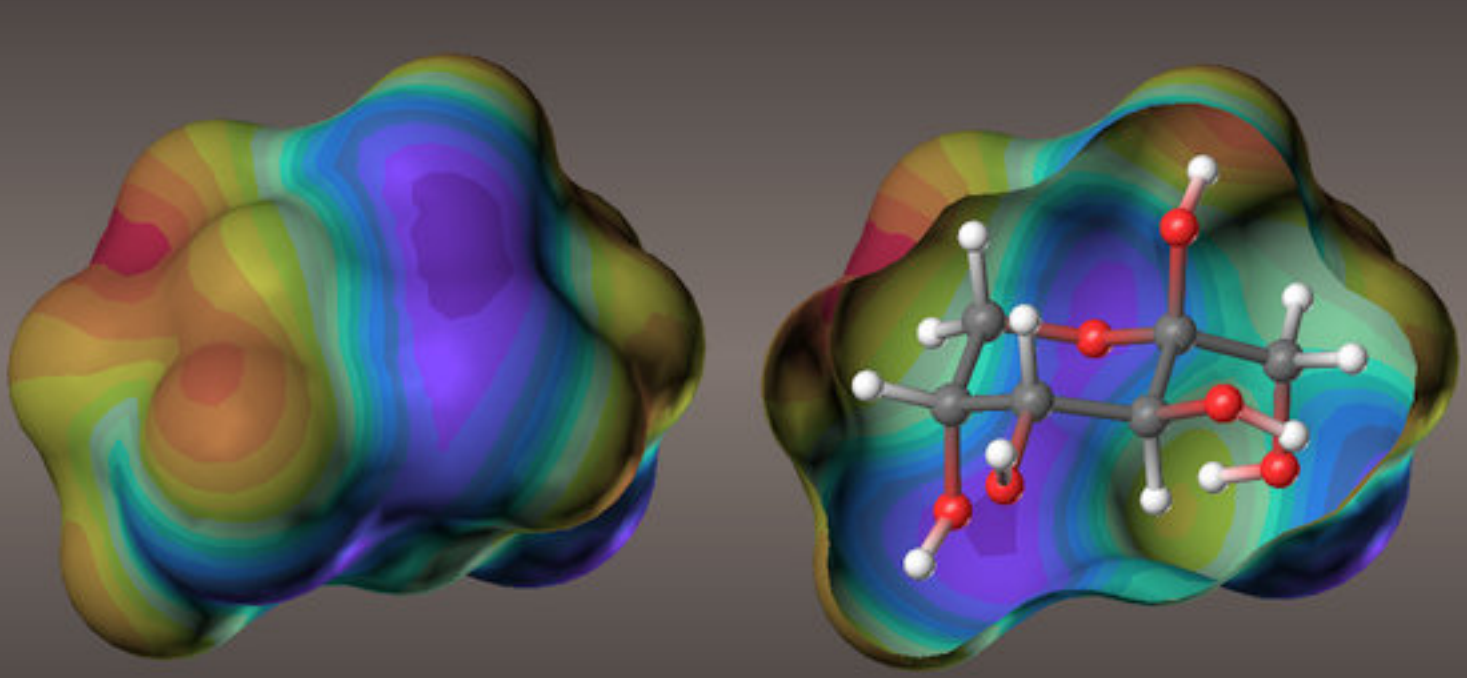

MOLCAD

ORGANIC CHEMISTRY

INTRODUCTION

All chemical substances can be classified into two groups--inorganic and organic. Organic compounds are those based on the element carbon. There are some inorganic compounds that also contain carbon--carbon dioxide, carbon monoxide, carbonic acid, etc. All organic compounds contain carbon and hydrogen and perhaps another element like nitrogen, oxygen, or sulfur. Organic compounds contain carbon and hydrogen and have a carbon-hydrogen bond.

Wöhler's synthesis of urea (H_2NCONH_2), in 1828 started the structural theory of organic chemistry.

Cyanides, cyanates, thiocyanates, carbides, carbonates, bicarbonates are not organic

Even though organic compounds are composed of only a few elements there are many more organic compounds (estimated to be about two million) than inorganic compounds (about 50 000). There are three primary reasons for this:

1. Carbon atoms can bond together to form chains. Carbon atoms are the only atoms that can effectively do this. The number of carbon atoms in each chain can vary widely. This property is called polymerism.

2. The bonds between carbon atoms in these chains are covalent bonds. Each carbon atom must share four pair of electrons and form four covalent bonds. However, the bonds between two carbon atoms may be single, double, or triple covalent bonds. That is, two carbon atoms may share one, two, or three pairs of valence electrons.

3. It is possible for the same number of atoms of carbon and other elements to have more than one arrangement; that is, more than one compound can be formed from the same number of atoms. This property is called isomerism.

THE IMPORTANCE OF ORGANIC COMPOUNDS

What's so important about carbon and its compounds? All living things contain carbon compounds. The building units of living matter -- carbohydrates, proteins, and fats--are all carbon-containing compounds. All foods are organic compounds.

Carbon becomes part of our foods and eventually a part of our bodies, because of a unique chemical reaction that occurs in green plants called photosynthesis. Light, carbon dioxide, and water react to produce a sugar called glucose and oxygen gas. The sugar made by plants travels throughout the animal world in food chains as animals eat plants and larger animals eat smaller animals. At each step, the sugar from photosynthesis is modified and combined with other materials. The resulting chemical compounds include new sugars, proteins, fats, starches, and cellulose.

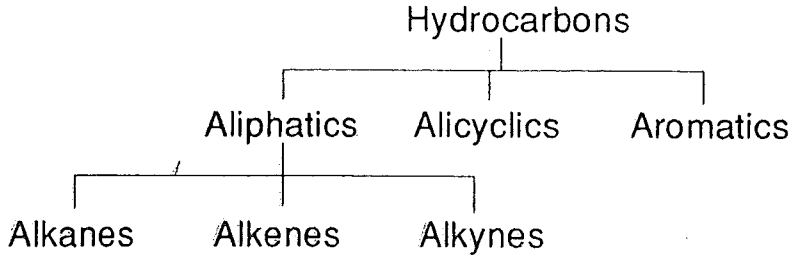
All living things eventually die. The dead organisms may become food for other organisms, or they may become trapped and buried in the earth. As a result of intense heat and pressure over long periods of time, some buried organic compounds have been converted into fossil fuels. Over millions of years these organic deposits have formed peat, coal and petroleum. Petroleum is not only a source of fuel, but also the starting material for the manufacture of plastics, fabrics, and industrial chemicals.

Probably every organic compound we know contains carbon that was once part of a living organism, or a product of a living organism. Because plants "recycle" carbon atoms from the atmosphere, a continuing source of organic compounds is available.

HYDROCARBONS

Hydrocarbons are organic compounds containing only the elements hydrogen and carbon. Because of the large number of hydrocarbons, they are classified into groups as shown by the classification scheme below:

Examples:
Aliphatics
- propane
Alicyclics
- cyclopropane
Aromatics
- propylbenzene



Aliphatic hydrocarbons are those containing chains of carbon atoms. The chains may be open or branched chain structures. The three families of hydrocarbons are determined by the type of bonds that exists between the carbon atoms.

The aliphatic hydrocarbons form homologous series. A homologous series is one in which the formula of each member differs from that of the preceding member in a constant, regular way, such as a CH_2 unit.

NOMENCLATURE OF HYDROCARBONS

The tremendous number of carbon compounds poses a major problem when it comes to naming them. The problem is overcome by using a systematic method of nomenclature developed by the International Union of Pure and Applied Chemistry. The IUPAC rules will be used for naming all organic compounds. In this system, the following stems for naming organic compounds containing up to 10 carbon atoms in a straight chain are used.

NUMBER OF CARBON ATOMS	STEM NAME	ALKYL GROUP NAME	MULTIPLIER
1	meth	methyl	-
2	eth	ethyl	di
3	prop	propyl	tri
4	but	butyl	tetra
5	pent	pentyl	penta
6	hex	hexyl	hexa
7	hept	heptyl	hepta
8	oct	octyl	octa
9	non	nonyl	nona
10	dec	decyl	deca

There are three types of formulas used in working with organic compounds:

1. Molecular formulas indicate the total number of each type of atom in a molecule.

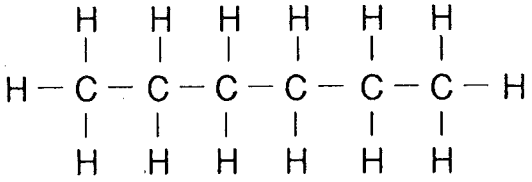
   Example, C_6H_{14}.

2. Condensed structural formulas show the number of hydrogen atoms bonded to each carbon atom in a molecule.

   Example, $CH_3–CH_2–CH_2–CH_2–CH_2–CH_3$

3. Structural formulas indicate how hydrogen and carbon atoms are bonded to each other in a molecule, using a dash (-) to represent a bond.

   Example,



In order to write the formula of an organic compound from its name, it is crucial to remember the following points:

- each carbon atom must form four bonds
- each hydrogen atom must form one bond
- each nitrogen atom must form three bonds
- each oxygen atom must form two bonds
- each sulfur atom must form two bonds

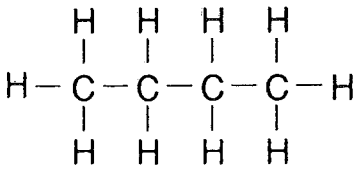
NOMENCLATURE OF ALKANES

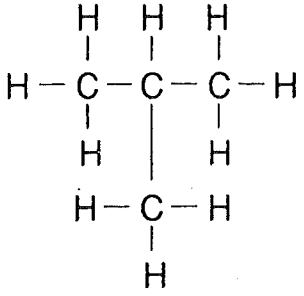
When there are four or more carbon atoms per molecule, it is possible to have more than one structure for the same molecular formula. This property is called isomerism and the molecules are said to isomers of one another. Isomers have different physical and chemical properties.

As the number of carbon atoms per molecule increases, the number of possible isomers increases.

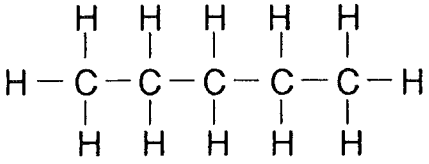
FORMULA	NUMBER OF POSSIBLE ISOMERS
CH_4	1
C_2H_6	1
C_3H_8	1
C_4H_{10}	2
C_5H_{12}	3
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75

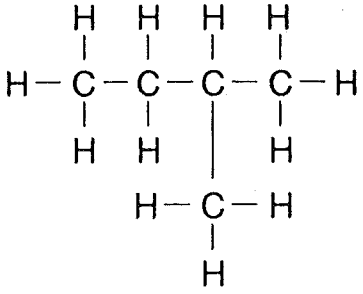
Isomers of C_4H_{10}:

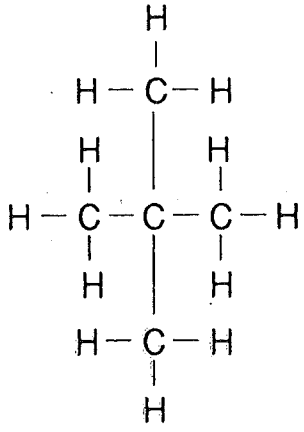




Isomers of C_5H_{12}



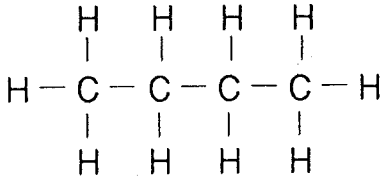




The following rules are used by IUPAC to name the alkanes and distinguish between isomers.

1. For straight chain alkanes, name the longest continuous chain of carbon atoms in the molecule by naming the stem for the appropriate number of carbon atoms plus the suffix "ane."

   Example:



butane

2. For branched chain alkanes, number the carbon atoms of the longest continuous chain starting at the end closest to the branching.

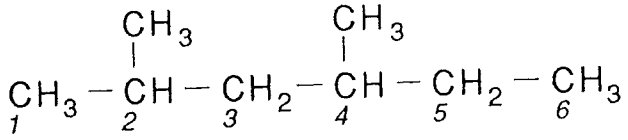
3. Locate the branch by the number of the carbon atom to which it is attached on the main chain.

4. Name the branch. The branches are called alkyl groups and are named by using the appropriate stem plus the suffix "yl." The position and name of the alkyl branches are given first in the overall name.

5. If more than one of the same alkyl groups are present as branches, the number of these branches is indicated by the prefix multipliers di-, tri-, tetra-, penta-, etc. The location of each of these alkyl groups is indicated by a number, using the lowest numbers possible.

The italicized numbers under the carbon atoms represent the atom's number in the longest chain

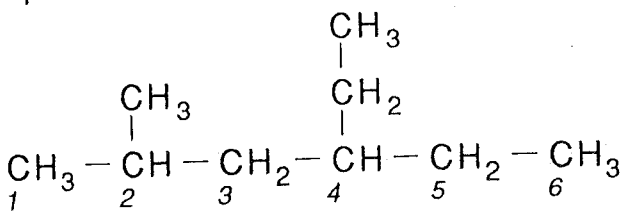
Example:



2,4-dimethylhexane

6. If different alkyl groups are present as branches, assign the lowest numbers possible to locate each branch. The order of the branches is arranged alphabetically, regardless of their number, on the longest chain..

Example:



4-ethyl-2-methylhexane

ALKANES

Alkanes are saturated compounds. Each carbon has only single bonds.

Alkanes have a general formula of C_nH_{2n+2}, where "n" represents an integer 1 to up 100 or more. All carbon-carbon bonds in alkanes are single bonds. This means the maximum number of hydrogen atoms are bonded to each carbon, and the molecule is said to be saturated.

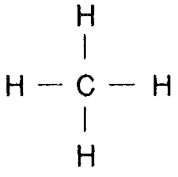
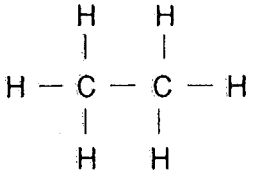
Alkanes form a homologous series:

ALKANE	FORMULA
methane	CH_4
ethane	C_2H_6
propane	C_3H_8
butane	C_4H_{10}
pentane	C_5H_{12}
hexane	C_6H_{14}
heptane	C_7H_{16}
octane	C_8H_{18}
nonane	C_9H_{20}
decane	$C_{10}H_{22}$

* * * * * * * * * *

Problems: Alkanes

1. Complete the following table:

NAME	MOLECULAR FORMULA	CONDENSED STRUCTURAL FORMULA	STRUCTURAL FORMULA
methane	CH_4	CH_4	
			

NAME	MOLECULAR FORMULA	CONDENSED STRUCTURAL FORMULA	STRUCTURAL FORMULA
		$CH_3 - CH_2 - CH_3$	
butane			
	C_6H_{14}		
		$CH_3–CH_2–CH_2–CH_2–CH_2–CH_2–CH_3$	

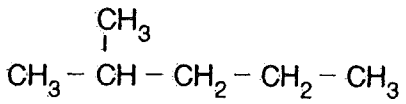
2. Draw structural formulas for and name the five isomers of C_6H_{14}.

3. Name each of the following compounds:

a. $CH_3 - CH_2 - \underset{\displaystyle CH_3}{\underset{|}{CH}} - CH_2 - CH_3$

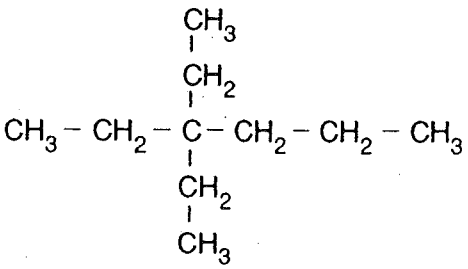
b. $CH_3 - CH_2 - \underset{\displaystyle CH_3}{\underset{|}{CH}} - \underset{\displaystyle CH_3}{\underset{|}{CH}} - CH_3$

c.



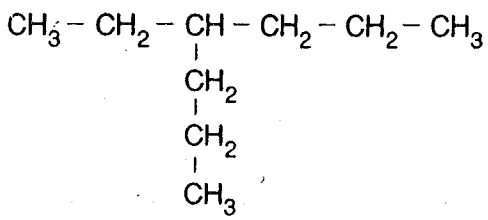
c. 3,4-diethyl-3-methylhexane

d.



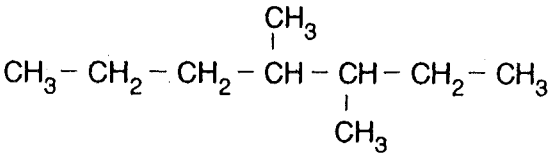
d. 3-ethyl-4,5-dipropyloctane

e.



e. 2,2,3,3-tetramethylheptane

f.



f. 3-ethyl-2,3,4-trimethylhexane

4. Write structural formulas for the following compounds:

a. 3-ethylhexane

b. 2,4-dimethylhexane

g. 2,2,3,3,4,4-hexamethylpentane

h. 3-ethyl-4-propylnonane

i. 4-propyloctane

j. 2,2-dimethylpropane

* * * * * * * * * *

ALKENES

Alkenes are unsaturated compounds.

There is at least one double bond in the molecule.

The general formula for an alkene is C_nH_{2n}. These hydrocarbons all contain at least one carbon-carbon double bond. Hydrocarbons that do not contain the maximum number of hydrogen atoms possible are said to be unsaturated with hydrogen. A hydrocarbon containing a carbon-carbon double bond is, therefore, unsaturated. All alkenes have the suffix of -ene to indicate the presence of a double bond. Alkenes form a homologous series:

ALKENE	FORMULA
Ethene	C_2H_4
Propene	C_3H_6
Butene	C_4H_8

The double bond takes the lowest carbon number possible.

The parent chain must fully contain the double bond even if it is not the longest continuous sequence of C's

Because there is a double bond in an alkene molecule, there is a new type of isomerism that can exist--different structures exist because of the position of the double bond. To name these compounds, indicate the position of the double bond with the number of the carbon that precedes the bond. Numbering the double bond takes precedence over the position of branches.

Example:

$$\underset{1}{CH_2}=\underset{2}{CH}-\underset{3}{CH_2}-\underset{4}{CH_3}$$

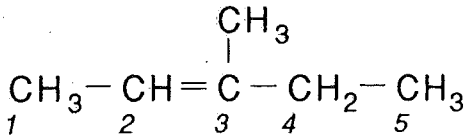
1-butene

$$\underset{1}{CH_3}-\underset{2}{CH}=\underset{3}{CH}-\underset{4}{CH_3}$$

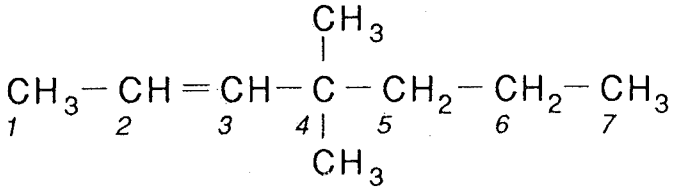
2-butene

Branches on alkene molecules are indicated and named as they are on alkane molecules.

Example,



3-methyl-2-pentene

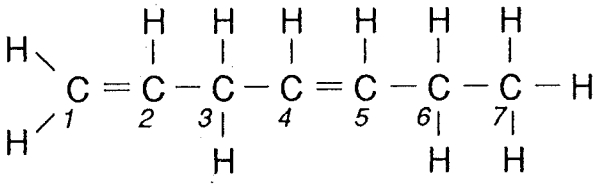


4,4-dimethyl-2-heptene

Alkadienes are isomers of alkynes.

It is possible for a molecule to have more than one double bond. Note that the formula for these compounds does not fit the general formula for an alkene, but they are still considered to be alkenes. To name this type of molecule, indicate the positions of the double bonds with numbers and place a multiplier in the suffix.

Example,

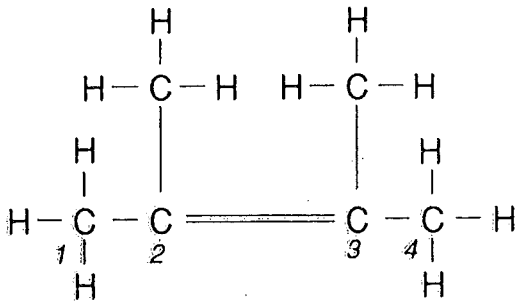


1,4-heptadiene

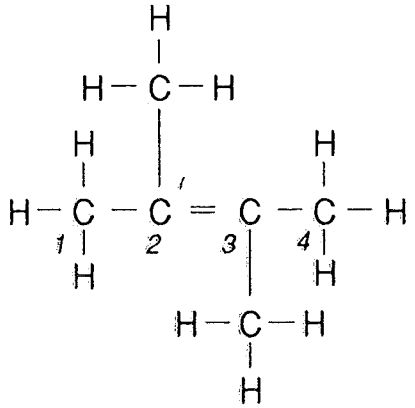
CIS AND TRANS ISOMERS

This type of isomer will occur in a double bond compound (an alkene).

Carbon atoms cannot rotate between a double bond.



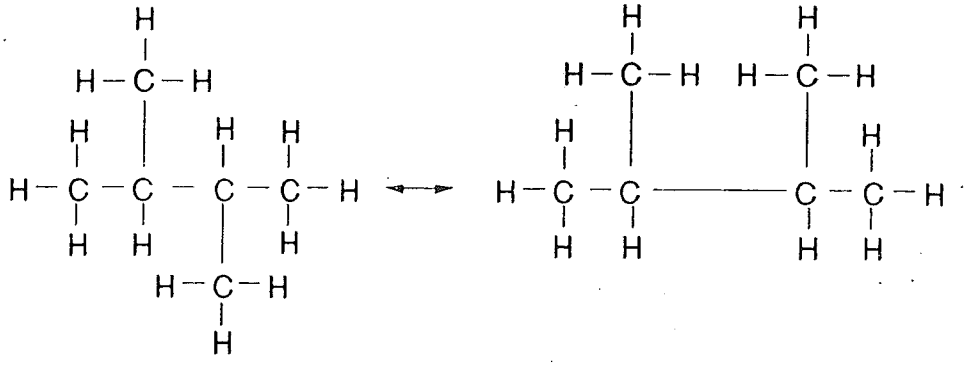
cis 2,3-dimethyl-2-butene



trans 2,3-dimethyl-2-butene

The unsaturated bond between the two carbons to which the methyl groups are attached cannot twist to produce the other isomer. In a saturated bond (single bond), the groups can twist to allow the methyl groups to be either opposite or adjacent to each other.

These two molecules are the same. Rotation can take place around a single C – C bond.



ALKYNES

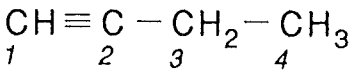
Alkynes will contain a triple bond.

Alkynes are somewhat similar to alkenes in that they are unsaturated hydrocarbons. These hydrocarbons all contain at least one carbon-carbon triple bond. The general formula for an alkyne is C_nH_{2n-2}. The suffix of -yne indicates the presence of a triple bond. Alkynes form a homologous series.

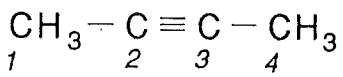
ALKYNE	FORMULA
ethyne	C_2H_2
propyne	C_3H_4
butyne	C_4H_6
pentyne	C_5H_8

The rules for nomenclature are similar to the alkenes.

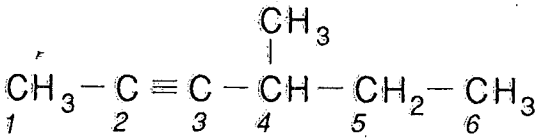
Example,



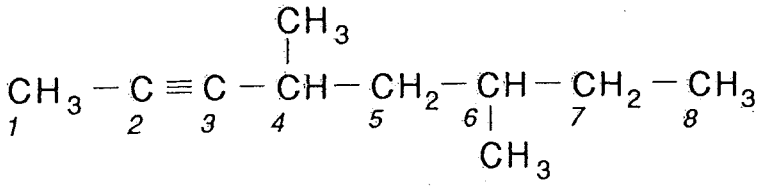
1-butyne



2-butyne



4-methyl-2-hexyne



4,6-dimethyl-2-octyne

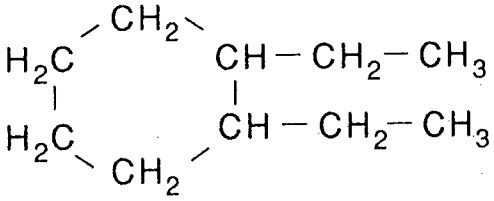
NOMENCLATURE OF CYCLIC HYDROCARBONS

Some hydrocarbons form closed ring molecules. These are known as cyclic hydrocarbons or the alicyclics. The following rules can be applied.

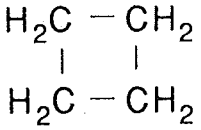
1. Name the largest ring of carbon atoms in the molecule by naming the stem for the appropriate number of carbons in the ring plus the appropriate suffix depending on whether there are single, double, or triple bonds. The entire name has a prefix of "cyclo" to indicate the ring or cyclic structure.

2. Alkyl branches are indicated by numbering the atoms in the ring in a clockwise manner, starting at the first branch and numbering to give the lowest numbers possible.

Examples:



1,2-diethylcyclohexane



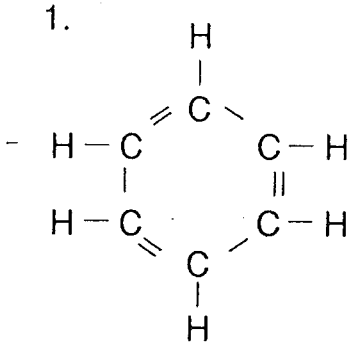
cyclobutane

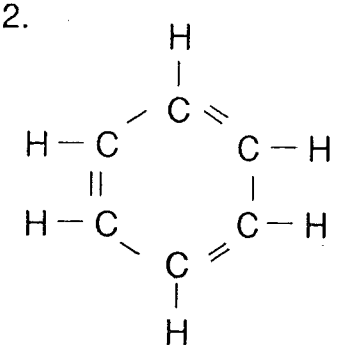
AROMATIC HYDROCARBONS

In 1825 the English scientist, Michael Faraday, purified and analyzed an oily liquid given to him by the Portable Gas Company of London. Because of his careful work, he is credited with the discovery of benzene. Several of the aromatic, pleasant-smelling oils obtainable from plant sources were also found to consist of molecules similar in some ways to benzene. Benzene is called the "prototypical" aromatic compound.

The molecular formula of benzene is C_6H_6. Any compound which has only six hydrogen atoms for six carbon atoms must be unsaturated. However, benzene does not react like other unsaturated hydrocarbons such as hexene or cyclohexene. The structure of benzene is now described by a resonance theory.

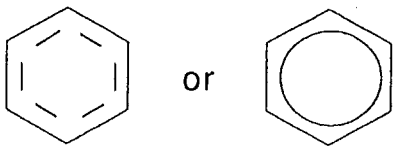
It is possible to draw two structures for benzene differing only in the locations of electron pairs:

1. 

2. 

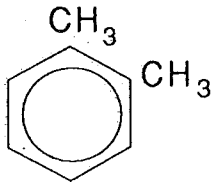
These structures are not identical. The C-1 to C-2 bond in structure 1 is a single bond, and in structure 2 it is a double bond.

The resonance theory suggests that whenever it is possible to draw two or more structures differing only in the location of the electrons, neither structure adequately represents the molecule. However, a good approximation of the molecular structure of benzene can be obtained by thinking of it as being a resonance hybrid or "average" of the two structures. The two classical structures are not considered as being real themselves. Rather, they are said to be the contributing structures. The resonance hybrid is often written as:



Benzene is a new type of molecule, an aromatic compound. Benzene is more stable than expected in comparison to alicyclic compounds. In fact, any compound that exhibits resonance is more stable that might be expected.

Derivatives of benzene are named by numbering the carbons atoms in the ring in a clockwise manner, starting at 1 for the first grouping.



1,2-dimethylbenzene

* * * * * * * * * *

Problems: Alkenes, Alkynes, Aromatics

1. Give the IUPAC name for each of the following compounds:

a. $CH_3-CH_2-CH_2-CH=CH-CH_3$

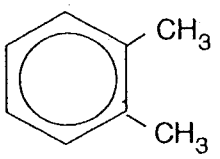
b. $CH_3-CH=C(CH_3)-CH_3$

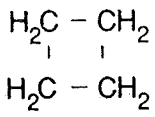
c. $CH_2=CH-C(CH_3)(CH_3)-CH_2-CH_3$

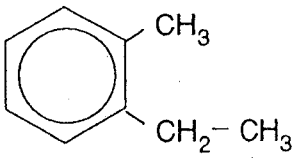
d. $CH_3-CH=CH-CH(CH_2CH_3)-CH_2-CH_3$

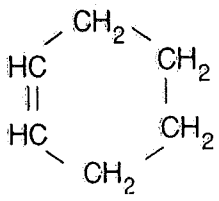
e. $CH\equiv C-CH(CH_3)-CH_3$

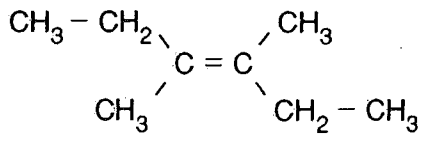
f. $CH_3-C\equiv C-CH(CH_2CH_3)-CH_3$

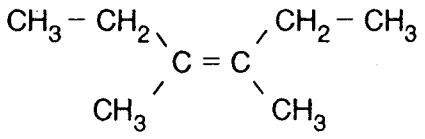
g. 

h. 

i. 

j. 

k. 

l. 

2. Draw the structural formulas and give names for three noncyclic isomers of C_5H_{10}.

3. Draw the structural formulas and give names for three noncyclic isomers of C_5H_8.

4. Draw structural formulas for:

a. 3-octene

b. 2,4-dimethyl-2-pentene

c. 4-ethyl-3-methyl-2-hexene

d. 2-methylpropene

e. 3,4-diethyl-1-hexyne

f. 5-ethyl-4-propyl-2-heptyne

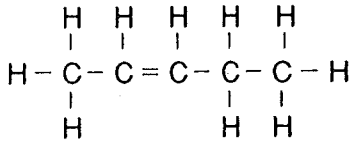
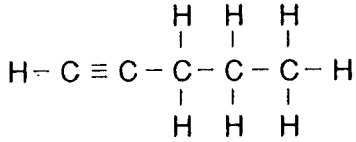
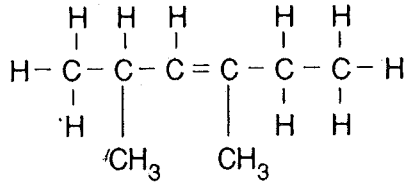
g. 1,4-dimethylbenzene

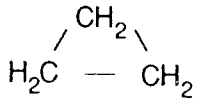
h. 1,3-diethylbenzene

i. cyclopentene

j. cyclohexyne

5. Complete the following table:

NAME	MOLECULAR FORMULA	STRUCTURAL FORMULA
2-pentene	C_5H_{10}	
		
	C_3H_4	
		

NAME	MOLECULAR FORMULA	STRUCTURAL FORMULA
2-methylpropene		
		
1,3-pentadiene		
1,3-dipropylbenzene		

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PHYSICAL PROPERTIES OF HYDROCARBONS

1. Melting and Boiling Points

Within a homologous series (e.g. the alkanes, the alkenes, or the alkynes) the melting and boiling points increase as the number of carbon atoms per molecule increases. Molecules of hydrocarbons are nonpolar. The London Dispersion forces between the molecules increase as the number of atoms, and therefore, the number of electrons in the molecule increases. Increased attractive forces between the bigger molecules require more energy to break the intermolecular London Dispersion forces in order to melt and then boil the compound.

18

2. Solubility

Since hydrocarbons are nonpolar, they are not soluble in polar solvents such as water. Liquid alkanes, alkenes, and simple aromatics are good nonpolar solvents for other hydrocarbons.

CHEMICAL PROPERTIES OF HYDROCARBONS

Hydrocarbons can undergo a variety of reactions with the most common being combustion, substitution, and addition. Since these reactions involve the breaking and remaking of strong covalent bonds, they are generally slow in rate. Many of them require catalysts.

1. Combustion Reactions

All hydrocarbons burn by combining with oxygen. The products depend upon how much oxygen gas is available to support the combustion.

a. With a very short supply of oxygen the products of combustion are carbon, water vapor and heat.

$$C_3H_{8(g)} + 2O_{2(g)} \rightarrow 3C_{(s)} + 4H_2O_{(g)} + \text{heat}$$

b. With a limited supply of oxygen the products of combustion are carbon monoxide, water vapor and heat.

$$C_3H_{8(g)} + \frac{7}{2}O_{2(g)} \rightarrow 3CO_{(g)} + 4H_2O_{(g)} + \text{heat}$$

c. With an abundant supply of oxygen the products of combustion are carbon dioxide gas, water vapor and heat.

We will always assume complete combustion.

$$C_3H_{8(g)} + 5O_{2(g)} \rightarrow 3CO_{2(g)} + 4H_2O_{(g)} + \text{heat}$$

2. Substitution Reactions

Alkanes and aromatics undergo substitution reactions in which one or more hydrogen atoms are replaced by another atom or group of atoms. These reactions must generally be catalyzed. Common substitution reactions involve the substituting of halogen atoms for the hydrogen.

Examples:

$$CH_{4(g)} + Cl_{2(g)} \rightarrow \underset{\text{chloromethane}\\ \text{primary product}}{CH_3Cl_{(g)}} + HCl_{(g)}$$

The substitution process can continue until all hydrogen atoms have been replaced.

$$CH_3Cl_{(g)} + Cl_{2(g)} \rightarrow \underset{\text{dichloromethane}\\ \text{secondary product}}{CH_2Cl_{2(g)}} + HCl_{(g)}$$

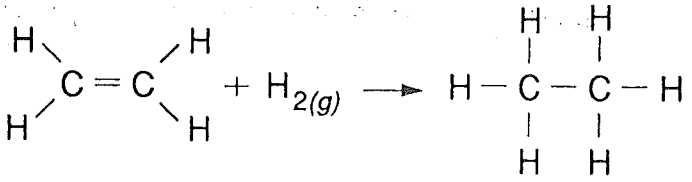
$$CH_2Cl_{2(g)} + Cl_{2(g)} \rightarrow \underset{\text{trichloromethane}\\ \text{tertiary product}}{CHCl_{3(g)}} + HCl_{(g)}$$

$$CHCl_{3(g)} + Cl_{2(g)} \rightarrow \underset{\text{tetrachloromethane}\\ \text{final product}}{CCl_{4(g)}} + HCl_{(g)}$$

3. Addition Reactions

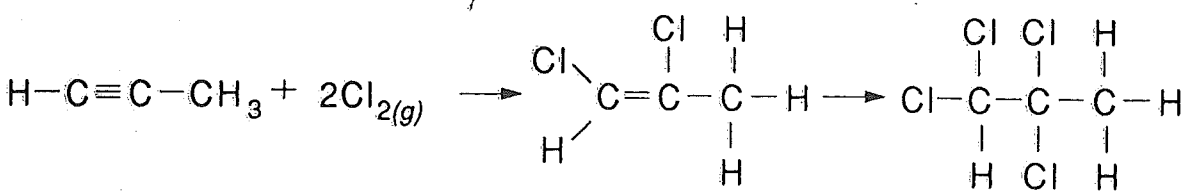
Alkenes and alkynes, the unsaturated hydrocarbons, have chemically reactive double and triple bonds. These unsaturated bonds undergo what is called addition reactions, where another compound reacts with the unsaturated hydrocarbon and is added onto it by breaking the double or triple bond and forming single bonds. Alkenes and alkynes commonly undergo addition reactions with hydrogen, the halogens and hydrogen halide compounds.

Example 1: Hydrogen addition.



It is difficult to stop at an intermediate step.

Example 2: Halogen addition.



1,1,2,2-tetrachloropropane

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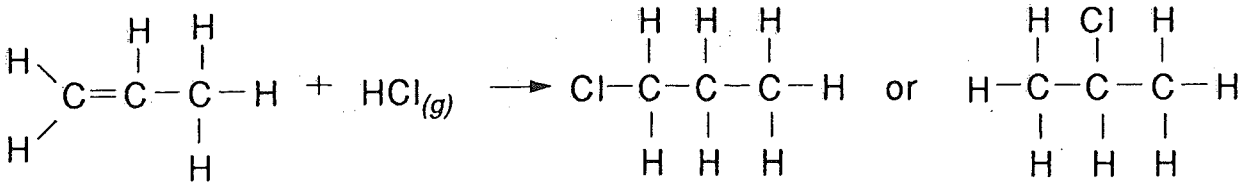
Example 3: Hydrogen halide addition



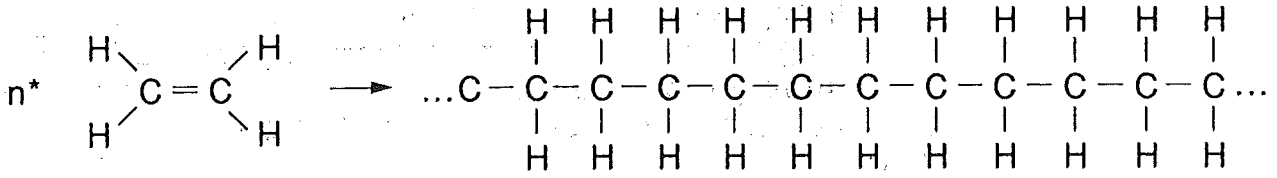
1-chloropropane 2-chloropropane

4. Addition Polymerization

A polymer is a giant molecule made from thousands of smaller alkene molecules called monomers. It can be compared to a chain-link fence. A chain fence is made up of individual links joined together. Similarly, many large molecules (often called macromolecules) are composed of smaller units, linked together by chemical bonds. The combination of thousands of monomers produces a polymer (from the Greek, poly=many, meros=part).

The polymer results from repeated addition of monomers to the growing polymer chain. Each monomer is added at the double bond. The most common monomers are ethene (ethylene) and substituted ethenes, known as vinyl monomers.

Example:



ethene polyethene or polyethylene

*"n" represents a large number of about 1000 or more.

* * * * * * * * * *

Problems: Hydrocarbon Reactions

1. Write a balanced equation to represent the following **combustion** reactions:

   a. Combustion of butane in very short supply of oxygen.

   b. Combustion of hexene in limited supply of oxygen.

   c. Combustion of propane in abundant supply of oxygen.

   d. Combustion of benzene in very short supply of oxygen.

   e. Combustion of ethyne in abundant supply of oxygen.

2. Write a balanced equation to represent the following **substitution** reactions. Represent the organic product with a structural formula and name it. (Primary or next product only)

   a. $C_2H_{6(g)} + Cl_{2(g)} \rightarrow$

   b. $CH_3Cl_{(g)} + Cl_{2(g)} \rightarrow$

   c. $CH_2Cl_{2(g)} + Cl_{2(g)} \rightarrow$

   d. $C_3H_{8(g)} + Br_{2(g)} \rightarrow$
   (Two possible products--show and name both)

   e. $C_4H_{10(g)} + F_{2(g)} \rightarrow$
   (Two possible products--show and name both)

3. Write a balanced equation to represent the following **addition** reactions. Represent the organic product with a structural formula and name it.

   a. ethene + $Br_{2(g)} \rightarrow$

b. propyne + $Cl_{2(g)}$ →

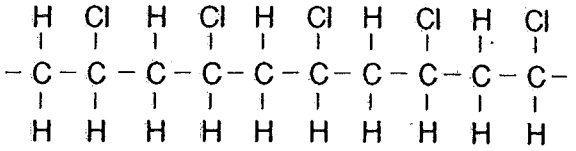
c. propyne + $2Cl_{2(g)}$ →

d. 1-butene + $HCl_{(g)}$ →
(Two possible products--show and name both)

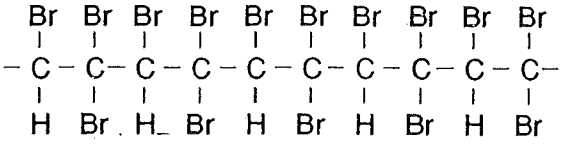
e. 2-butyne + $2HCl_{(g)}$ →
(Two possible products--show and name both)

4. Draw the structural formula and give an IUPAC name for the monomer that would produce the following addition polymers:

a.

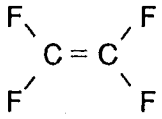


b.

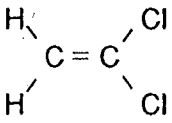


5. Draw a segment of the addition polymer that could be formed from these monomers:

a.



b.



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HYDROCARBON DERIVATIVES

A large number of hydrocarbons exist in nature or can be synthesized from other hydrocarbons. In addition, there are a great number of compounds that are formed from hydrocarbons that contain other atoms in addition to the carbon and hydrogen atoms. We call these hydrocarbon derivatives. It is the additional atoms that give these compounds their properties. The symbol "R" is often used to designate the hydrocarbon part of the molecule. These R-groups are often alkyl groups which are derived from the alkanes.

The atom or reactive groups of atoms attached to the alkyl group is called a functional group. The term "functional group" is applied to any reactive atom or group of atoms in an organic compound to distinguish it from those which do not react. Examples of functional groups are -OH (hydroxyl) for alcohols, -N- (nitrogen) for amines and -COOH (carboxyl) for acids.

It is the functional group that is responsible for the type of chemical reaction shown by a particular class of compounds. During a reaction, the hydrocarbon part usually remains unchanged, while the functional group is chemically reactive. The hydrocarbon derivatives includes such groups as alcohols, aldehydes, ketones, acids, esters, amines, amides, ethers, etc.

ALCOHOLS

The general formula for an alcohol is R-OH.

The functional group of an alcohol is -O-H.

Alcohols can be synthetically prepared by oxidizing (adding oxygen) to an alkane hydrocarbon.

The simplest member of the family is methanol, CH_3OH. Methanol is a colorless liquid with a pleasant odor. It is a good fuel and is often used for that purpose. It is also used as a solvent and as an antifreeze compound. Methanol is highly poisonous, and even small quantities can cause blindness and death. Methanol is often sold under the common names of methyl alcohol, wood alcohol, or methyl hydrate.

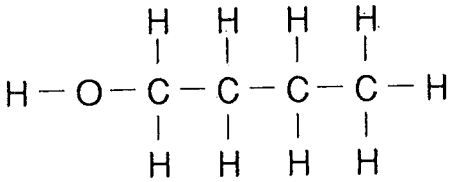
The most familiar member of the alcohol family is ethanol, C_2H_5OH, also called ethyl alcohol or grain alcohol. It is colorless, has a pleasant odor and a sharp taste, and burns with a colorless flame. Ethanol is a good solvent for many organic compounds. A solution of iodine in ethanol is called tincture of iodine, and is used as an antiseptic for wounds. The active ingredients of certain cough syrups are also dissolved in ethanol. All alcohol beverages contain ethanol in varying concentrations, from about 4% to as high as 75% by volume. Like other members of the alcohol family, ethanol is poisonous. A concentration of only 0.40% in the blood of an individual can cause death.

Some alcohols have more than one hydroxyl group per molecule. 1,2-ethanediol (ethylene glycol) is a two-carbon, saturated molecule which has two hydroxyl groups. It is used as an antifreeze in the ratio of 1:1 by volume with water. The resultant solution has a lower freezing point and a higher boiling point than water.

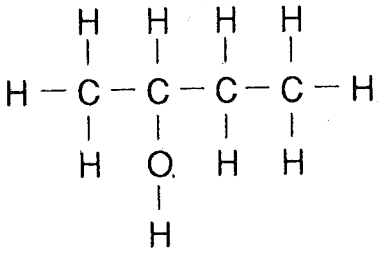
ALCOHOL NOMENCLATURE

Alcohols are named by taking the corresponding alkane name, dropping the last "e" and adding a suffix of "-ol." The position of the alcohol functional group is indicated by numbering the carbon atoms. If more than one alcohol functional group is present, the appropriate multiplier is used before the suffix. Any branches are named as they would on a hydrocarbon.

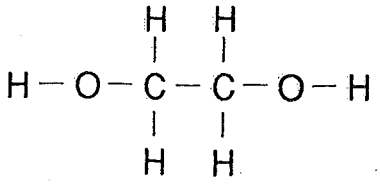
Examples:



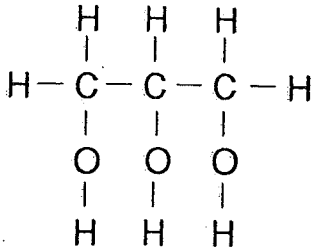
1-butanol



2-butanol

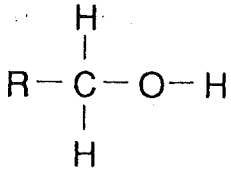


1,2-ethanediol
(ethylene glycol)

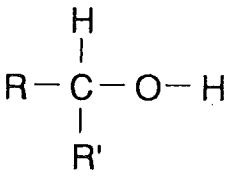


1,2,3-propanetriol
(glycerol)

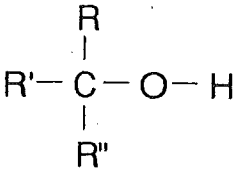
There are three degrees of alcohols, primary, secondary, and tertiary. In a primary alcohol the carbon bonded to the oxygen is bonded to only one other carbon (or no carbons in the case of methanol). In a secondary alcohol the carbon bonded to the oxygen is bonded to two other carbon atoms. In a tertiary alcohol the carbon bonded to the oxygen is bonded to three other carbon atoms.



primary



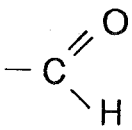
secondary



tertiary

ALDEHYDES

The general formula for an aldehyde is R-CHO.

The functional group of an aldehyde is 

Aldehydes are formed by the oxidation or dehydrogenation of a primary alcohol. This reaction gives this group its name--alcohol dehydrogenation.

ALDEHYDE NOMENCLATURE

Aldehydes are named by taking the corresponding alkane name, dropping the last "e" and adding a suffix of "-al." Any branches are named as they would be on a hydrocarbon.

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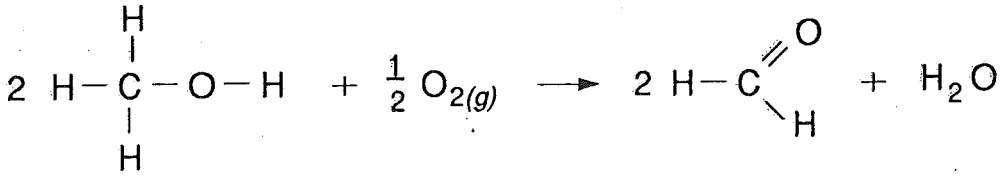
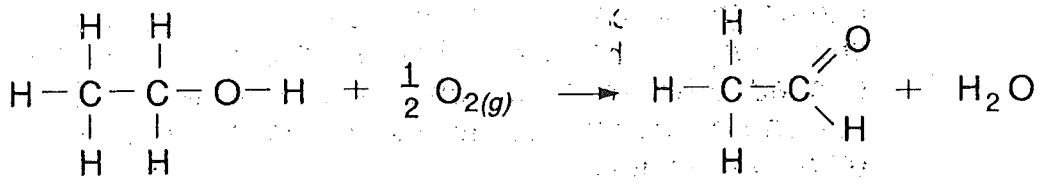


methanol

methanal
(formaldehyde)

A solution of methanal (formaldehyde) in water is called formalin. This solution is used as a biological preservative and embalming fluid.

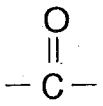


ethanol

ethanal
(acetaldehyde)

KETONES

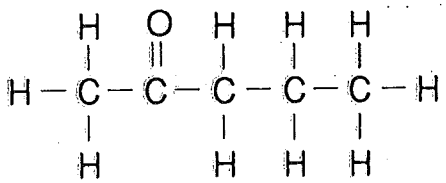
The general formula of a ketone is R-CO-R'

The functional group of a ketone is 

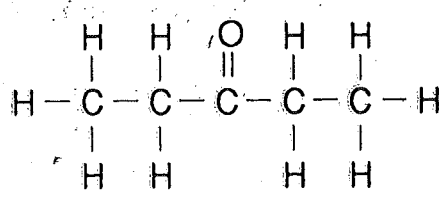
Ketones are formed by the oxidation (dehydrogenation) of a secondary alcohol.

KETONE NOMENCLATURE

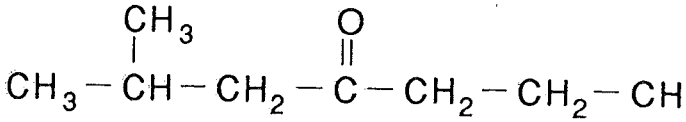
Ketones are named by dropping the last "e" from the alkane name and replacing it with a suffix of "-one." The position of the functional group is indicated by numbering the carbon atoms in the chain.



2-pentanone



3-pentanone



2-methyl-4-heptanone

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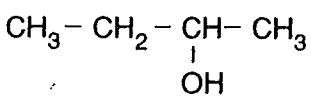
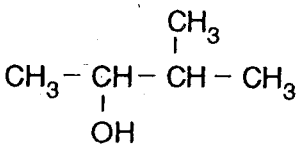
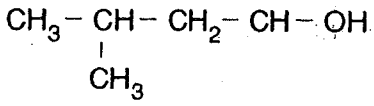
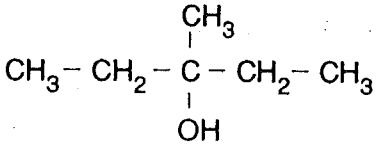
Problems: Alcohols, Aldehydes and Ketones

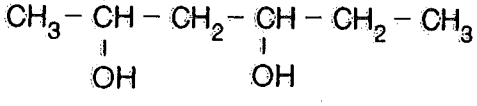
1. Name the following alcohols:

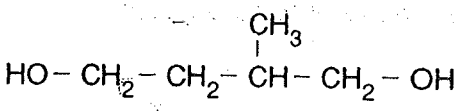
a. 

b. 

c. 

d. 

e. 

f. 

2. Draw structural formulas for the following alcohols:

a. 3-heptanol

b. 2-pentanol

c. 2-methyl-2-butanol

d. 2,2-dimethyl-1-propanol

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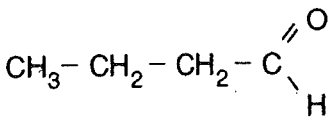
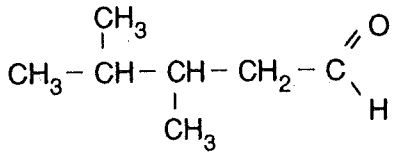
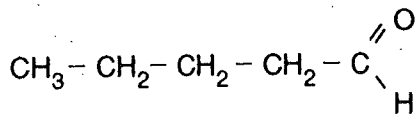
e. 3-methyl-3-heptanol

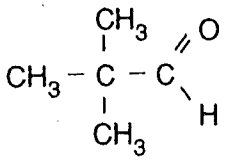
f. 3,3-dimethyl-1-pentanol

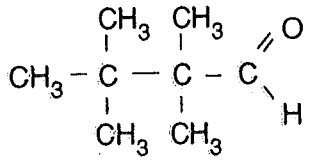
3. Name the following aldehydes:

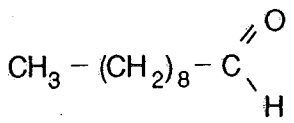
a. 

b. 

c. 

d. 

e. 

f. 

4. Draw structural formulas for the following aldehydes:

a. 2,2-dimethylpentanal

b. heptanal

c. butanal

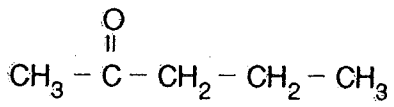
d. 2,2,3,3-tetramethylbutanal

e. 3-ethyl-2-methyloctanal

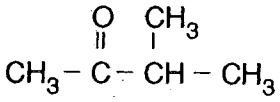
f. 2,3-dichloropropanal

5. Name the following ketones:

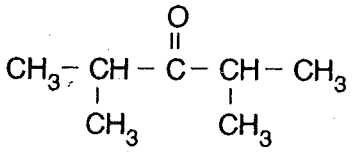
a.



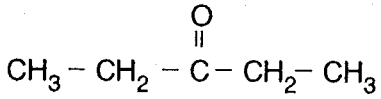
b.



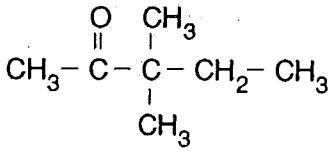
c.



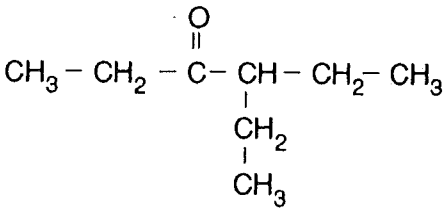
d.



e.



f.



6. Draw structural formulas for the following ketones:

a. 2-heptanone

b. 3-heptanone

c. 2,2-dimethyl-3-pentanone

d. 3,3-dimethyl-2-butanone

e. 3,4-dimethyl-2-pentanone

f. 4-methyl-3-hexanone

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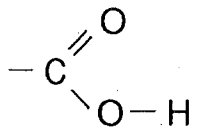
CARBOLIC ACIDS

The general formula of a carboxylic acids is R-COOH.

The functional group of a carboxylic acid is 

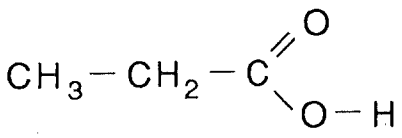
Carboxylic acids are formed by oxidizing aldehydes.

The first member of the organic acid family is methanoic acid, HCOOH. Methanoic acid, commonly called formic acid, is an acrid-smelling liquid which is the irritative component in the sting of bees and the "bite" of many ants. Ethanoic acid, CH_3COOH, commonly called acetic acid, is the acid found in vinegar.

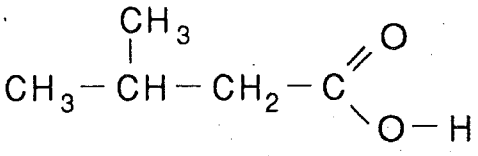
The carboxylic acids figure prominently in metabolic processes. They are also used by living systems as building blocks for the manufacture of larger molecules such as fats and steroids.

CARBOXYLIC ACID NOMENCLATURE

Carboxylic acids are named by taking the corresponding alkane name, dropping the last "e", replacing it with the suffix "-oic" and adding the word "acid." Branches are named as they would be on a hydrocarbon molecule. The carbon atom in the functional group is number one.

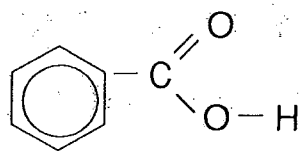


propanoic acid



3-methylbutanoic acid

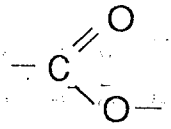
The acid functional group may also replace one of the six hydrogen atoms of the benzene ring. This produces benzoic acid.



benzoic acid

ESTERS

The general formula of esters is R-COO-R'.

The functional group of an ester is 

Esters are formed by a reaction between carboxylic acids and alcohols, which is called esterification. The reaction is usually slow and is catalyzed with concentrated sulfuric acid to help remove the water.

ESTERIFICATION

$$R-COOH + H-O-R' \rightarrow R-COO-R' + HOH$$

carboxylic acid + alcohol → ester + water

Esters have many commercial uses ranging from cosmetics, perfumes, and artificial flavors to synthetic fibers. Many vegetable oils are complex esters. The flavors and odors of fruits such as apples, oranges, and bananas are due to the presence of esters.

NAME	SOURCES OR TYPICAL USE
ethyl methanoate	rum flavor and odor
pentyl propanoate	apricot flavor and odor
ethyl butanoate	used in artificial peach, pineapple and apricot flavors
octyl ethanoate	orange flavor and odor
pentyl ethanoate	pear flavor and odor
1-methylpropyl ethanoate	strawberry flavor and odor
methylsalicylate	wintergreen flavor and odor

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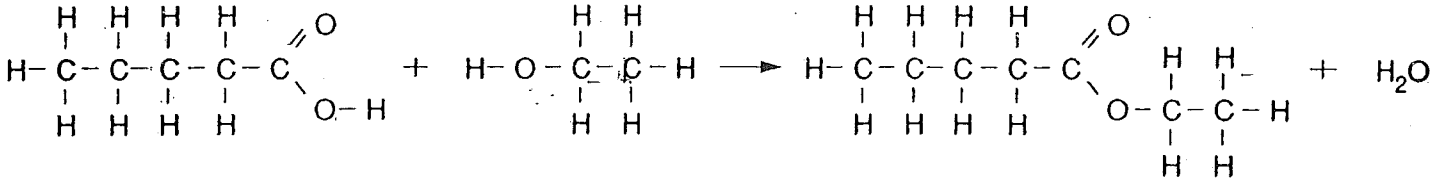
NOMENCLATURE OF ESTERS

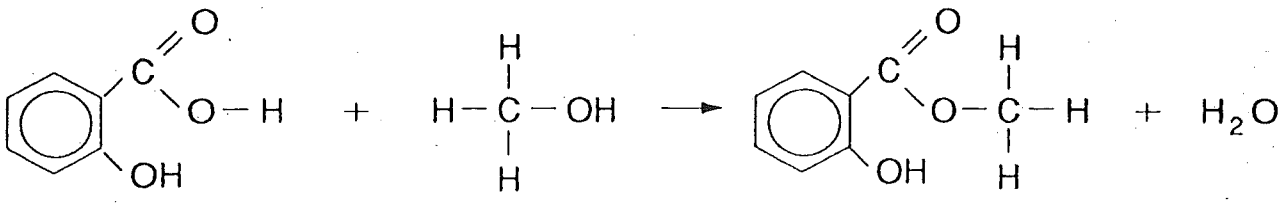
1. The alcohol part of the ester is named as an alkyl group first.

2. The acid part of the ester is named second. In naming the acid part, drop the ending "ic" and replace it with "ate."

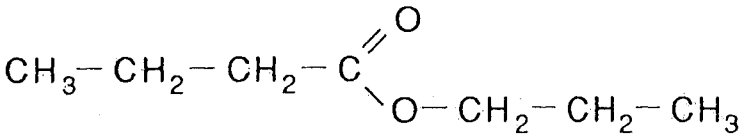
Examples:



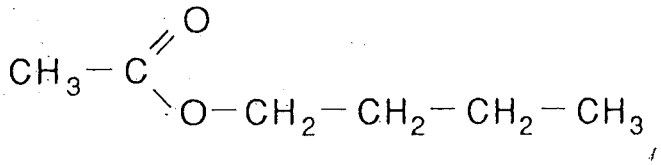
pentanoic acid ethanol ethyl pentanoate



salicylic acid methanol methylsalicylate



propyl butanoate



butyl ethanoate

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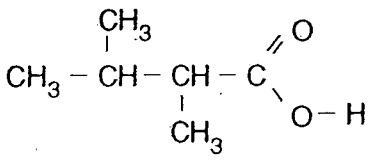
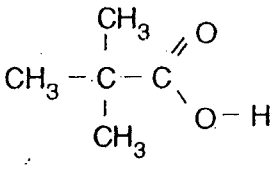
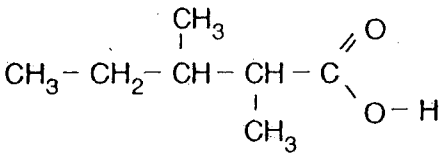
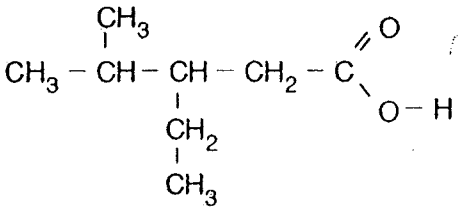
Problems: Carboxylic Acids and Esters

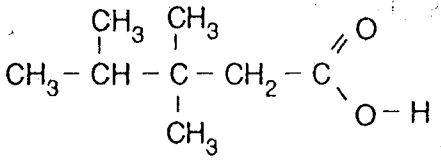
1. Name the following carboxylic acids:

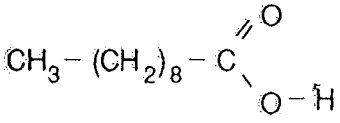
a. 

b. 

c. 

d. 

e. 

f. 

2. Draw structural formulas for the following carboxylic acids:

a. hexanoic acid

b. heptanoic acid

c. 2,2-dimethylbutanoic acid

d. 3,3-dimethylpentanoic acid

e. 3-ethylheptanoic acid

f. 3-methylbenzoic acid

3. Write structural formulas and give the IUPAC name for the esters formed in these esterification reactions:

a. methanoic acid + ethanol →

b. butanoic acid + 2-propanol →

c. ethanoic acid + 1-pentanol →

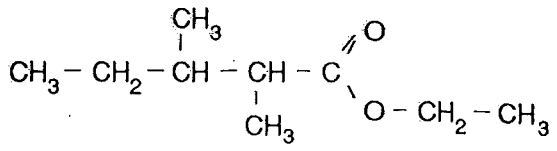
d. propanoic acid + 1-butanol →

e. benzoic acid + ethanol →

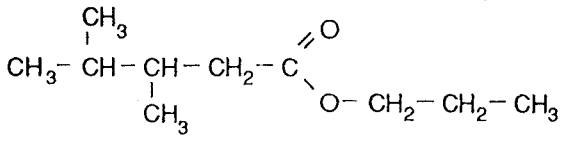
f. hexanoic acid + 2-butanol →

4. Name the following esters:

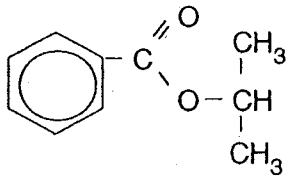
a.



b.



c.



5. Write the equations to describe the making of

a. pentyl propanoate (apricot flavor)

b. octyl ethanoate (orange flavor)

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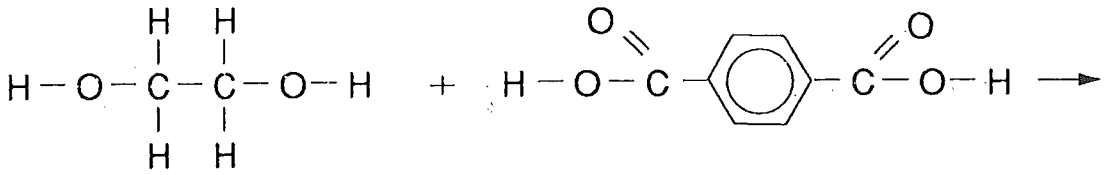
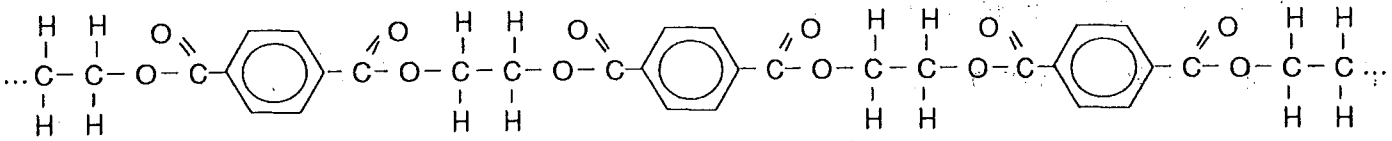
CONDENSATION POLYMERIZATION

In a condensation polymerization reaction simpler molecules (monomers) combine to form a giant molecule (polymer) and a bi-product. Each time a bond is formed between the monomer molecules a molecule of the bi-product is formed. For example, 1,4-benzenedicarboxylic acid reacts with 1,2-ethanediol to form a polyester. The giant molecule contains many ester functional groups--a polyester.



1,2-ethanediol + 1,4-benzenedicarboxylic acid →

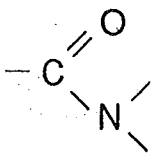


A Polyester

Condensation polymerization also occurs between carboxylic acids and amines to form a polyamide.

AMIDES

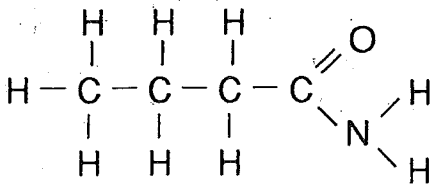
The general formula for an amide is $RCONR_2$

The functional group of an amide is 

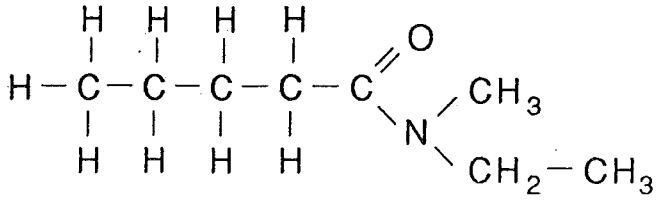
Amides are formed from the reaction of a carboxylic acid with ammonia.

AMIDE NOMENCLATURE

Drop the last "e" from the corresponding alkane name and replace it with the suffix of "-amide." Name any alkyl groups bonded to the nitrogen atom first.



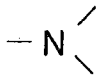
butanamide



methyl-ethyl-pentanamide

AMINES

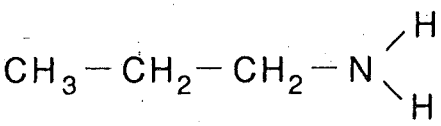
The general formula of an amine is R_3N

The functional group of an amine is 

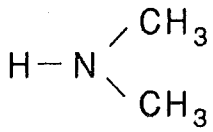
Amines are most commonly formed from the reaction of alkyl halides with ammonia.

AMINE NOMENCLATURE

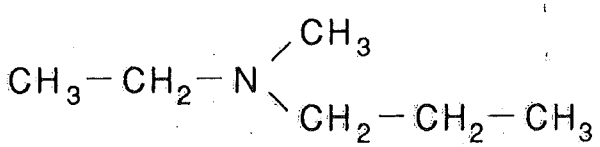
Name the alkyl groups that are bonded to the nitrogen functional in increasing order of size.



propylamine
(primary amine)



dimethylamine
(secondary amine)

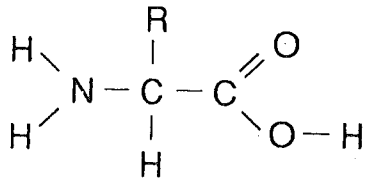


methyl-ethyl-propylamine
(tertiary amine)

The amine is said to be primary with one alkyl group only bonded to the nitrogen atom. With two alkyl groups bonded to the nitrogen atom it is a secondary amine, and with three alkyl groups bonded to the nitrogen atom it is a tertiary amine.

AMINO ACIDS

The general formula for an amino acid is:



The functional groups for amino acids are both the amine and carboxylic acid functional groups.

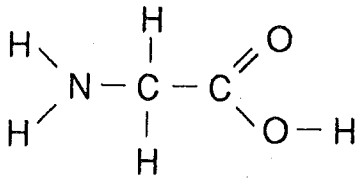
AMINO ACID NOMENCLATURE

Since there are only twenty amino acids known in nature, they each have individual names and there is no systematic way of naming them.

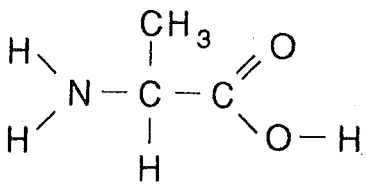
IMPORTANCE OF AMINO ACIDS

Amino acids are the monomers that form protein molecules. The acid end of one molecule bonds to the amine end of another form an amide bond or link. Proteins can have thousands of these monomer units.

Examples:



glycine



alanine

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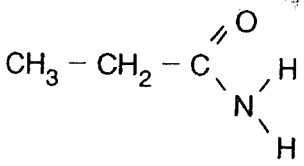
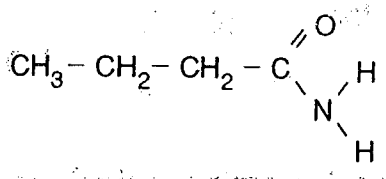
Problems: Amides and Amines

1. Name the following amides:

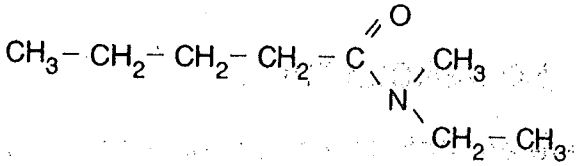
a.



b.



c.



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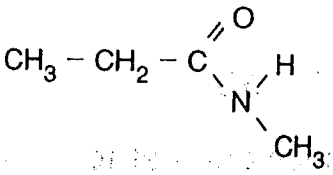

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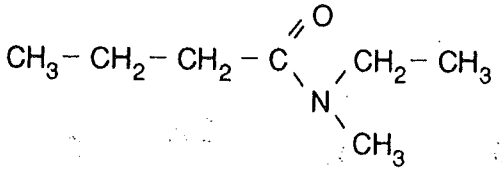

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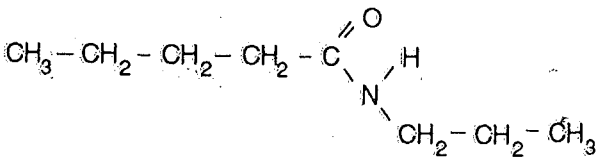


2. Draw structural formulas for the following amides:

a. ethanamide

b. methylpropanamide

c. methylethylpropanamide

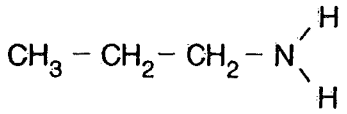
d. dimethylhexanamide

e. ethylpropylhexanamide

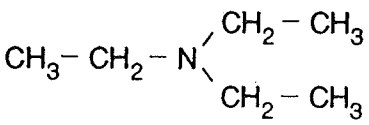
f. heptanamide

3. Name the following amines:

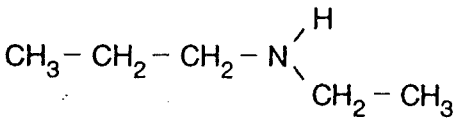
a.



b.



c.



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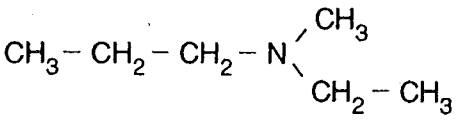

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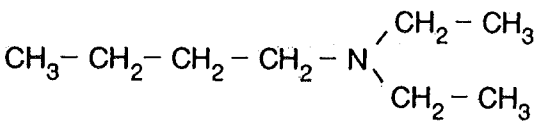

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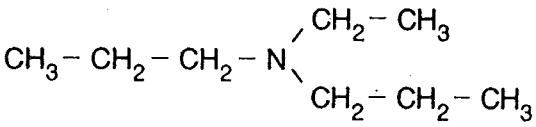


b. diethylmethylamine

c. tripropylamine

d. dimethylbutylamine

e. heptylamine

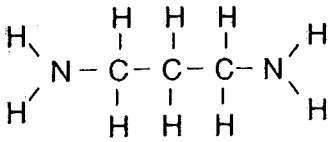
f. methyloctylamine

4. Draw structural formulas for the following amines:

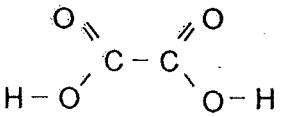
a. ethylmethylamine

5. Classify the amines in questions 3 and 4 as primary, secondary, or tertiary amines.

6. Two monomers are reacted in a condensation polymerization reaction:



and



1,3-diaminopropane oxalic acid

Draw a segment of the polyamide that can be formed by the condensation polymerization of these two monomers.

* * * * * * * * * * *

Multiple Choice Test: Organic Chemistry

1. Esters are formed by reaction of

   A. an alkane and an alkene
   B. an organic acid and an inorganic acid
   C. an organic acid and an alcohol
   D. an alcohol and water

2. Which of the following is likely to have the highest boiling point?

   A. CH_4
   B. C_4H_{10}
   C. CH_3CH_3
   D. C_7H_{16}

3. Which of the following is likely to be most soluble in water?

   A. CH_4
   B. CH_3OH
   C. $C_{14}H_{30}$
   D. C_6H_6

4. The carbon-carbon bonds in benzene are

   A. identical to the carbon-carbon bonds in cyclohexane
   B. identical to the carbon-carbon bonds in cyclohexene
   C. a hybrid between a double and single bond
   D. easily broken in chemical reactions

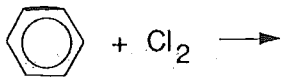
5. Which of the following is NOT a property of alkanes?

   A. They are soluble in water.
   B. They have weak intermolecular attraction
   C. The boiling point increases as the number of carbons increase.
   D. They are unreactive at room temperature.

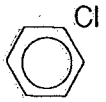
6. The coefficients for the balanced equation for the reaction
   $\_\_C_5H_{12} + \_\_O_2 \rightarrow \_\_CO_2 + \_\_H_2O$ are

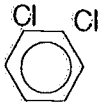
   A. 1, 8, 5, 6
   B. 0, 8, 5, 6
   C. 1, 16, 5, 6
   D. 2, 16, 10, 12

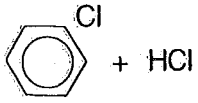
7. The product(s) of the reaction

   is (are)

   A. 

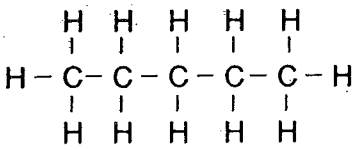
   B. 

   C. 

   D. no reaction occurs

8. Which compound is not an isomer of the other three compounds?

A.



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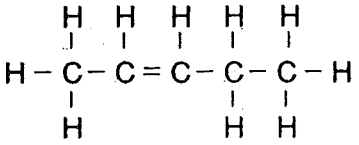

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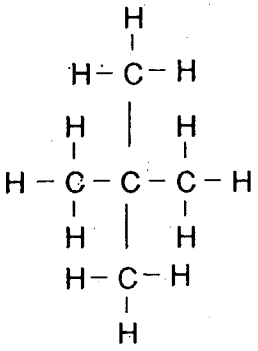
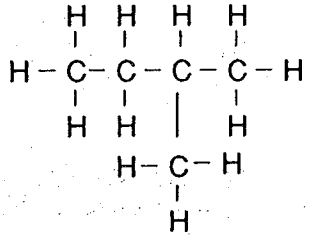


D.



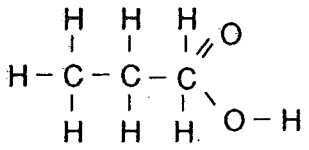
9. Which of the following is a homologous series?

A. C_2H_6, C_2H_4, C_2H_2
B. C_2H_2, C_3H_5, C_4H_8
C. C_2H_6, C_3H_8, C_4H_{10}
D. C_2H_2, $C_2H_2O_2$, $C_2H_2O_2N_2$

10. The balanced equation for the combustion of 2-methyl-1-butene is

A. $C_5H_{12} + 8O_2 \rightarrow 5CO_2 + 6H_2O$
B. $2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$
C. $2C_5H_{10} + 15O_2 \rightarrow 10CO_2 + 10H_2O$
D. $2C_6H_{14} + 19O_2 \rightarrow 12CO_2 + 14H_2O$

11. 1.



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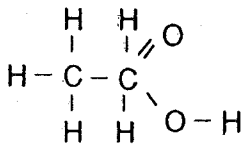
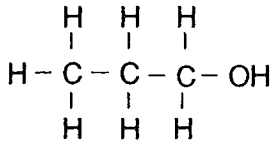
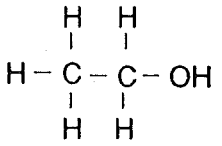


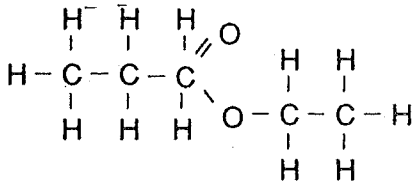
3.



4.



Which of the above two reactants will form the following compound:

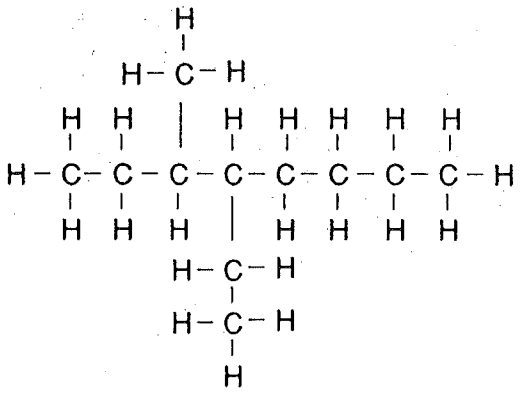


A. 1 and 3
B. 1 and 4
C. 2 and 4
D. 2 and 3

12. The name of the compound formed in question 11 is:

A. ethyl propanote
B. 3,3,dioxypentane
C. propyl ethanate
D. propylethylester

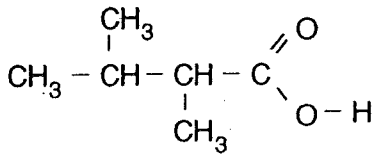
13. The name of the following compound is



A. 5-methyl-6-methyloctane
B. 3-methyl-4-ethyloctane
C. 4-ethyl-3-methyloctane
D. 3-methyl-5-butylhexane

Use the following compounds to answer the next two questions.

1.



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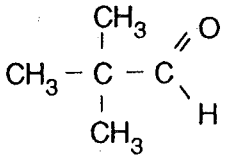

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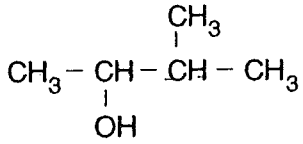

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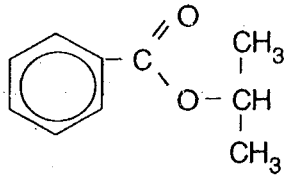

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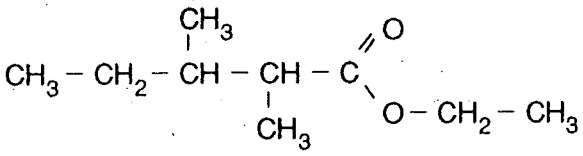

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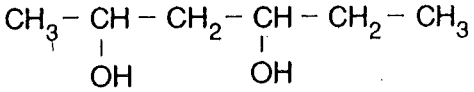


14. A compound(s) which is an alcohol is(are)

A. 1 only
B. 2 only
C. 3 and 6
D. 4 and 5

15. A compound(s) which is an ester is(are)

A. 1 only
B. 2 only
C. 3 and 6
D. 4 and 5

16. A compound which is an aldehyde is

A. 1
B. 2
C. 4
D. 6

---

17. The saturated compound is

A. propene
B. octane
C. 3-heptyne
D. 2-butene

18. When Cl_2 is mixed with propane, what type of reaction will occur?

A. a combustion reaction
B. a substitution reaction
C. an addition reaction
D. no reaction

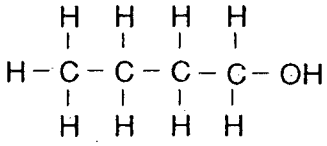
19. When Cl_2 is mixed with propene, what type of reaction will occur?

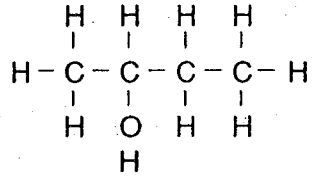
A. a combustion reaction
B. a substitution reaction
C. an addition reaction
D. no reaction

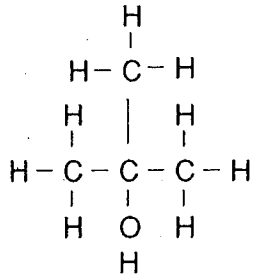
20. The formula which represents an alkyne is

A. C_5H_8
B. C_5H_{12}
C. C_5H_{10}
D. C_5H_{12}

21.







Which is the UNTRUE statement about the above three alcohols?

A. They are isomers of each other.
B. They all have the same physical and chemical properties.
C. They are examples of primary, secondary and tertiary alcohols.
D. They all have the same molar mass.

22. When methanol is combined with oxygen gas as shown in the equation below, the missing product will be

$$2CH_3OH_{(l)} + \frac{1}{2}O_{2(g)} \rightarrow 2\,\_\_\_\_\_ + H_2O_{(l)}$$

A. $CO_{2(g)}$
B. $CH_2O_{(l)}$
C. $CH_{4(g)}$
D. $CO_{(g)}$

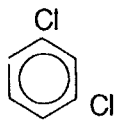
23. Cis and trans isomers can occur in an

A. alkane
B. alkene
C. alkyne
D. aromatic

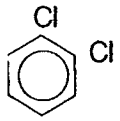
24. An artificial rum flavoring is ethylmethanoate. Ethylmethanoate is

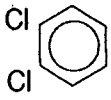
A. an acid
B. an alcohol
C. an ester
D. a ketone

25. The structural formula for 1,3-dichlorobenzene is

A. 

C. 

B. 

D. 

Answer Key

1. C	2. D	3. B	4. C
5. A	6. A	7. C	8. B
9. C	10. C	11. B	12. A
13. B	14. C	15. D	16. B
17. B	18. B	19. C	20. A
21. B	22. B	23. B	24. C
25. A			

NAME:_____

BLOCK: ___; DATE: _____

ORGANIC COMPOUNDS - A REVIEW

I. DRAW EACH ORGANIC MOLECULE:

1. 2-methylhexane

2. bromocyclopentane

3. trans-3-methyl-~~trans~~-2-heptene

4. 6-bromo-4-ethyl-1-octyne

5. 1,2 dibromo-3-propylbenzene

6. ~~Trans~~-3-nonene

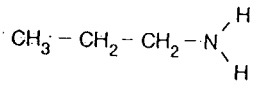
7. Cis-3,4-dimethyl-3-hexene

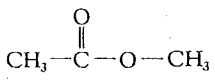
8. 3-pentanol

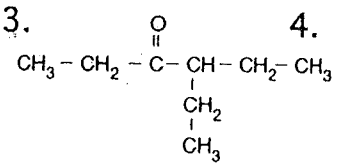
9. 5-ethyl-4-propyl-2-heptyne

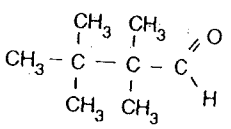
10. 2,2-dimethyl-1-propanol.

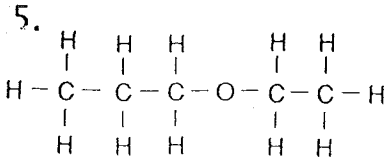
II. IDENTIFY THE FUNCTIONAL GROUP OF EACH MOLECULE SHOWN BELOW:

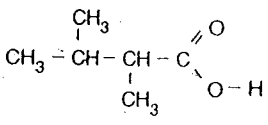
1. 

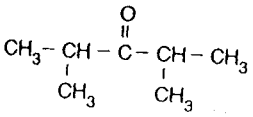
2. 

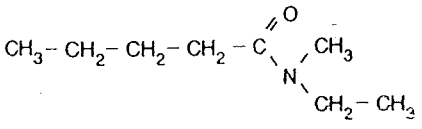
3. 

4. 

5. 

6. 

7. 

8. 

III. NAME EACH MOLECULE SHOWN BELOW:

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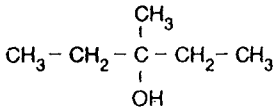

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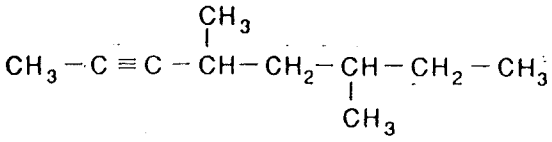

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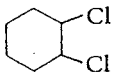

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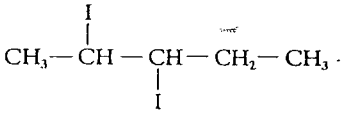

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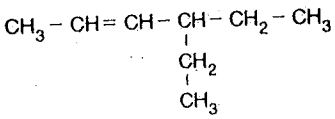

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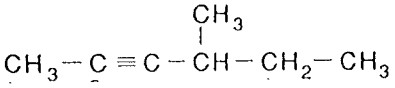

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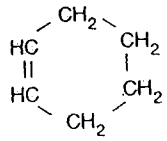

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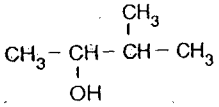

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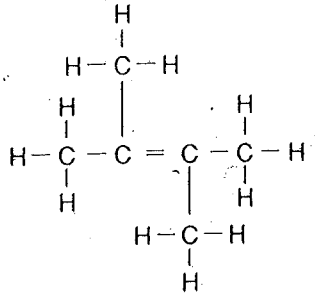

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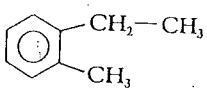

NAME:_____

BLOCK: ___; DATE: _____

REACTIONS OF ORGANIC COMPOUNDS

FORMING ESTERS

PURPOSE: To prepare several different esters and to identify them by odour.

BACKGROUND INFORMATION:

Esters can be prepared by reacting an alcohol (-OH) with an organic acid (-COOH). Organic acids tend to have a sharp, pungent or biting odour (ex. ethanoic acid = vinegar; butanoic acid = smelly feet odour) while alcohols also tend to have sharp or unpleasant odours. Esters on the other hand generally smell pleasant and are often used as flavouring/scent agents in fruit or floral products.

A typical esterification reaction is shown below:

MATERIALS: (per group of 4)

- dropper bottles of alcohols and acids;
- thermometer
- 6 small test tubes
- goggles
- 2 large beakers and hotplate
- 3, 50 mL beakers
- wash bottle
- test tube tongs

PROCEDURE:

1. Fill the large beaker half full of water and heat to about 70°C.
2. Label your test tubes (A to F).
3. Place 1 mL (2 droppers full, about a baby finger's depth) of each acid and alcohol into 3 test tubes.
4. Add 4 drops of 18.0 M H_2SO_4.
5. Place an inverted 50 mL beaker over top of the mouth of each test tube in case of any eruption of the reactants during heating.
6. Place the test tubes in the water bath and heat for about 10 minutes.
7. After 10 minutes of heating, remove the test tubes and place them in a second beaker full of cold tap water to cool.
8. After they have cooled for a few minutes, use the wash bottle to increase the volume in each test tube to about half full.
9. Detect the presence of the ester by 'wafting' the odour of the compound towards you.
10. Describe the odour in the table below.
11. Swap test tubes with another groups and smell their esters.

OBSERVATIONS:

Test Tube	Organic Acid	Alcohol	Odour of ester
A	1 mL ethanoic acid	1 mL ethanol	
B	1 g salicylic acid	1 mL methanol	
C	1 mL butanoic acid	1 mL ethanol	
D	1 mL ethanoic acid	1 mL 1-pentanol	
E	1 mL ethanoic acid	1 mL 1-octanol	
F	1 mL butanoic acid	1 mL 1-pentanol	

ANALYSIS:

Complete the chart below for of the 3 esters that your group smelled:

Structure of acid	Structure of alcohol	Structure of ester