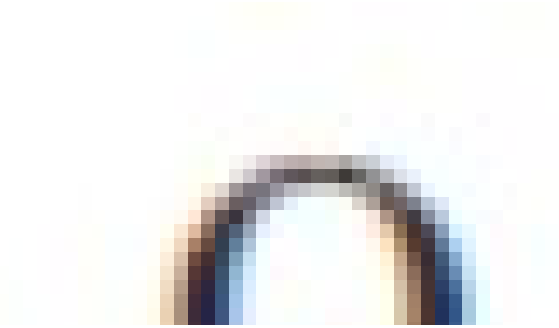


2-methoxybutane



1-ethoxy-3-methylpentane

- Ethers in which the oxygen atom is incorporated into a three-membered ring are called **epoxides** or **oxiranes**.

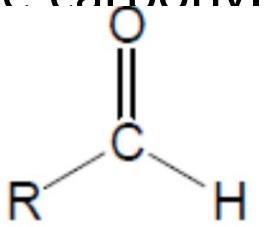


7.Carbonyl Compounds

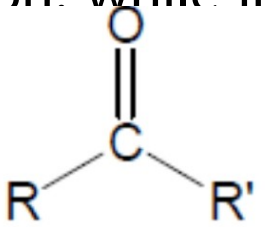
❖The **carbonyl group**, a carbon double bonded to oxygen, is probably the most important functional group found in organic compounds. Compounds containing carbonyl groups, called **carbonyl compounds,** are abundant in nature

Aldehydes and Ketones

- ❖ Aldehydes (RCHO) and ketones (R_2CO) are similar in structure in that both classes of compounds possess a **C=O** bond, called a ***carbonyl group***
- ❖ The carbon and oxygen in the carbonyl group are **sp^2**-hybridized, with bond angles of 120°.
- ❖ In **ketones**, two carbon groups are attached to the carbonyl carbon, while in **aldehydes** at least one hydrogen is attached to the carbon



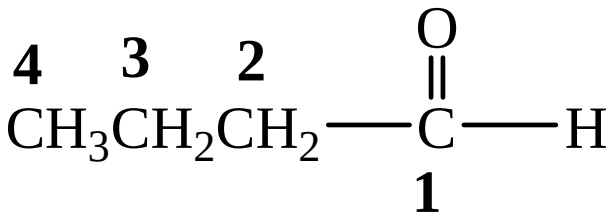
aldehyde



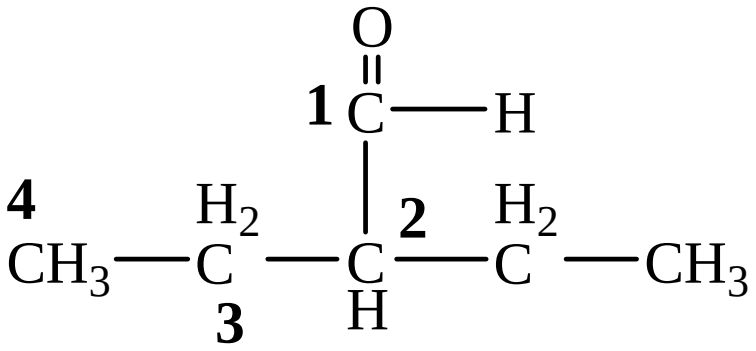
ketone

Nomenclature of Aldehydes

- Select the longest carbon chain **containing the carbonyl carbon** and the **-e** ending of the parent alkane name is replaced by the suffix **-al**.
- The carbonyl carbon is always numbered "1." (It is not necessary to include the number in the name.)



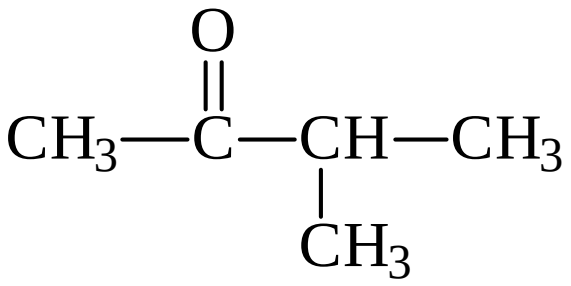
Butanal



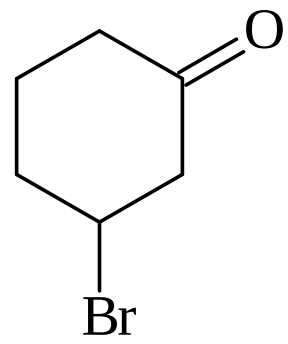
2-ethyl Butanal

IUPAC Names for Ketones

- Select the longest carbon chain *containing the carbonyl carbon* and number the chain starting with the end closest to the ketone group (i.e., the carbonyl carbon should have the lowest possible number).
- Replace -*e* with –*one* and indicate the position of the carbonyl with a number
- For cyclic ketones the carbonyl carbon is assigned the number ‘1’ **Example:-**



3-methyl-2-butanone



3-bromocyclohexanone

Physical Properties of Aldehydes and Ketones

Boiling Points

- ✓ The boiling point of aldehydes and ketones is higher than that of non-polar compounds (hydrocarbons) but lower than those of corresponding alcohols and carboxylic acids as aldehydes and ketones do not form H- bonds with themselves

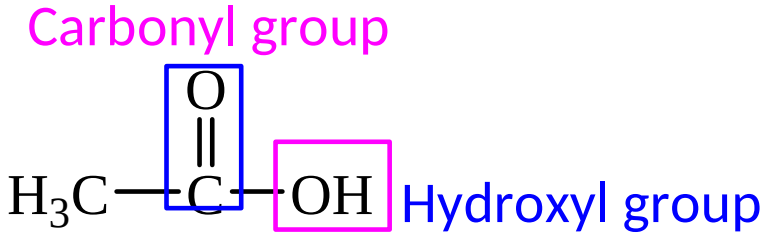
Solubility

- ✓ The **lower members** (up to 4 carbons) of aldehydes and ketones are ***soluble*** in water due to ***H-bonding***
- ✓ The higher members ***do not dissolve*** in water because the ***hydrocarbon part is larger and resists the formation of hydrogen bonds with water molecules***

Chemical Properties:-Both aldehydes and ketones contain carbonyl group, therefore they undergo same reactions like nucleophilic addition reactions, oxidation, reduction, halogenation

8. Nomenclature of Carboxylic Acids

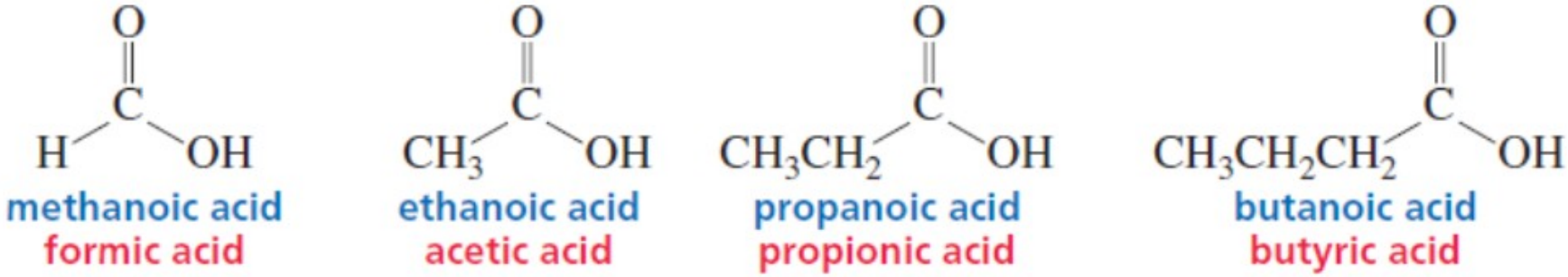
- Contains a ***carboxyl group***, which is a *carbonyl group (C=O)* attached to a hydroxyl group (—OH)



- In **systematic nomenclature**, a **carboxylic acid** is named by replacing the terminal "e" of the **alkane** name with **"oic acid"**

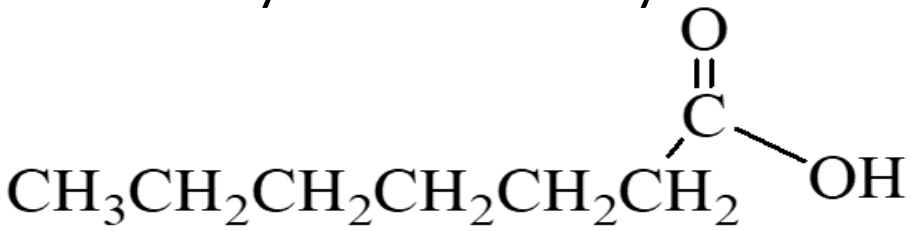
- Carboxylic acids containing six or fewer carbons are **frequently** called by their **common names**

Example:-



- In systematic nomenclature, the position of a substituent is designated by a number. The carbonyl carbon of a carboxylic acid is always the C-1 carbon

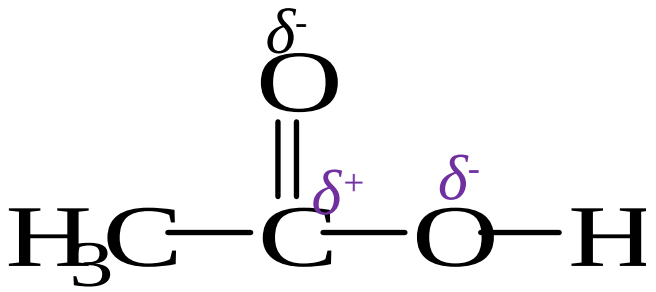
Example:-



heptanoic acid

Properties of Carboxylic Acids

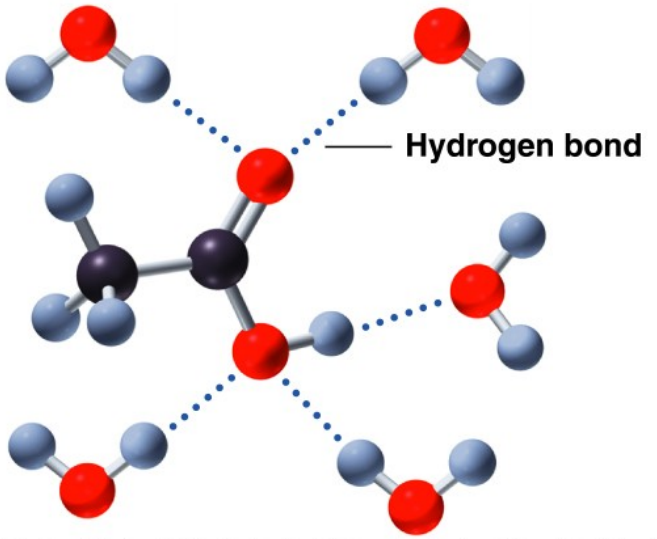
Carboxylic acids are strongly polar. Have two polar groups: - **hydroxyl (–OH)** and **carbonyl (C=O)**



Solubility in Water

- ✓ Carboxylic acids form hydrogen bonds with many water molecules.
- ✓ With 1-4 carbon atoms are very soluble in water.

Water molecules



Timberlake, *General, Organic, and Biological Chemistry.* Copyright © Pearson Education Inc., publishing as Benjamin Cummings

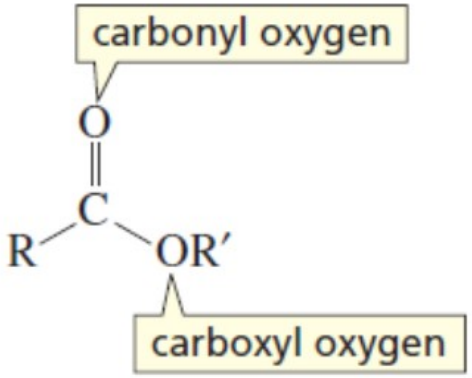
Table Physical Properties of Selected Carboxylic Acids

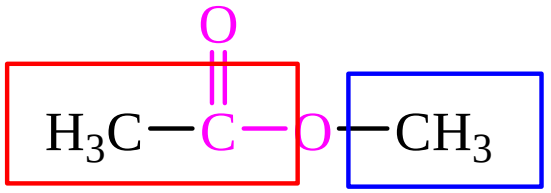
IUPAC name	bp (°C)	Solubility in Water
Methanoic acid	101	Very soluble
Ethanoic acid	118	Very soluble
Propanoic acid	141	Very soluble
Butanoic acid	164	Very soluble
Pentanoic acid	187	Slightly soluble
Hexanoic acid	205	Slightly soluble
Benzoic acid	250	Slightly soluble

- ✓ Carboxylic acids with higher molecular weights are solids at room temperature

9. Nomenclature of Esters

✓ An ester is a compound that has an OR′ group in place of the OH group of a carboxylic acid. In naming an ester, the name of the group (R′) attached to the carboxyl oxygen is stated first, followed by the name of the acid, with "**ic acid**" replaced by "**ate**."

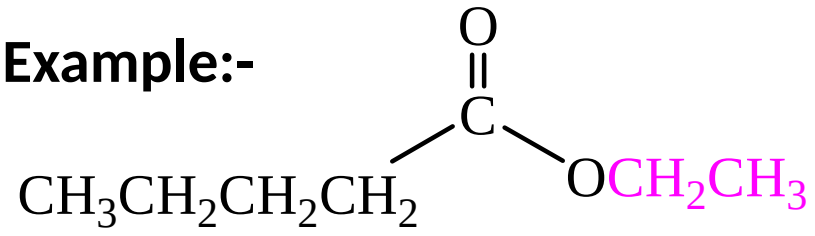




IUPAC: methyl ethanoate

Common: methyl acetate

Example:-



ethyl pentanoate

Physical Properties of Ester

Esters are colourless, pleasant smelling liquids, lower esters are fairly soluble in water.

The solubility of esters in water decreases rapidly with increase in the mass.

The boiling points of methyl and ethyl esters are lower than those of the corresponding parent acids

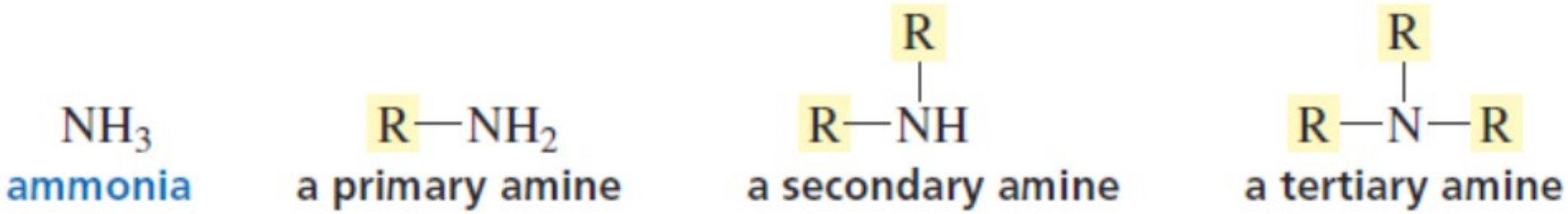
Chemical Properties of Esters

Esters are less reactive than acyl chlorides and acid anhydrides. It react slowly with ammonia to form amides and alcohols

It also undergo hydrolysis slowly to form the parent carboxylic acid and alcohol

10. Amines and Amide

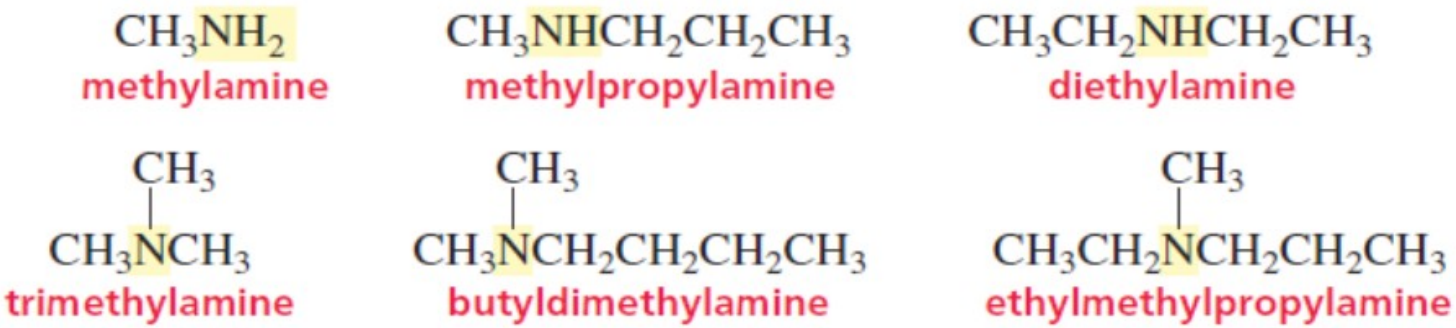
- ***Amines*** are compounds in which one or more of the **hydrogens of ammonia** have been replaced by ***alkyl*** groups. Smaller amines are characterized by their fishy odors
- There are **primary amines**, **secondary amines**, and **tertiary amines**. The classification depends on ***how many alkyl groups are bonded to the nitrogen***.
- Primary amines have one alkyl group bonded to the nitrogen, secondary amines have two, and tertiary amines have three.



- Notice that the number of alkyl groups *attached to the nitrogen* determines whether an amine is primary, secondary, or tertiary

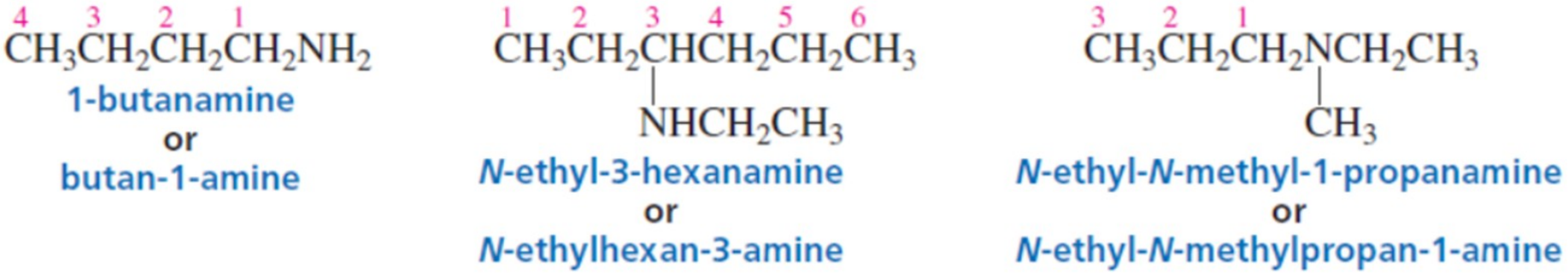
✓The common name of an amine consists of the names of the alkyl groups bonded to the nitrogen, in *alphabetical* order, followed by "amine"

Example:-



✓ The **IUPAC** system uses a suffix to denote the amine functional group. The "**e**" at the end of the name of the parent hydrocarbon is replaced by "**amine**"

✓ The name of any alkyl group ***bonded to nitrogen*** is preceded by an "***N***" (in italics) ***to indicate that the group is bonded to a nitrogen rather than to a carbon***

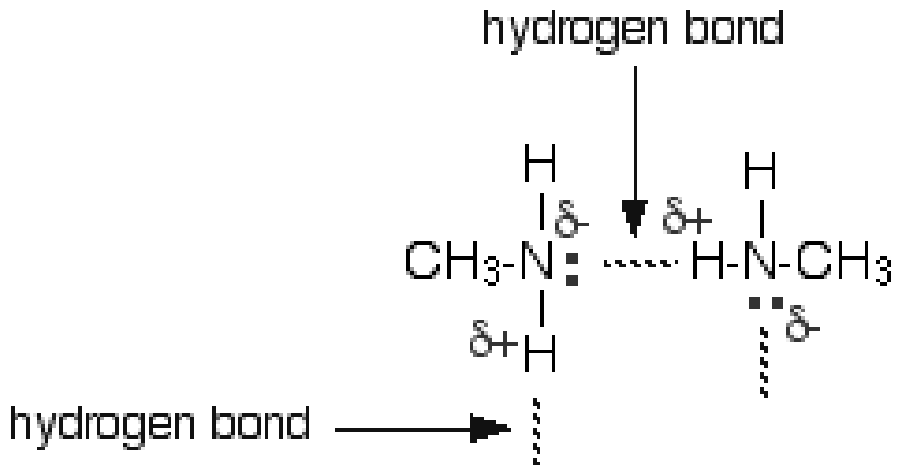


Boiling points

type	formula	boiling point (°C)
primary	CH_3NH_2	-6
primary	$CH_3CH_2NH_2$	16.6
primary	$CH_3CH_2CH_2NH_2$	48.6
secondary	$(CH_3)_2NH$	7.4
tertiary	$(CH_3)_3N$	3.5

- ***The reason for the higher boiling points of the primary amines is that***

  - ✓ they can form *hydrogen bonds* with each other
  - ✓ Van der waals dispersion forces and dipole-dipole interactions.



The boiling points of the primary amines increase as you increase chain length because of the van der Waals dispersion forces between the bigger molecules

❖ The *boiling point of the secondary amine is a little lower than the corresponding primary amine*

- ✓ having the nitrogen atom in the middle of the chain rather than at the end makes the permanent dipole on the molecule slightly less.
- ✓ lower dipole-dipole attractions in the dimethylamine compared with ethylamine.

❖ ***hydrogen bonding between tertiary amine molecules is impossible. That's why the boiling point is much lower.***

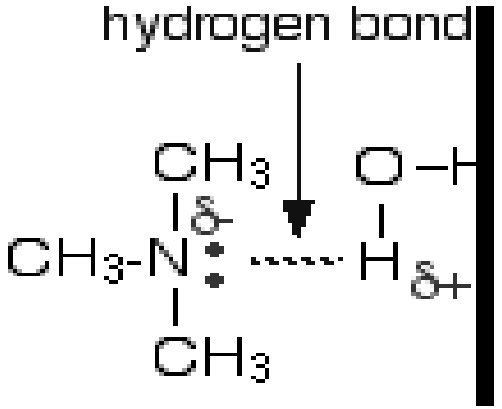
- ✓ trimethylamine has a much lower boiling point (3.5°C) than 1-aminopropane (48.6°C)

Solubility in water

- ✓ The small amines of all types are very soluble in water.
- ✓ All of the amines can form hydrogen bonds with water - even the tertiary ones.

- Although the tertiary amines don't have a hydrogen atom attached to the nitrogen and so can't form hydrogen bonds with themselves

- They can form hydrogen bonds with water molecules just using the lone pair on the nitrogen



- *Solubility falls off as the hydrocarbon chains get longer - noticeably so after about 6 carbons.*

Smell

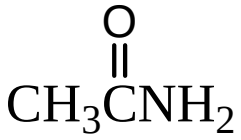
- The very small amines like methylamine and ethylamine smell very similar to ammonia, the amine smells are slightly more complex

- As the amines get bigger, they tend to smell more "fishy", or they smell of decay

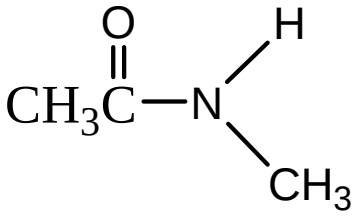
Nomenclature of Amides

- ✓ An **amide** has an NH_2, NHR, or NR_2 group *in place of the OH group of a carboxylic acid*. Amides are named by using the acid name, replacing "oic acid" or "ic acid" with "amide"
- ✓ If the amide nitrogen is bonded to an alkyl or aryl group, name the group and show its location on nitrogen by ***N-***

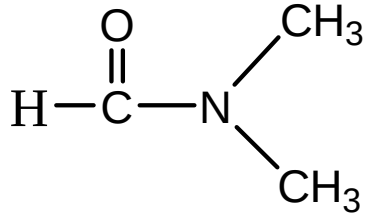
Example:-



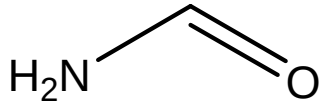
Acetamide
(a 1° amide)



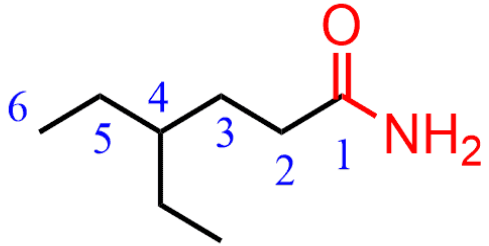
N-Methylacetamide
(a 2° amide)



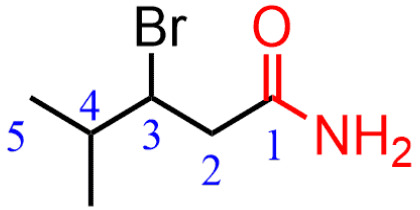
N,*N*-Dimethyl-form amide (DMF)
(a 3° amide)



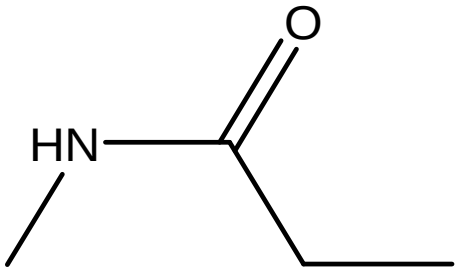
methanamide or formamide



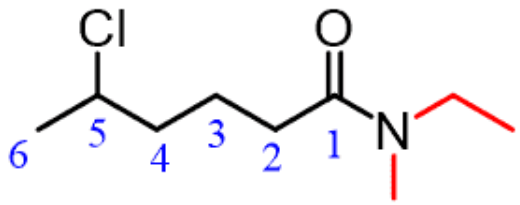
4-ethylhexanamide



3-bromo-4-methylpentanamide



N-Methylpropanamide



5-chloro-*N*-ethyl-*N*-methylhexanamide