

INDEPENDENT STUDY

Term 1

Objective – you are to learn how to name organic molecules according to the IUPAC rules.

The following sheets describe the naming process and although they are quite thorough there have been some changes regarding prioritising and alphabetizing of substituents in the name of the molecule. For this reason some of the examples will be named slightly improperly. Make the corrections according to clarification by your teacher.

TIMELINE

Quiz 1 – ane, ene, yne, cyclo

Quiz 2 – halo, amino, nitro

In Class Assignment – lab, work period

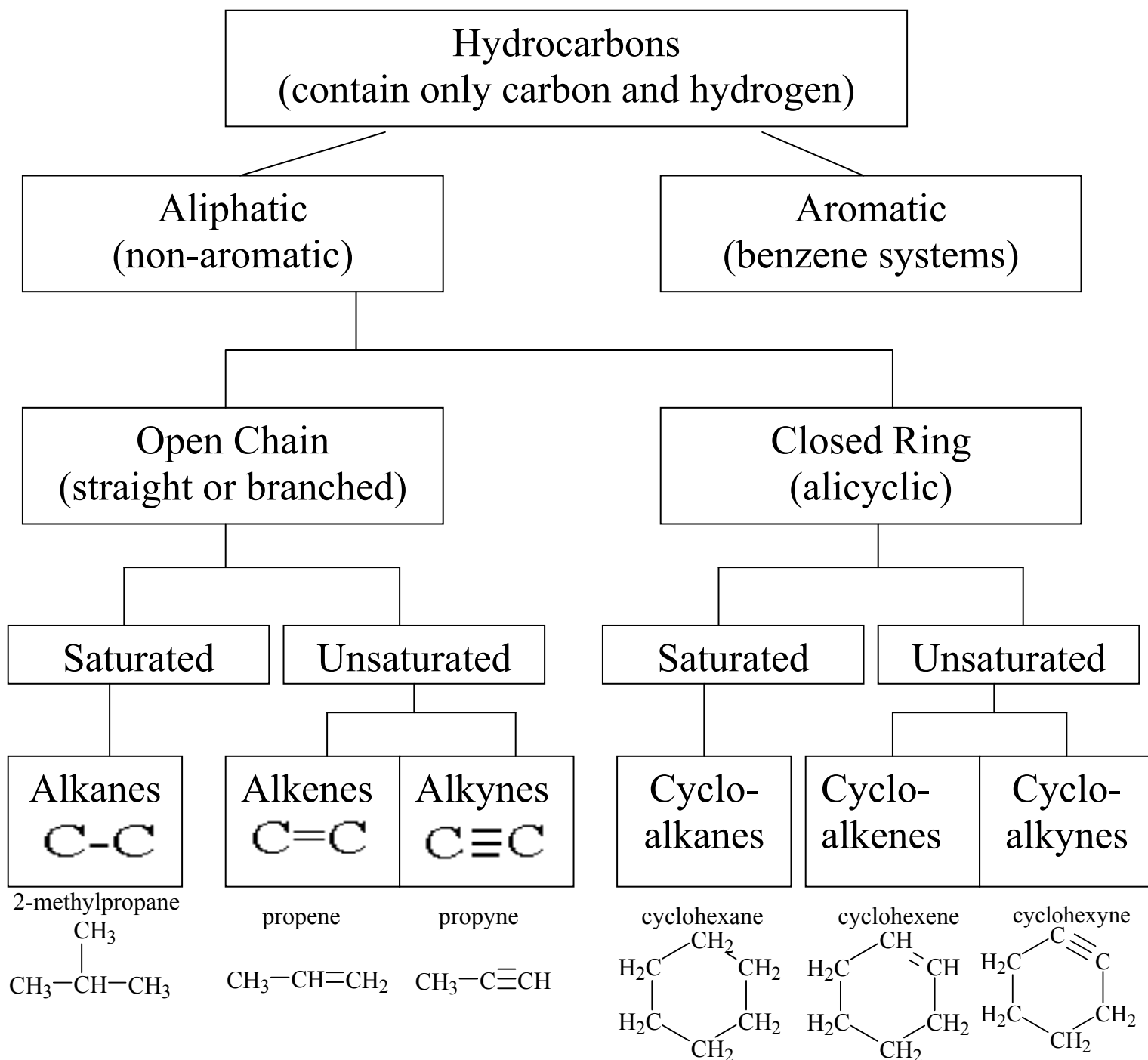
Test 1 – ane, ene, yne, cyclo, halo, amino, nitro

Quiz 3 – ether, alcohol, aldehyde, ketone

Quiz 4 – carboxylic acid, ester, amide, aromatics

Test 2 – everything

Classification of Hydrocarbons



Aliphatic – chains or rings that do not contain alternating bonds

Aromatic – rings that contain alternating double bonds

Saturated – all C-C bonds are single bonds

Unsaturated – at least one C-C bond is double or triple

Which is bad for you-saturated or unsaturated? Why?

I.U.P.A.C. RULES for NAMING ALKANES

1. The longest continuous chain is chosen as the root name of the compound.

Branches !!

The Unbranched Alkanes

Name	Alkyl Name	# of C's	Formula	Structure
Methane	methyl	1	CH ₄	CH ₄
Ethane	ethyl	2	C ₂ H ₆	CH ₃ CH ₃
Propane	propyl	3	C ₃ H ₈	CH ₃ CH ₂ CH ₃
Butane	butyl	4	C ₄ H ₁₀	CH ₃ (CH ₂) ₂ CH ₃
Pentane	pentyl	5	C ₅ H ₁₂	CH ₃ (CH ₂) ₃ CH ₃
Hexane	hexyl	6	C ₆ H ₁₄	CH ₃ (CH ₂) ₄ CH ₃
Heptane	heptyl	7	C ₇ H ₁₆	CH ₃ (CH ₂) ₅ CH ₃
Octane	octyl	8	C ₈ H ₁₈	CH ₃ (CH ₂) ₆ CH ₃
Nonane	nonyl	9	C ₉ H ₂₀	CH ₃ (CH ₂) ₇ CH ₃
Decane	decyl	10	C ₁₀ H ₂₂	CH ₃ (CH ₂) ₈ CH ₃

2. The numbering of the carbon chain starts from the end of the chain which gives the lowest numbering system to all of the substituents. Numbering can start from either end!
3. The substituents are then named in alphabetical order.
4. Numbers and words are separated by a dash. ex: 3-ethyl
5. Numbers are separated by a comma. ex. 3,3-dimethyl
6. Every substituent must have a number. If there are two or more of the same substituent a prefix is used to indicate the number of identical substituents. ex. 1,1,4-trimethyl
7. The last substituent and the root name are one word.
8. In the alphabetical order, prefixes such as di, tri, tetra etc. do not count but iso and cyclo do count.
9. If the parent forms a ring, use the prefix "cyclo" before the parent name.
10. Cis isomers are substituents on the same side of a double bond and trans isomers have substituents on opposite sides of the double bond.

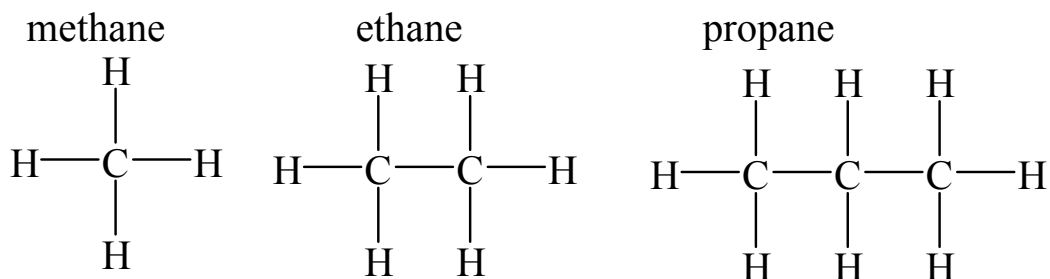
Organic Chemistry

Organic chemistry is defined as the chemistry of CARBON. The properties of organic compounds are governed by:

- a series of carbon atoms linked together to form a stable, almost completely unreactive framework or molecular skeleton to which we add
- a series of different reactive groups which determine the basic chemistry of the molecule.

PART 1 – ALKANES, ALKENES, ALKYNES AND CYCLO

Carbon atoms have four bonds. The basic hydrocarbons are shown in the previous chart but the structures are as follows:



A hydrocarbon containing only single bonds is called an **alkane**.

An alkane is said to be SATURATED since all the carbon atoms in an alkane are bonded to four other atoms (four bonds is the maximum number of bonds for carbon) and hence its bonding capacity has been used up, or saturated.

The general formula for an alkane is $\text{C}_n\text{H}_{2n+2}$.

In order to build up complicated hydrocarbons we attach groups of carbon atoms called an ALKYL GROUP or a SIDE CHAIN or a SUBSTITUENT to the main carbon backbone. To do this a hydrogen must be removed from the parent chain. The alkyl group is already one hydrogen short so the bond happens where the hydrogen is missing.

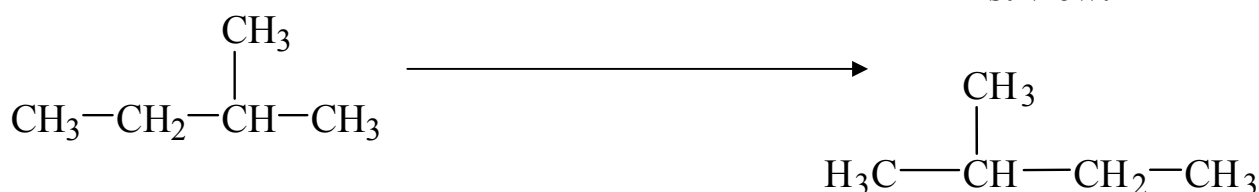
Ex:	<u>Parent</u>	<u>alkyl group</u>
	methane = CH ₄	methyl = -CH ₃
	ethane = CH ₃ -CH ₃	ethyl = -CH ₃ -CH ₂

Note: The name of the hydrocarbon group is obtained by changing the “ane” ending to an “yl” ending. Alkyl groups cannot exist on their own. They must be attached to some molecule.

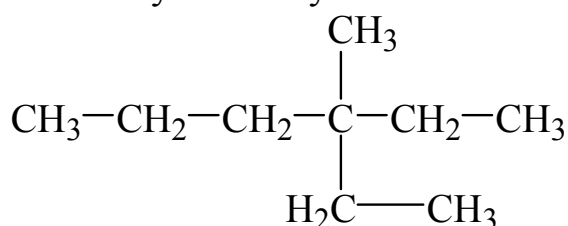
Examples

2-methylbutane (note - this is one word!)

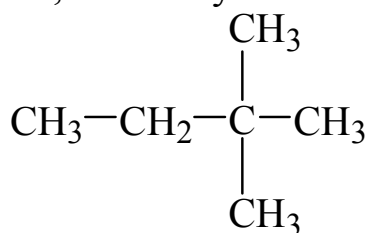
The structure can be viewed from the other side but this is identical to the first view.



3-ethyl-3-methylhexane

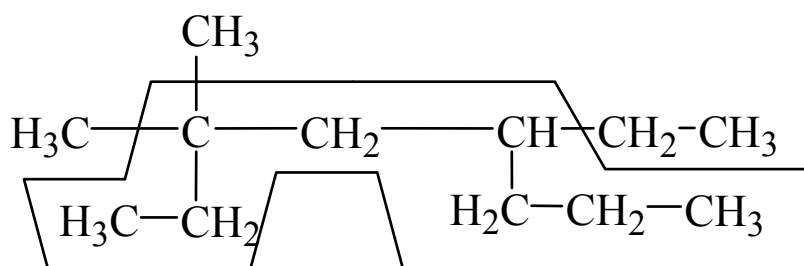


2,2-dimethylbutane

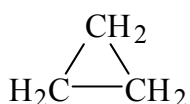


NOT: 2-dimethylbutane or
2-methyl-2-methylbutane

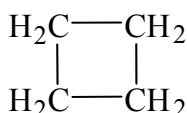
5-ethyl-3,3-dimethyloctane



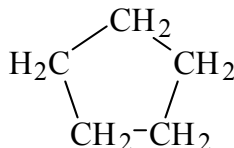
cyclopropane



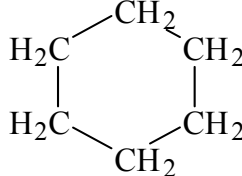
cyclobutane



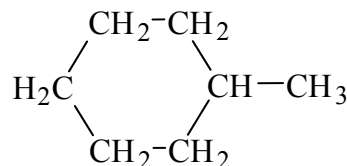
cyclopentane



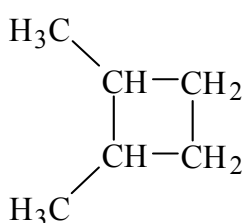
cyclohexane



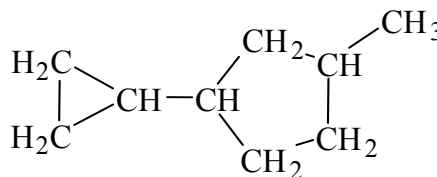
methylcyclohexane



1,2-dimethylcyclobutane



1-cyclopropyl-3-methylcyclopentane



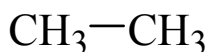
Note:

- 1) No number is used for a single substituent on a ring since all ring positions are equivalent.
- 2) When more than one substituent is present, the first is placed at the "1" position of the ring. (lowest numbering system possible)
- 3) A cyclic substituent is named like a simple straight chain substituent except for the prefix "cyclo"
- 4) Substituents with no number are assumed to be on carbon#1.
ie: 1-cyclopropylhexane is the same as cyclopropylhexane.

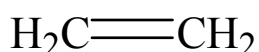
Unsaturated Hydrocarbons: Alkenes and Alkynes

If insufficient numbers of atoms are available to give each carbon four bonds then the hydrocarbon is said to be unsaturated and the molecule will have DOUBLE (alkene) or TRIPLE (alkyne) bonds.

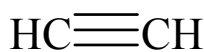
ethane



ethene



ethyne



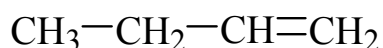
unsaturated

To indicate that a hydrocarbon contains a double bond we change the ANE ending of the parent to ENE. The parent name for a complex hydrocarbon is determined by the longest chain

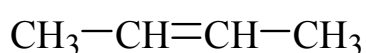
CONTAINING THE DOUBLE OR TRIPLE BOND. The position of the DOUBLE OR TRIPLE BOND HAS TO BE NUMBERED AS LOW AS POSSIBLE. This lowest numbering for the multiple bond takes priority over the lowest numbering system rule. You will see that any time the parent name changes its ending those substituents that changed the ending have this priority over the normal lowest numbering system rule.

Examples

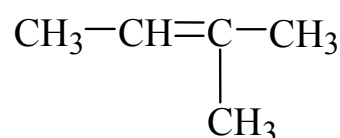
1-butene



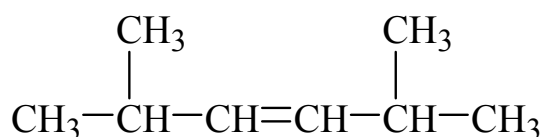
2-butene



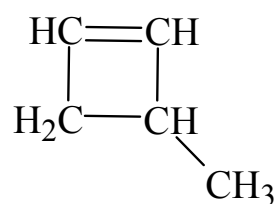
2-methyl-2-butene



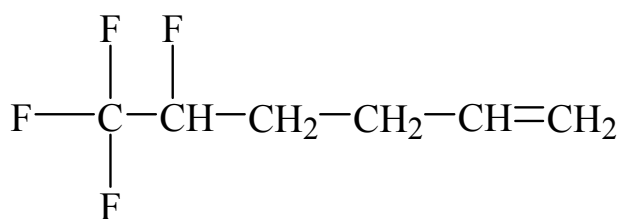
2,5-dimethyl-3-hexene



3-methylcyclobutene

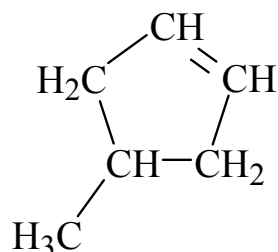


5,6,6,6-tetrafluoro-1-hexene



(not 1,1,1,2-tetrafluoro-5-hexene)

4-methylcyclopentene



Note:

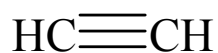
- 1) The location of the double bond is given as the lowest carbon of the double bond ie: 1-butene above.
- 2) In cycloalkenes and cycloalkynes the multiple bond **must** be carbon 1 and carbon 2. You cannot have a multiple bond between the first and last carbon of a ring in order to get a lower numbering system for the substituents.

The general formula for alkenes is C_nH_{2n} .

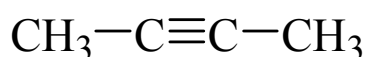
To indicate a triple bond the “ANE” ending of the parent is changed to “YNE”. The same naming procedure as alkenes is followed and the same priority is applied to triple bonds (alkynes).

Examples

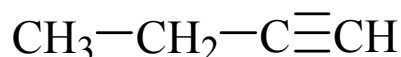
ethyne



2-butyne



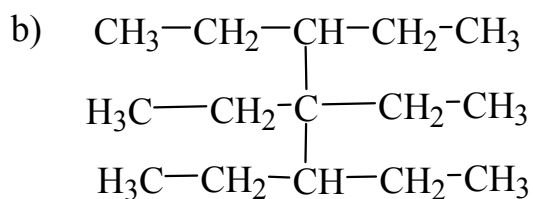
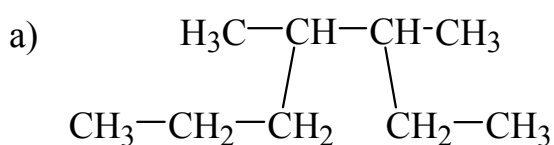
1-butyne

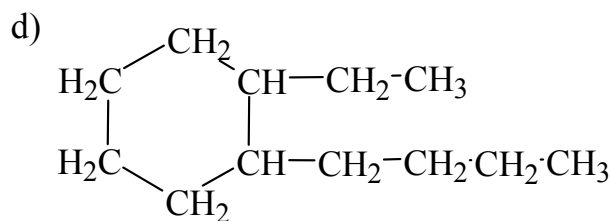
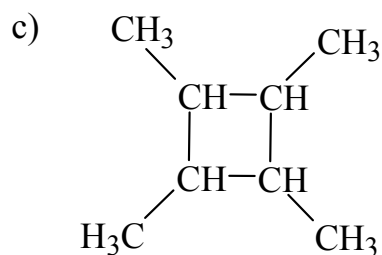


Exercises

1. Draw and name the 5 different isomers of C_6H_{14} . An isomer is a compound with the same molecular formula but a different connectivity of the atoms. ie: two molecules with the exact same atoms but with different structures.
2. Draw and name the 9 different isomers of C_7H_{16} .
3. Draw and name all the isomers of C_8H_{18} which have a single side chain.
4. Draw and name all the isomers of C_8H_{18} which have two side chains.
5. Draw the following:

a) 2-methyloctane	b) 4-ethyloctane
c) 2,3-dimethyloctane	d) 4-propylnonane
e) 2,3,4,5-tetramethylhexane	f) 4,6-diethyl-5-propylnonane
g) propylcyclopropane	h) 2-cyclopropylpropane
i) 3,3-diethylpentane	j) 1,2-dicyclobutylethane
6. Name the following.





7. Draw the following.

a) 1-hexyne

b) 3-heptene

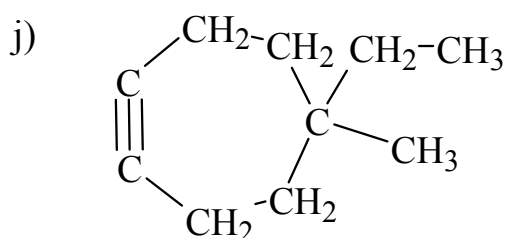
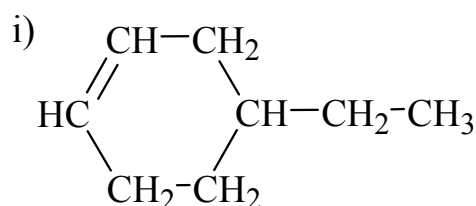
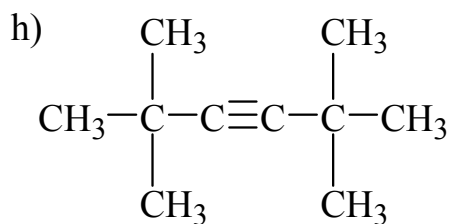
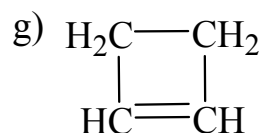
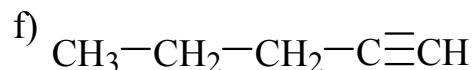
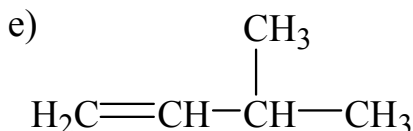
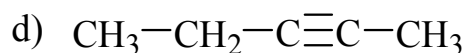
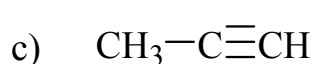
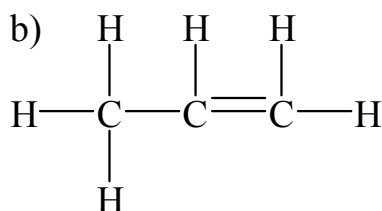
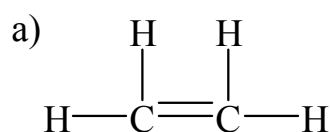
c) 3-methyl-2-pentene

d) 3-cyclopropyl-1-pentene

e) 1,2,3-trimethylcyclopropene

f) 1,1-dicyclopropyl-2-methyl-1-propene

8. Name the following.



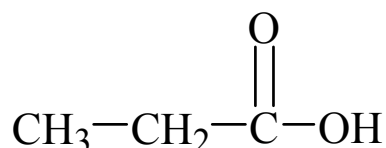
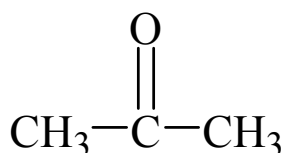
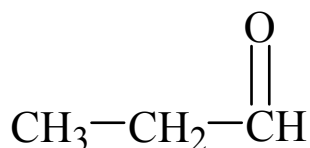
- 9) What is wrong with the following?
- a) 2-ethene
 - b) 2,2,2-trimethylpropane
 - c) 3,5-dimethyl-4-ethyl-4-hexene

Functional Groups

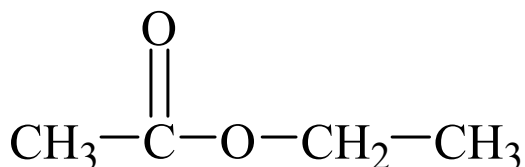
We shall now consider the special reactive groups called **FUNCTIONAL GROUPS** which can be attached to the hydrocarbon skeleton of the molecule. Each of the functional groups serves a special chemical function.

The functional groups we shall consider are:

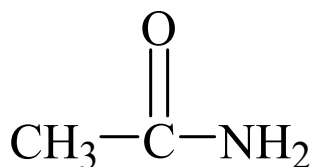
1. Halogens: F, Cl, Br, I
2. Amino: NH_2 , NHR , NR_1R_2 (R_1 and R_2 are alkyl groups)
3. Nitro: NO_2
4. Ether: $\text{R}_1\text{-O-R}_2$
5. Alcohol: OH
6. Aldehyde:
7. Ketone:
8. Carboxylic Acid



9. Ester:



10. Amide



PART 2 – HALO, AMINO, NITRO

Halogen, amine and nitro compounds are named in the same manner as hydrocarbons.

F = fluoro

Cl = chloro

Br = bromo

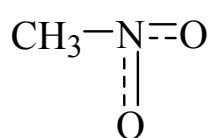
I = iodo

NH_2 = amino

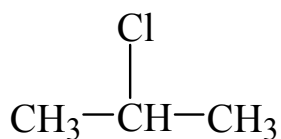
NO_2 = nitro

Examples

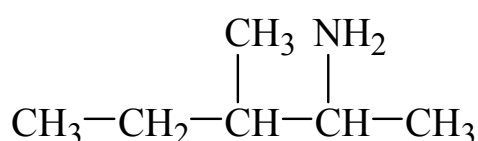
nitromethane



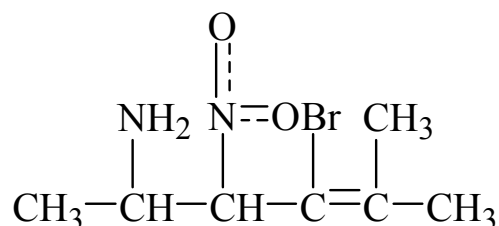
2-chloropropane



2-amino-3-methylpentane



5-amino-3-bromo-2-methyl-4-nitro-2-hexene

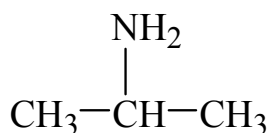


There is a special kind of substituted amino group which we must also consider. If one or more of the hydrogens on the NH_2 group are replacing by other groups we adopt the following naming scheme.

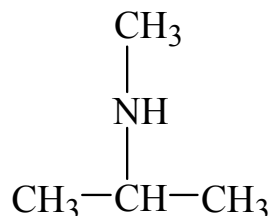
- 1) The names of the substituents on the amino group immediately precede the word amino in proper alphabetical order.
- 2) The alphabetical order for the molecule goes by the “a” of the amino not the letter of the group substituted onto the amino.

Examples

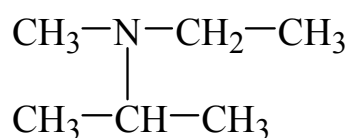
2-aminopropane



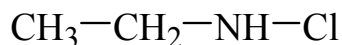
2-(methylamino)propane



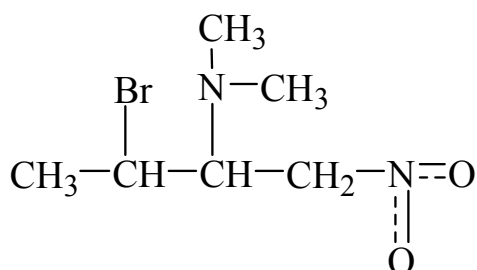
2-(ethylmethylamino)propane



(chloroamino)ethane



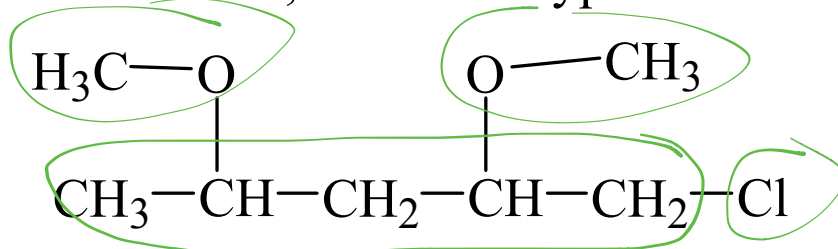
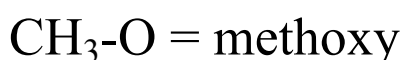
2-(dimethylamino)-3-bromo-1-nitrobutane



The dimethylamino group is only one word because it is only one substituent on the carbon chain.

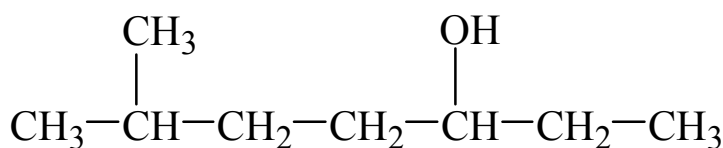
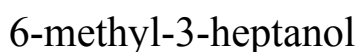
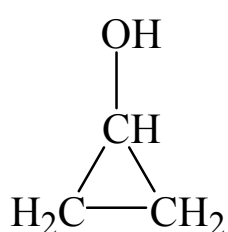
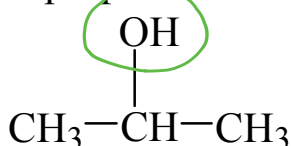
PART 3 – ETHER, KETONE, ALDEHYDE, ALCOHOL

An ETHER molecule consists of two hydrocarbon groups joined together by an oxygen atom. The larger of the two hydrocarbon groups is taken to be the parent hydrocarbon. The smaller group, together with the oxygen atom, is renamed by changing the ANE ending to OXY. The naming is similar to that of normal hydrocarbons. Ethers do not have priority in the numbering system. Examples



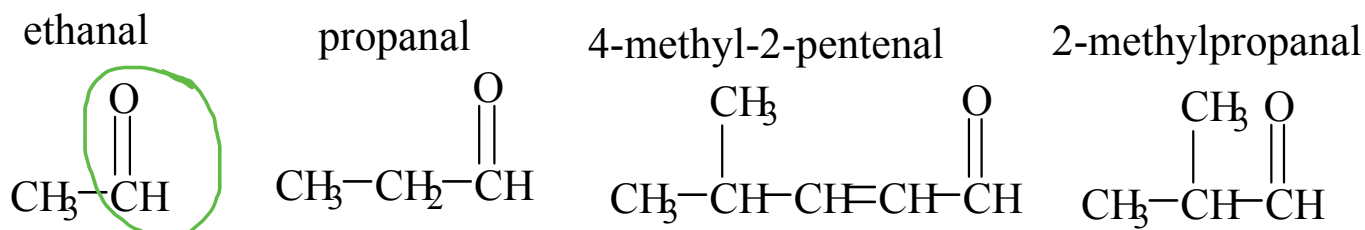
An ALCOHOL is an organic compound with an OH group. It is named as a derivative of the longest continuous carbon chain containing the OH group. The ANE of the parent group is changed to ANOL (ENE → ENOL; YNE → YNOL). The chain is numbered so as to give the OH group the lowest possible number. The ending of the parent is changed so the priority discussed earlier is in effect.

Examples



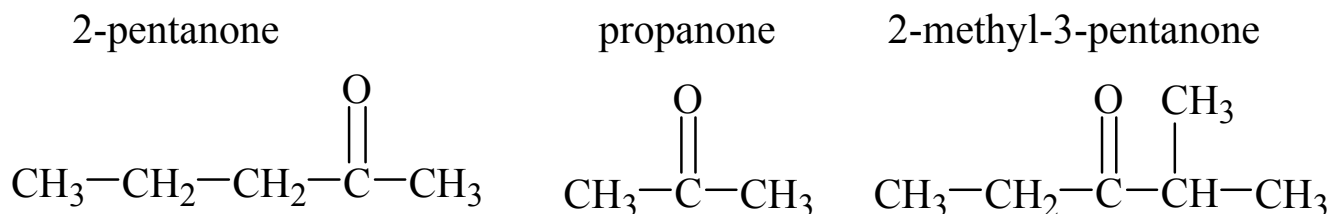
An ALDEHYDE is a hydrocarbon chain containing a double bonded oxygen on the end of the carbon chain. The C=O group is called the CARBONYL GROUP. The C=O group is always carbon number one as priority is in effect again. The parent name goes from ANE to ANAL. (ENE → ENAL; YNE → YNAL)

Examples



A KETONE is a hydrocarbon containing a carbonyl group that is not at the end of the chain. Again priority is in effect as the ending for the parent goes from ANE to ANONE. (ENE → ENONE; YNE → YNONE). The position of the carbonyl group is indicated by a number preceding the parent name.

Examples



PART 4 – CARBOXYLIC ACID, ESTER, AMIDE, AROMATIC

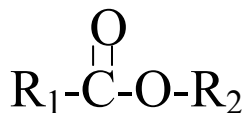
A CARBOXYLIC ACID is an organic compound containing a

$\overset{\text{O}}{\underset{\text{||}}{\text{C}}}-\text{OH}$ group (often shortened to COOH). The COOH group is called a CARBOXYL GROUP. Carboxylic acids are named by changing ANE to ANOIC ACID. Since the parent name is changed prioritization is again in effect and the carbon of the carboxyl group is always numbered as “1”.

Examples

CH₃COOH=ethanoic acid or H₂C=CH-CH₂COOH=3-butenic acid
 Br-CH₂-CH₂-COOH=3-bromopropanoic acid

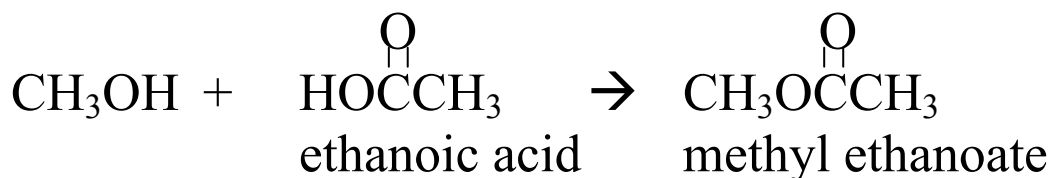
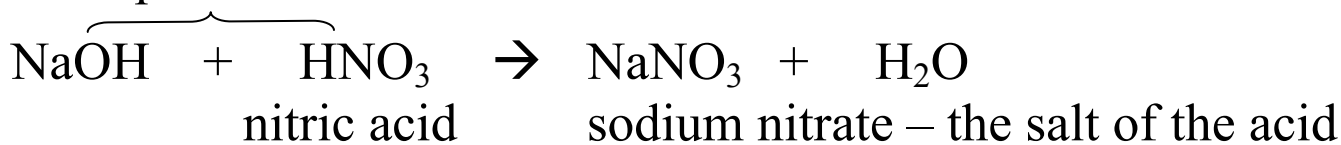
An ESTER is a compound made by combining a carboxylic acid with an alcohol and is written as



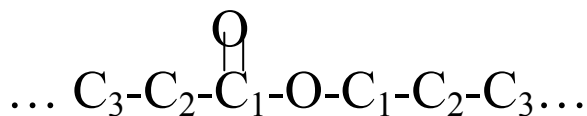
Esters are named like inorganic salts. The hydrocarbon part of the alcohol is named first AS A SEPARATE WORD, followed by the name of the acid with the IC ACID changed to ATE. Note in all of the naming thus far, the ester is the only name to contain a space!

Note: Numbering of the acid part starts with the carbon of the carboxyl group as number 1. The alkyl group is numbered with the carbon nearest the carboxyl group as number 1. There are two number sets for the same molecule.

Example

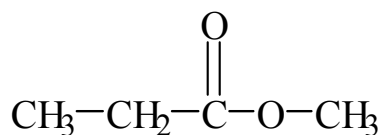


Numbering is as follows

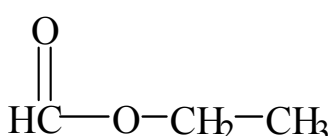


Examples

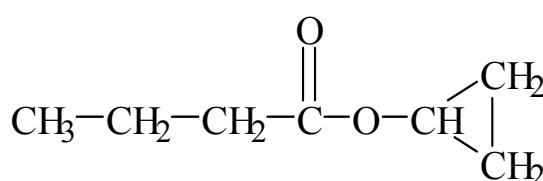
methyl propanoate



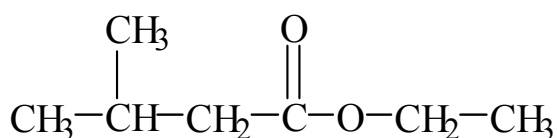
ethyl methanoate



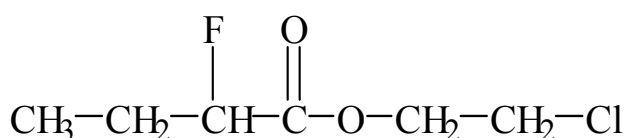
cyclopropyl butanoate



ethyl 3-methylbutanoate



2-chloroethyl 2-fluorobutanoate

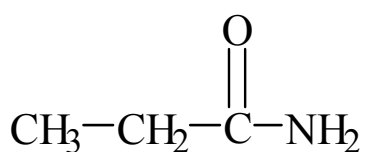


An AMIDE is an organic compound containing a $\begin{array}{c} \text{O} \\ \parallel \\ \text{C}-\text{NH}_2 \end{array}$

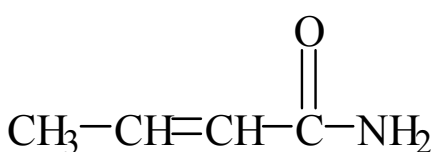
at the end of the chain. Amides are named by dropping the ANE and adding ANAMIDE. Since the parent name changes, priority is in effect for the numbering system with the C of the amide group always being carbon number “1”.

Examples

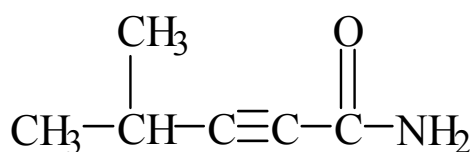
propanamide



2-butenamide



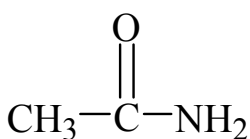
4-methyl-2-pentynamide



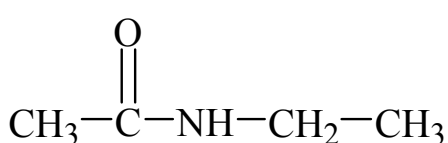
Amides can also have the hydrogen on the amide group substituted with another functional group. When this happens the functional group is numbered as “N-“ to show that it is on the amide part of the molecule. This “N-“ is just a number and goes in the name of the molecule following the normal alphabetizing rules for substituents.

Examples

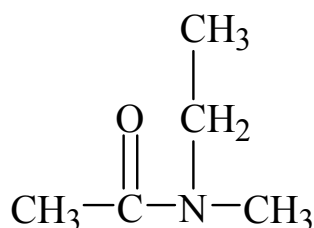
ethanamide



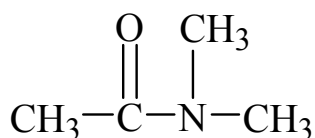
N-ethylethanamide



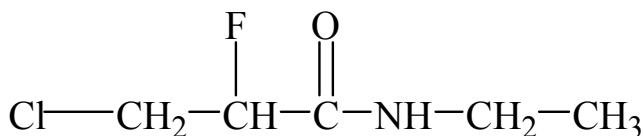
N-ethyl-N-methylethanamide



N,N-dimethylethanamide



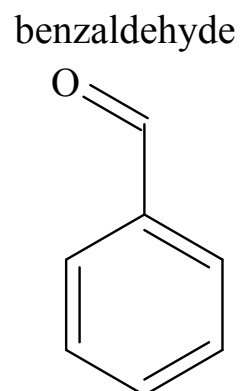
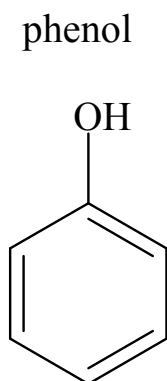
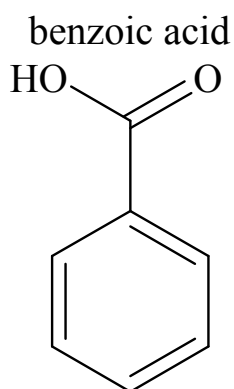
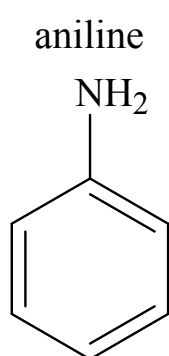
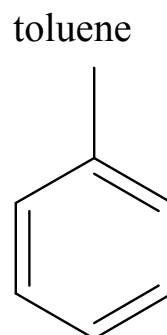
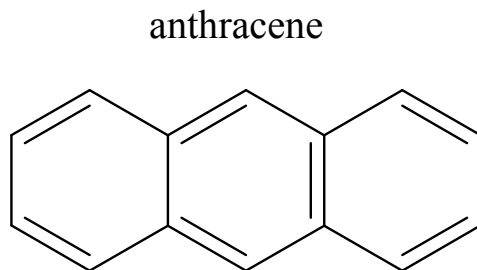
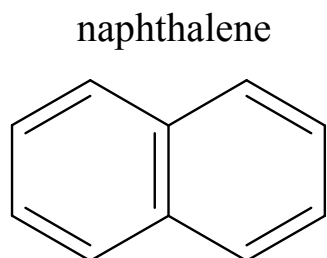
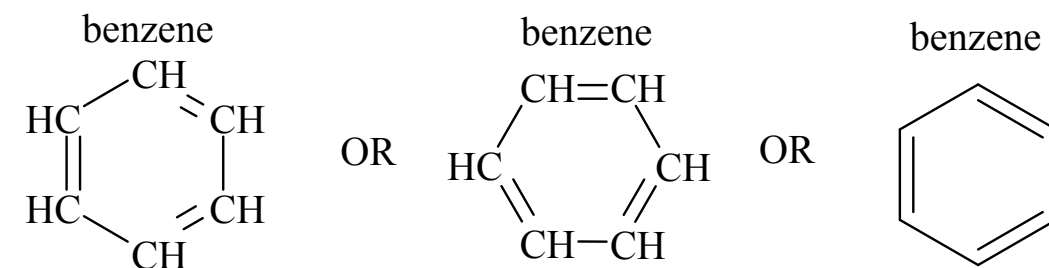
3-chloro-N-ethyl-2-fluoropropanamide



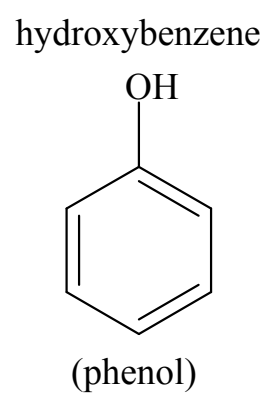
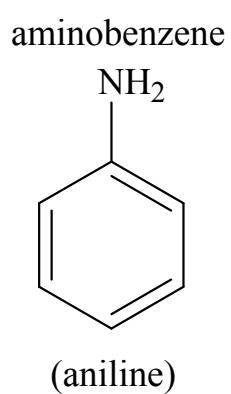
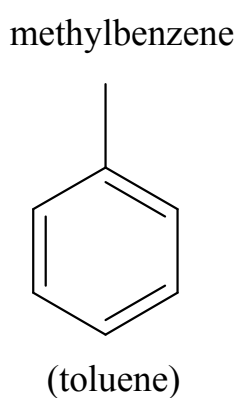
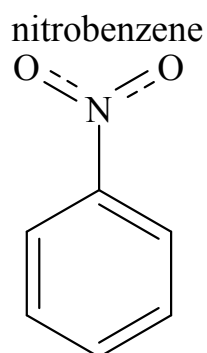
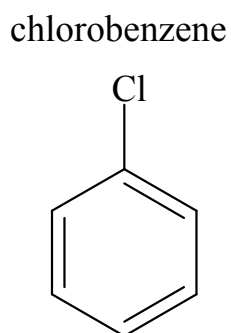
An AROMATIC compound can be thought of as compounds containing at least one BENZENE ring. The alternating double bond structure of aromatics gives them special properties like stability and distinctive odours – hence the term aromatic.

Examples

Naming aromatics.



1) Single substituents

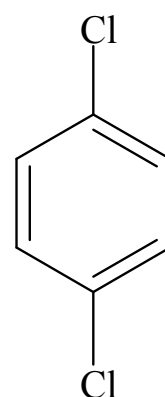
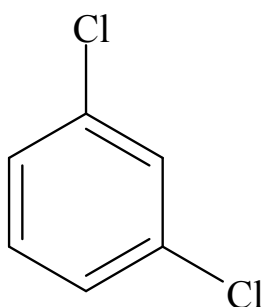
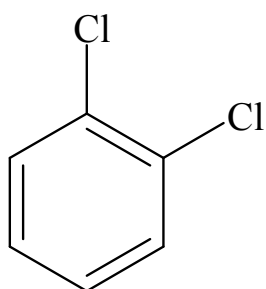


2) Two substituents

There are two methods one with numbers and one that gives the position of the substituents with respect to each other.

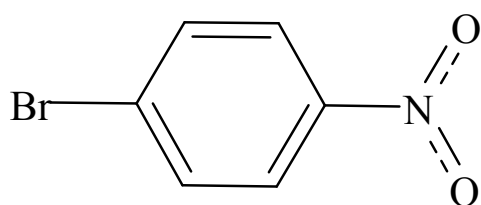
Method A – relative position.

o-dichlorobenzene m-dichlorobenzene p-dichlorobenzene
OR ortho dichlorobenzene OR meta dichlorobenzene OR para dichlorobenzene

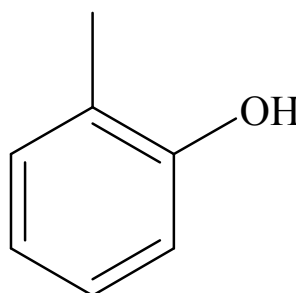


Examples

p-bromonitrobenzene

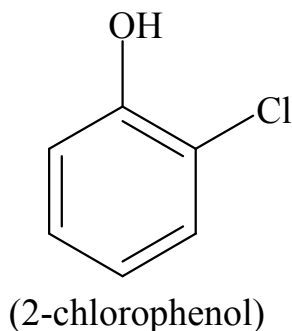


o-hydroxymethylbenzene

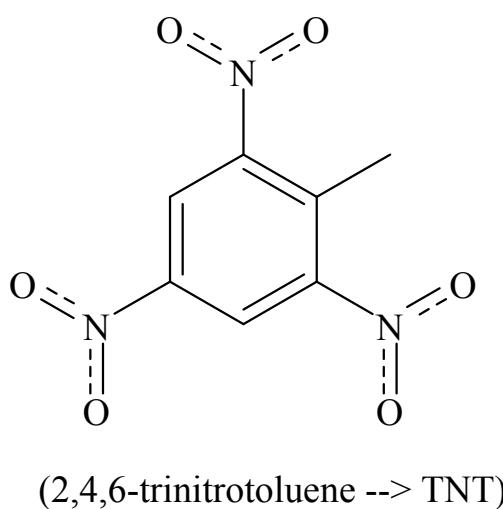


Method B – numbering

2-chloro-1-hydroxybenzene



2-methyl-1,3,5-trinitrobenzene



Exercises

I. Halo, Amino, Nitro

1) Name the following:

- a) $\text{CH}_3\text{CH}_2\text{Br}$ b) $\text{Cl-CH}_2\text{CH}_2\text{-Cl}$ c) $\text{CH}_3\text{-NH}_2$
d) $\text{I}_2\text{CHCH}_2\text{I}$ e) $\text{ClC}\equiv\text{CCH}_2\text{NH}_2$ f) $\text{CF}_3\text{-CCl}_3$
g) $\text{CH}_3\text{-NH-CH}_3$ h) $\text{ClCH}_2\text{-CH}_2\text{-N(CH}_3)_2$

2) Draw the following:

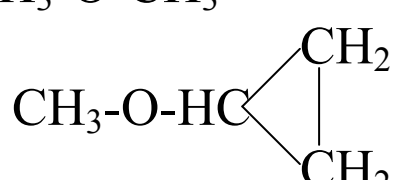
- a) 2-nitrobutane b) trichloromethane
c) 1,3-dinitrocyclobutane d) 2,3-diamino-2-pentene
e) 1-amino-3-bromo-5-ethyl-2-methyl-4-nitro-2-heptene
f) 1,4-diamino-1-cyclohexene g) 3-methylaminopentane
h) 2-ethylpropylamino-3-chloro-1-hexene

II. Ethers

3) Draw the following:

- a) 1-propoxypentane b) 1,2-dimethoxyethane
c) 2,3-diethoxybutane d) cyclobutoxybutane
e) 1,3,5-triethoxycyclohexane

4) Name the following:

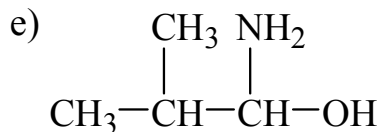
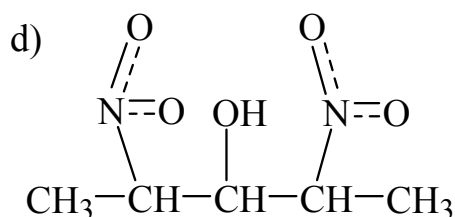
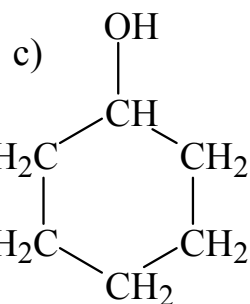
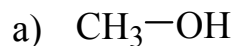
- a) $\text{CH}_3\text{-O-CH}_3$ b) $\text{Cl-CH}_2\text{CH}_2\text{-O-CH}_3$
c)  d) $\text{CH}_3\text{-O-CH}_2\text{CH=CHCH(Cl)-CH}_3$

III. Alcohols

5) Draw the following:

- a) 3-pentanol b) ethenol c) cyclopentanol
d) 3-amino-1-cyclobutenol
e) 3-bromo-2,3-dimethyl-2-butanol

6) Name the following:



IV. Aldehydes and Ketones

7. Draw the following:

a) methanal

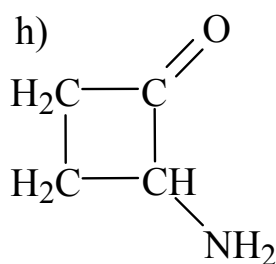
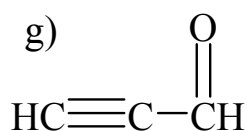
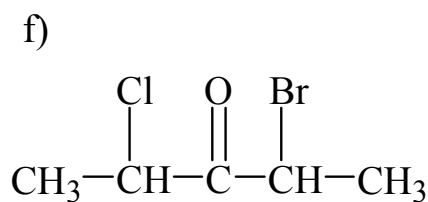
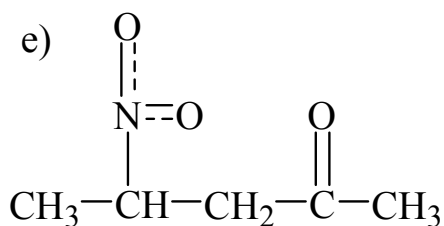
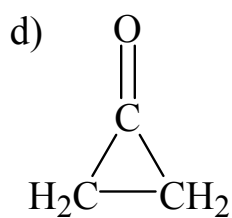
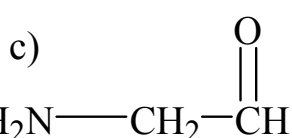
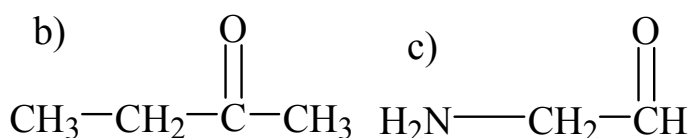
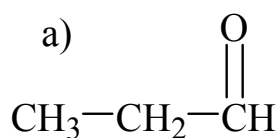
b) 2-aminopropanal

c) 2-ethylhexanal

d) 2-cyclopentenone

e) 3-cyclopropyl-4-methyl-2-pentanone

8. Name the following:



V. Carboxylic Acids

9) Draw the following:

- a) butanoic acid
- b) 2-aminoethanoic acid
- c) trifluoroethanoic acid
- d) 2-chloro-2-pentenoic acid

10) Name the following:

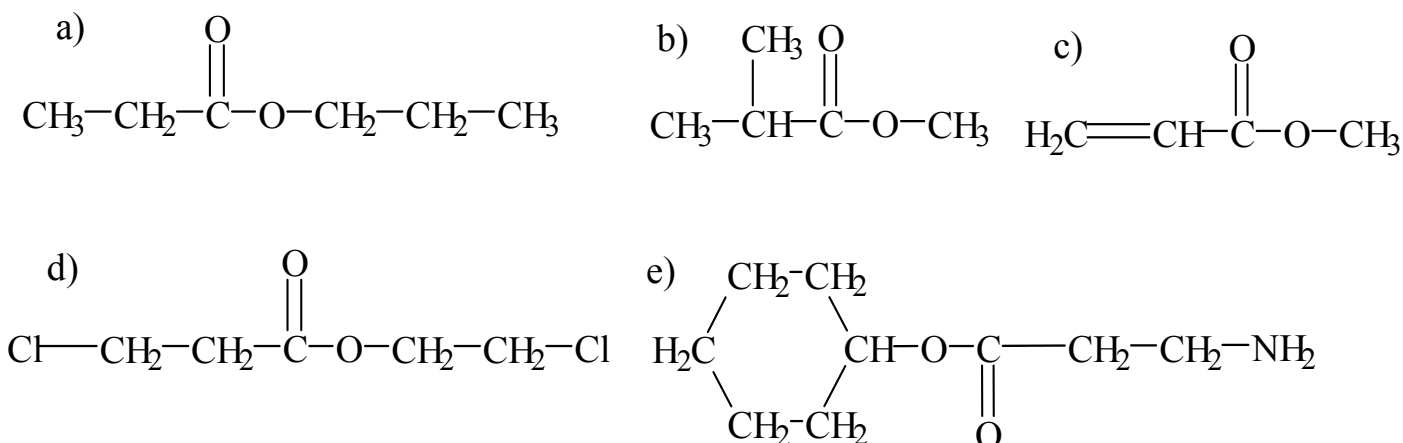
- a) H-COOH
- b) $\text{CH}_3\text{CH}_2\text{CH}=\text{CH-COOH}$
- c) $\begin{array}{c} \text{CH}_3 \\ | \\ \text{CH}_3-\text{C}-\text{COOH} \\ | \\ \text{CH}_3 \end{array}$
- d) $\begin{array}{c} \text{Cl} \\ | \\ \text{CH}_3-\text{C}-\text{COOH} \\ | \\ \text{Br} \end{array}$

VI. Esters

11) Draw the following:

- a) methyl methanoate
- b) ethyl butanoate
- c) ethyl ethanoate
- d) hexyl pentanoate
- e) 2-chloro ethanoate
- f) ethyl 2-chloroethanoate
- g) 2-methylpropyl propanoate

12) Name the following:

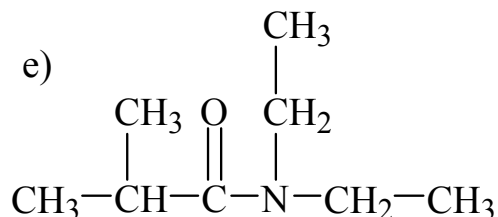
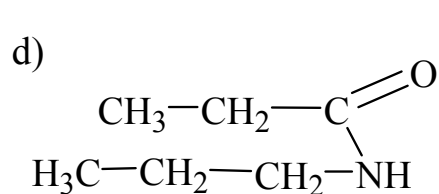
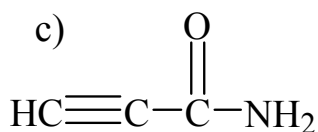
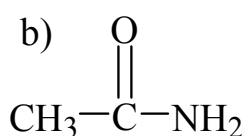
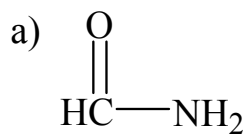


VII. Amides

13. Draw the following:

- a) pentanamide
- b) 2-methylbutanamide
- c) chloromethanamide
- d) N-methylmethanamide
- e) cyclopropylethanamide
- f) 2-chloro-N-ethyl-N-methylbutanamide
- g) N,N-diethylhexanamide

14. Name the following:



VIII. Aromatic compounds

15. Draw the following:

a) 1,2,3-trimethyl-5-propylbenzene

b) p-dihydroxybenzene

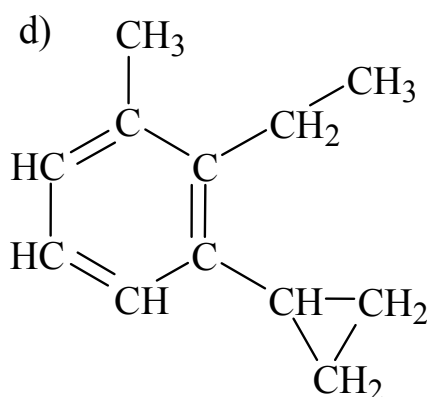
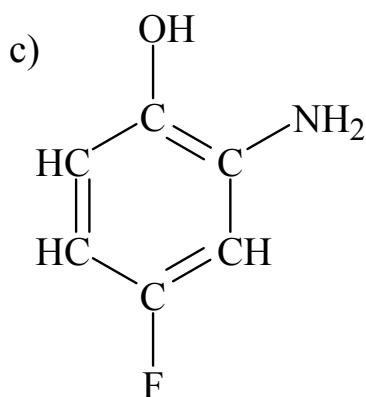
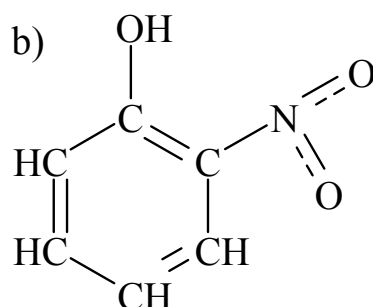
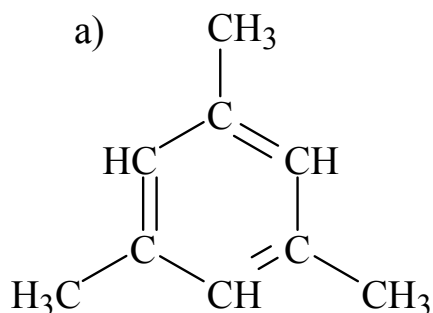
c) 1,2,3,5-tetrachlorobenzene

d) o-diaminobenzene

e) 1-chloro-2-hydroxy-4-methoxybenzene

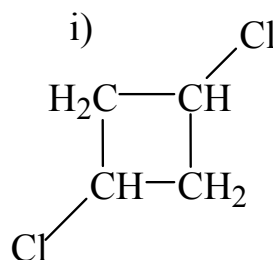
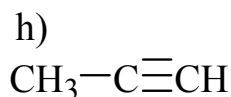
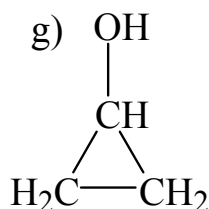
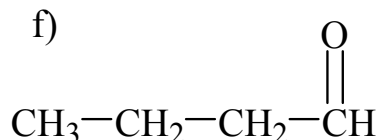
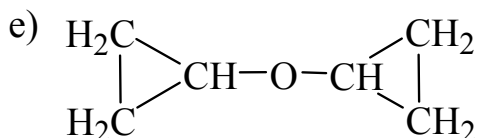
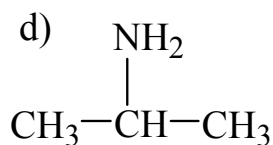
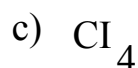
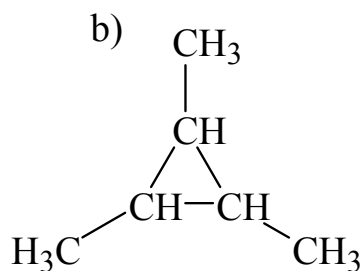
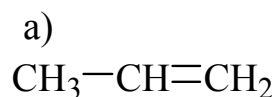
f) m-methylethylbenzene

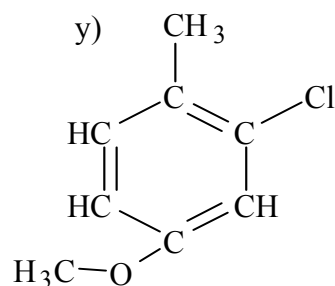
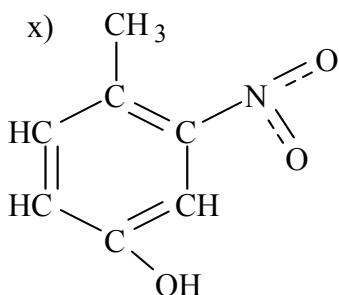
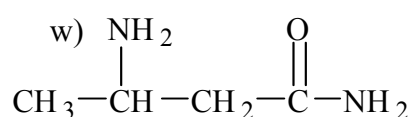
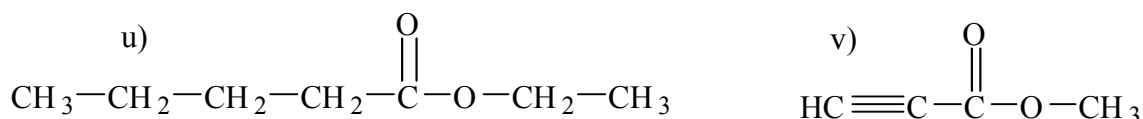
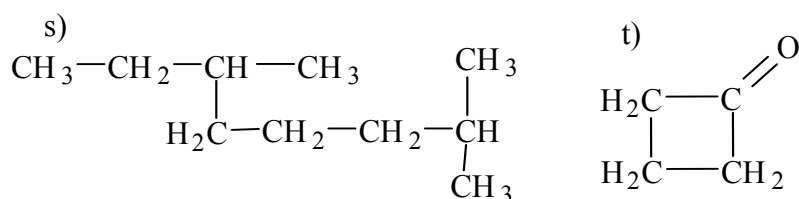
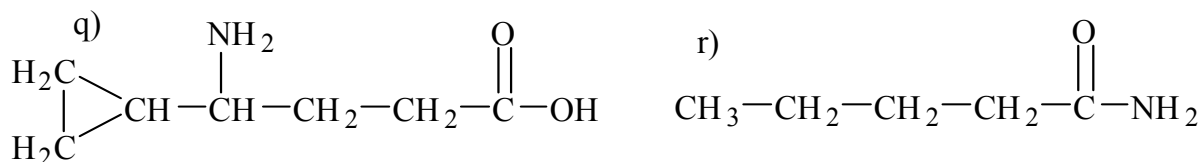
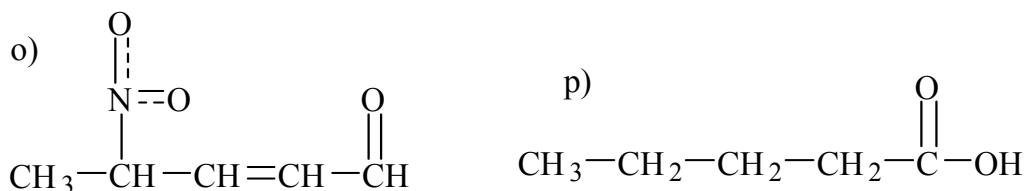
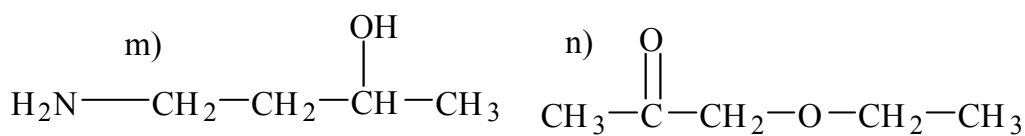
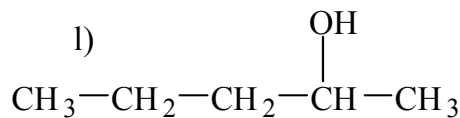
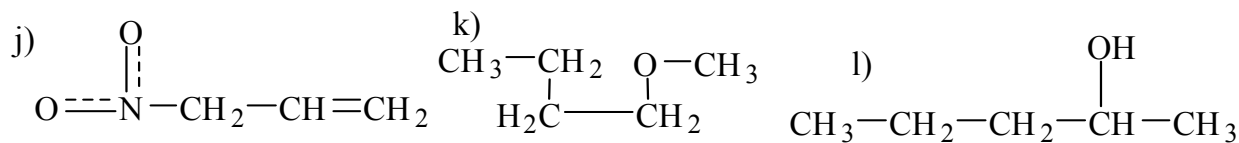
16. Name the following:



17. Write and name the 4 isomers of $C_3H_6Cl_2$.
18. Write and name the 6 isomers of $C_4H_8Cl_2$.
19. Draw and name all the isomers (appr. 10) of C_5H_{10} .
20. Skip 21. Skip
22. Draw the following:
 - a) 2-aminopropanoic acid b) 3-chloro-2-buteneamide
 - c) 1,4-dicyclopropylcyclohexane
 - d) 1-amino-4,4-difluoro-2-pentanol
 - e) methyl 2,3-dimethoxypropanoate
 - f) 3-nitropropenal g) methanamide
 - h) meta bromochlorobenzene i) ethyl pentanoate
 - j) 4-nitro-3-butenal k) 3-cyclopentenone
 - l) methoxybenzene m) dichloroethanoic acid
 - n) 3,4,5,6-tetramethylnonane o) p-diaminobenzene

23. Name the following:





24) Draw the following:

- | | |
|----------------------------------|--|
| a) 1,3-diaminohexane | b) 3,5-diethyl-4,4-dimethylheptane |
| c) 3-cyclopropoxybutanoic acid | d) cyclopentanone |
| e) 2-bromo-3-chloro-2-butenamide | f) ethyl hexanoate |
| g) 1,2,3-trihydroxybenzene | h) 4-ethyl-2-methyl-3,3-dicyclopropyl-1-hexane |
| i) o-dinitrobenzene | j) cyclooctane |
| l) 1,3,4-triaminobenzene | k) 3-pentynal |
| m) dinitromethane | |
| n) chloromethanoic acid | o) 1-bromo-2-pentanone |

25) Name the following:

