NOMENCLATURE OF ORGANIC COMPOUNDS

Organic chemistry is the chemistry of carbon compounds. Carbon has the ability to bond with itself to form long chains and, as a result, millions of compounds from simple hydrocarbons to large biomolecules such as proteins, lipids, carbohydrates, and nucleic acids. Originally it was believed that these compounds had to come from a living organism, now they are synthesized in the laboratory.

The simplest organic compounds are composed of carbon and hydrogen and are known as hydrocarbons. There are four types, or classes, of hydrocarbons:

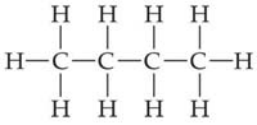
Alkanes: contain all C-C single bonds. These are known as **saturated hydrocarbons**.

Alkenes: contain at least one C=C double bond.

Alkynes: contain at least one C≡C triple bond. Both alkenes and alkynes are known as **unsaturated hydrocarbons**

Aromatic hydrocarbons: contain a benzene structure

Lewis structures of alkanes look like this:



These are also called structural formulas. Since these take up a lot of space, condensed structural formulas are used.

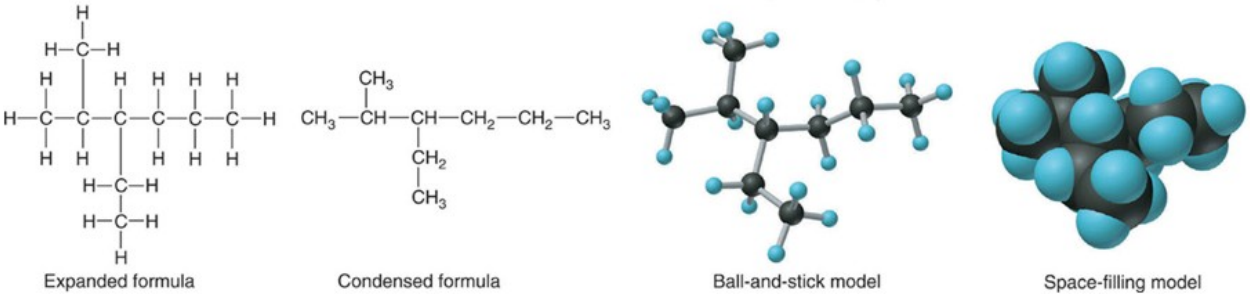
$H_3C—CH_2—CH_2—CH_3$

or

$CH_3CH_2CH_2CH_3$

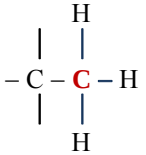
Even simpler than condensed structures are skeletal or line structures:

There are a range of structures used to represent organic compounds:

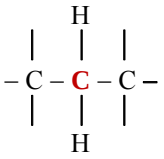


Before we start naming organic compounds, it is important to understand how carbon atoms are bonded. Every carbon atom will try to form 4 bonds.

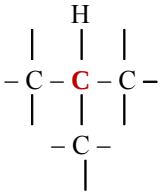
A carbon atom on the end of a chain of single bonded carbon atoms will be bonded to one carbon atom and three hydrogen atoms:



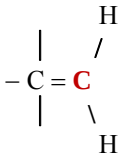
A carbon atom in the middle of a chain of single bonded carbon atoms will be bonded to two carbon atoms and two hydrogen atoms.



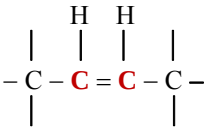
A carbon atom bonded to 3 other single bonded carbon atoms will be bonded to one hydrogen.



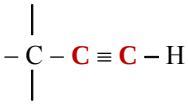
A carbon atom on the end of a chain that is double bonded to another carbon atom be bonded to two hydrogen atoms.



A carbon atom in the middle of a chain of that is double bonded to another carbon atom will be bonded to one carbon atom and one hydrogen atom.



A carbon atom on the end of a chain that is triple bonded to another carbon atom will be bonded to one hydrogen atom. The second carbon atom in that chain is only bonded to another carbon atom, but no hydrogen atoms.

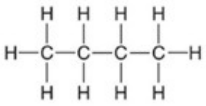
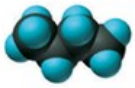
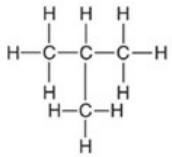
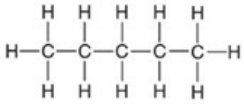
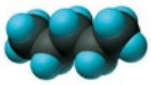
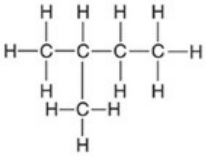
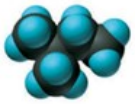
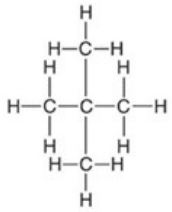


I. Naming Saturated Hydrocarbons - The Alkanes

The names of the alkanes are derived from the Greek prefix for the particular number of carbon atoms in the compound with an -ane ending. The names of the first ten alkanes are given in the following table.

Molecular Formula	Condensed Structural Formula	Name	Boiling Point (°C)
CH_4	CH_4	Methane	−161
C_2H_6	CH_3CH_3	Ethane	−89
C_3H_8	$CH_3CH_2CH_3$	Propane	−44
C_4H_{10}	$CH_3CH_2CH_2CH_3$	Butane	−0.5
C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$	Pentane	36
C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$	Hexane	68
C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	Heptane	98
C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Octane	125
C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Nonane	151
$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Decane	174

Not all the alkanes are straight chained compounds, as shown in the previous table, they can have side chains or branches. These variations of compounds which have the same number of carbon and hydrogen atoms, but a different arrangement are known as **isomers**. Some isomers are shown in the diagram below.

Systematic Name (Common Name)	Condensed Formula	Expanded Formula	Space-filling Model	Density (g/mL)	Boiling Point (°C)
Butane (*n*-butane)	$CH_3—CH_2—CH_2—CH_3$			0.579	−0.5
2-Methylpropane (isobutane)	$CH_3—CH(CH_3)—CH_3$			0.549	−11.6
Pentane (*n*-pentane)	$CH_3—CH_2—CH_2—CH_2—CH_3$			0.626	36.1
2-Methylbutane (isopentane)	$CH_3—CH(CH_3)—CH_2—CH_3$			0.620	27.8
2,2-Dimethylpropane (neopentane)	$CH_3—C(CH_3)_2—CH_3$			0.614	9.5

Rules for Naming of Branched Hydrocarbons.

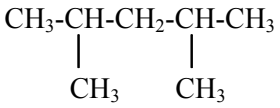
There are four parts to the name of a branched hydrocarbon

1. The **parent chain**: Tells how many carbons are in the longest continuous chain.
   meth = 1 eth = 2 prop = 3 but = 4 pent = 5
2. The **suffix**: Tells what type of compound it is.
   ane = an alkane ene = an alkene yne = an alkyne
3. The **prefix**: Tells what groups, or branches are attached to the parent chain.
   methyl = $– CH_3$ ethyl = $– CH_2– CH_3$ propyl = $–CH_2–CH_2–CH_3$
4. The **location**: Tells where groups, or branches, are attached to the parent chain.

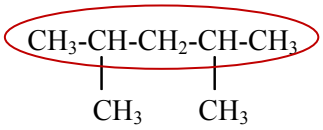
   2 = 2nd carbon atom 3 = 3rd carbon atom 4 = 4th carbon atom

   Note: alkyl groups, or branches cannot be located on the 1st or last carbon

Example 1:

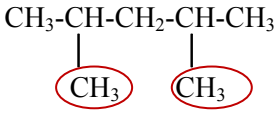


1. Select as the **parent chain** the LONGEST CONTINUOUS CHAIN of carbon atoms. The compound is considered to have been derived from the parent structure by the replacement of hydrogens by various alkyl groups.



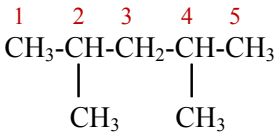
The longest continuous chain of carbon atoms in this example contains five carbon atoms. Since the carbon atoms in this compound all contain The alkane that contains five carbon atoms is **pentane**.

2. Identify the branches, or side chains, attached to the parent chain.



Both branches consist of single carbon atoms, there are called **methyl** groups

3. Starting from either end of the longest carbon chain, number the carbon atoms in the parent chain consecutively so that the alkyl groups (or branches) are attached to the carbon atoms with the lowest possible numbers.



For this compound, it makes no difference which end you start the numbering. In both cases the alkyl groups, or branches are attached to the second and fourth carbon atoms in the parent chain.

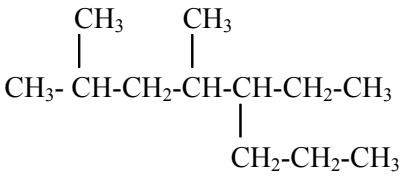
4. Name the compound in order of: number of carbon atom-alkyl group attached(number of carbon atom-alkyl group attached- etc...) name of parent compound. If there are several different alkyl groups attached to the parent chain, name them in order of increasing size or in alphabetical order.

The name for this compound looks like it would be called would be called 2-methyl-4-methylpentane, however, all branches with the same name are grouped together. The number of these branches have a prefix:

di = 2 tri = 3 tetra = 4 penta = 5

But, each branch needs a specified location, so, the correct name is **2,4-dimethylpentane**

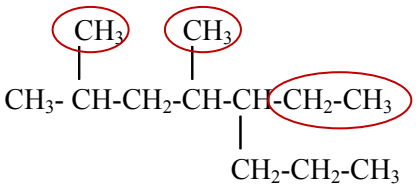
Example 2



In this compound, the longest continuous chain is **8 carbon atoms long**. Note that the longest continuous chain does not have to be straight. This longest chain is **oct-** (for 8 carbons)

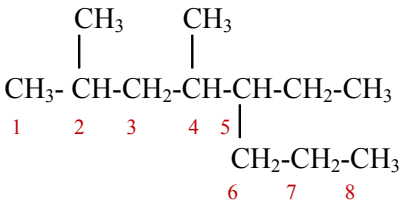
All the bonds are single bonds, so this is an alkane. The suffix is **-ane**

This parent chain is **octane**



There are three branches attached to the parent chain. Two of these are **methyl** groups and one is an **ethyl** group.

Number the carbon atoms, so that the groups are attached to the carbon atoms with the lowest possible numbers.



The two methyl groups in this compound are attached on the 2nd and 4th carbon atoms and the ethyl group is attached to the 5th carbon atom.

This compound is named **5-ethyl-2,4-dimethyloctane**. Note that the branches are named in alphabetical order.

II. Naming Unsaturated Hydrocarbons – Alkenes and Alkynes

Rules for Naming Alkenes and Alkynes

Alkenes contain at least one carbon to carbon double bond. The suffix used is **–ene**.

Alkynes contain at least one carbon to carbon triple bond. The suffix used is **–yne**.

Naming is the same as used for alkanes, except that the parent structure is the longest continuous chain of carbon atoms that contains the carbon-carbon double bond or triple bond. The name is derived by changing the suffix of the corresponding alkane name to **–ene** for an alkene and **–yne** for an alkyne and a number is added to denote the location of the multiple bond.

Example:

$CH_3–CH=CH–CH_3$

The longest continuous chain in this compound contains four carbon atoms. The parent structure would be named **but + ene** (to denote the double bond)

Number the carbon atoms in' the longest chain in such a way that the carbon atoms containing the double bond have the lowest possible numbers.

1 2 3 4
$CH_3–CH=CH–CH_3$

For this compound, the numbering should start on the left side so the double bond will be located between carbon atom no. 2 and carbon atom no. 3. Although the double bond involves two carbon atoms, its position is designated by the number of the first doubly-bonded carbon atom when numbering from the end of the parent chain nearest the double bond. So, this compound would be named **2-butene**.

Example:

$CH_3–CH_2–CH=CH_2$

In this compound the double bond is located between the 1st and 2nd carbon atoms. The compound is named **1-butene**.

Example:

$CH_3–CH=CH–CH=CH_2$

The longest continuous chain in this compound contains five carbon atoms. The parent structure would be named **pent-** however, the compound contains **two** carbon-carbon double bonds. The number of double bonds, if greater than 1, is denoted by a prefix added to the suffix.

di = 2 tri = 3 tetra = 4

The p[aren't chain is named **pentadiene** Note that an "a" is added to the name to make it easier to pronounce.

Number the carbon atoms in' the longest chain in such a way that the carbon atoms containing the double bond have the lowest possible numbers.

5 4 3 2 1
$CH_3–CH=CH–CH=CH_2$

For this compound, the numbering should start on the right side so the double bonds will be located between carbon atom no. 1 and carbon atom no. 2 and carbon atom no. 3 and carbon atom no. 4. The name of the compound is **1,3-pentadiene**

Example

$$CH_3–CH_2–C\equiv CH$$

The longest continuous chain in this compound contains four carbon atoms. The parent structure would be named **but + yne** (to denote the triple bond)

Number the carbon atoms in' the longest chain in such a way that the carbon atoms containing the triple bond have the lowest possible numbers.

$$\overset{4}{CH_3}–\overset{3}{CH_2}–\overset{2}{C}\equiv\overset{1}{CH}$$

For this compound, the numbering should start on the right side so the triple bond will be located between carbon atom no. 1 and carbon atom no. 2. This compound would be named **1-butyne**.

If the compound is branched, the name is determined similar to that used for the alkanes.

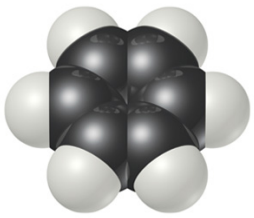
Example. CH_3-CH-CH=CH-CH_3 (with CH_3 branch on the CH)

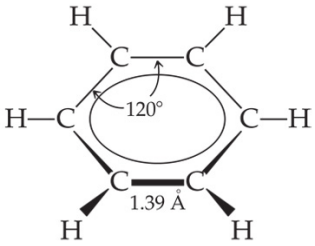
This compound is named **4-methyl-2-pentene**. Note that the double bond takes precedence in naming.

III. Naming Aromatic Compounds

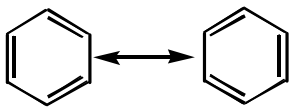
Aromatic Compounds are cyclic hydrocarbons containing a benzene structure.

AROMATIC
Benzene C_6H_6



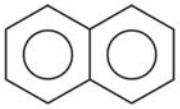


Benzene can be represented by the resonance structures:

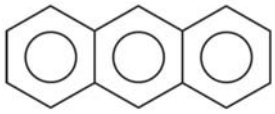


The actual structure of benzene, however, is a resonance hybrid of these two structure usually written as:

Benzene rings can be fused together. These compounds have common names.



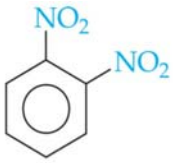
Naphthalene

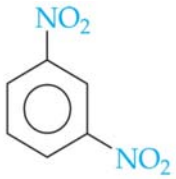


Anthracene

An aromatic compound which is formed by having an alkyl group attached to a benzene ring is named by prefixing the alkyl group name to the word benzene. An example of this is named **methylbenzene** or **toluene**

If there are only two groups attached to the benzene ring, their relative positions can be designated by numbers or by the terms ortho, meta. or para, abbreviated o-, m-, or p-.





1,2-dinitrobenzene	1,3-dinitrobenzene	1,4-dinitrobenzene
ortho-dinitrobenzene	meta-dinitrobenzene	para-dinitrobenzene

Ortho = the 1 and 2 positions on the ring (adjacent carbon atoms)
Meta = the 1 and 3 positions on the ring (alternate carbon atoms)
Para = the 1 and 4 positions on the ring (opposite carbon atoms)

IV. Naming Functional Group Compounds

Derivatives are formed by replacing one or more of the hydrogens in a hydrocarbon by a FUNCTIONAL GROUP. The functional group is responsible for giving what is ordinarily an inactive compound the characteristic chemical and physical properties of another class of compounds.

A. Halogen Derivatives of Hydrocarbons

Functional Group: - X (F, Cl, Br, I)

General Formula: R-X

Naming of Halides

Halogens attached to a hydrocarbon chain are named by replacing the -ine ending of the halogen name with **–o.** When naming a compound, halogens are named in the same manner as alkyl group branches.

Examples:

CH_3-Br	CH_3CH_2-I	$CH_3\underset{\displaystyle Cl}{\underset{\vert}{C}}HCH_3$	$CH_3CH_2\underset{\displaystyle Br}{\underset{\vert}{C}}HCH_2$–Br
bromomethane	iodoethane	2-chloropropane	1,2-dibromobutane

B. Oxygen Derivatives of the Hydrocarbons

These functional group compounds contain at least one oxygen atom in its structure.

1. Alcohols

Functional Group: –OH

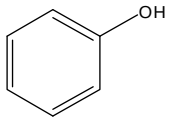
General Formula: R–OH

Naming of alcohols:
Number the-longest carbon chain so that the -OH group is attached to the carbon atom with the lowest possible number. Name the parent compound by using the alkane name and replacing the -e ending with an **-ol** ending. Indicate the position of the hydroxyl. group with a number in any alcohol containing three or more carbon atoms.

Examples:

CH_3OH	CH_3CH_2OH	$CH_3CH_2CH_2OH$	$CH_3\underset{\displaystyle OH}{\underset{\vert}{C}}HCH_3$
methanol	ethanol	1-propanol	2-propanol
(methyl alcohol)	(ethyl alcohol)	(propyl alcohol)	(isopropyl alcohol)

Aromatic alcohols are called phenols and contain the structure:



2. Ethers

Functional Group: –O–
General formula: R–O–R

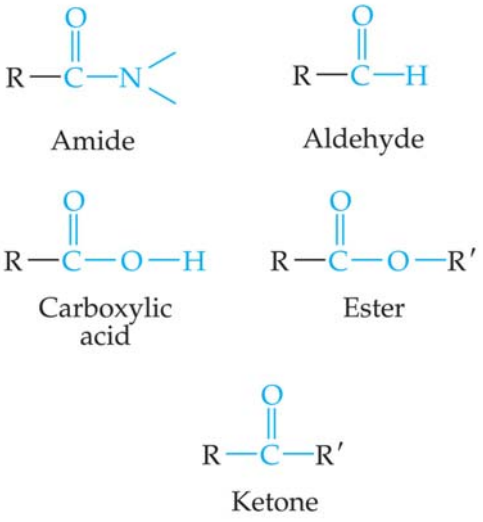
Naming of ethers
Ethers are commonly named by naming each group attached to the oxygen followed by the word **ether**. If one group has no simple name, the ether can be named as an <u>alkoxy</u> derivative of the larger group.

Examples:

CH_3-O-CH_3	CH_3-O-CH_2CH_3	CH_3CH_2-O-CH_2CH_3
dimethyl ether	methyl ethyl ether	diethyl ether
(methoxymethane)	(methoxyethane)	(ethoxyethane)

3. Carbonyl Compounds

Carbonyl compounds all contain a **= O**



This includes several types of compounds:

- Aldehydes
- Ketones
- Carboxylic acids
- Esters
- Amides

a) Aldehydes

Functional Group: –C(=O)–H

General formula: R–C(=O)–H or shorthand as –CHO (The oxygen is bonded to a terminal carbon atom)

Naming of aldehydes:
Number the-longest carbon chain starting with the -CHO group. Name the parent compound by using the alkane name and replacing the -e ending with an **-al** ending.

Examples:

H–C(=O)–H
methanal
(methyl aldehyde)

CH_3–C(=O)–H
ethanal
(ethyl aldehyde also known as acetaldehyde)

b) Ketones

Functional Group: –C(=O)–

General formula: R–C(=O)–R (The oxygen is bonded to a carbon atom in the middle of the chain)

Naming of Ketones:
Number the-longest carbon chain starting so that the –C=O group is attached to the carbon atom with the lowest number. Name the parent compound by using the alkane name and replacing the -e ending with an **-one** ending.

Examples:

propanone
(dimethyl ketone or acetone)

2-butanone
(methylethyl ketone)

c) Carboxylic acids

Functional Group: –C–OH

General formula: R–C–OH or shorthand as –COOH (The carboxyl group is bonded to a terminal carbon atom)

Naming of acids:
Number the-longest carbon chain starting with the -COOH group. Name the parent compound by using the alkane name and replacing the -e ending with an **–oic acid** ending.

Examples:

methanoic acid
(formic acid)

ethanoic acid
(acetic acid)

d) Esters

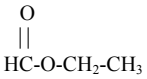
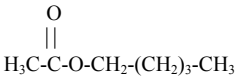
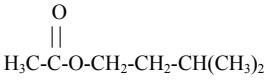
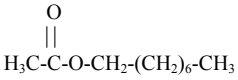
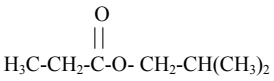
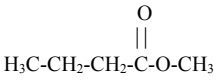
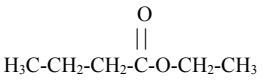
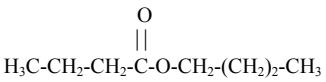
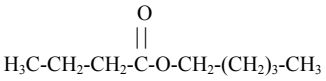
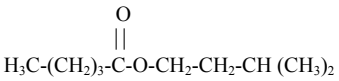
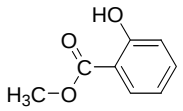
An ester is formed from the combination of a carboxylic acid and an alcohol. They are often highly aromatic compounds and are used for flavors and fragrances.

Functional Group: –C–O–

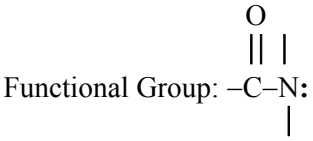
General formula: R–C–O–R' (The R' may be the same or different from R)

Naming of esters
Esters are usually named by naming the R' group [from an alcohol] as an akyl group first followed by the acid name [the R-C group] with ending **-oate**. Esters are often called by their common names.

Examples of esters and their flavor/odor properties are given in the table below.

Formula	Common name	IUPAC name	Flavor/odor
	ethyl formate	ethyl methanoate	rum
	n-amyl acetate	pentyl ethanoate	pears, bananas
	isoamyl acetate	3-methylbutyl ethanoate	pears, bananas
	n-octyl acetate	octyl ethanoate	oranges
	isobutyl propionate	2-methylpropyl propanoate	rum
	methyl butyrate	methyl butanoate	apples
	ethyl butyrate	ethyl butanoate	pineapples
	n-butyl butyrate	butyl butanoate	pineapples
	n-amyl butyrate	pentyl butanoate	apricots
	isoamyl valerate	3-methylbutyl butanoate	apples
	methyl salicylate	methyl 2-hydroxybenzoate	oil of wintergreen

e) Amides



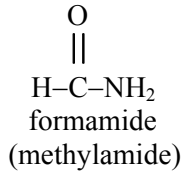
Functional Group: –C–N**:**

General formula: R–C–NH_2

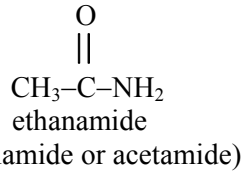
Naming of Amides

Amides are commonly named similar to a carboxylic acid, replacing the **–oic acid** suffix with **amide.**

Examples:

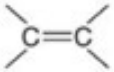
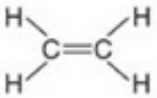
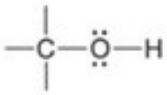
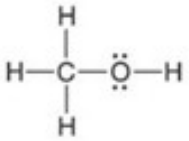
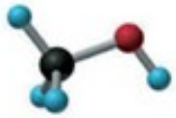
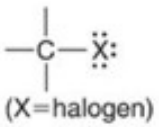
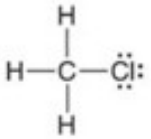
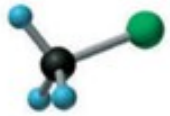
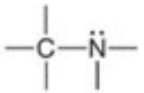
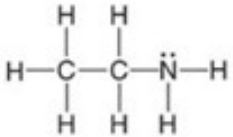
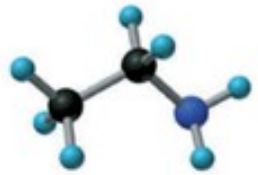
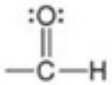
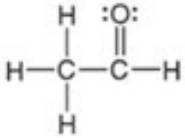
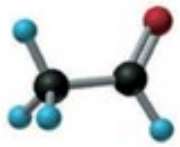


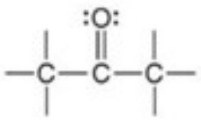
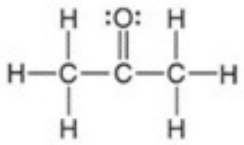
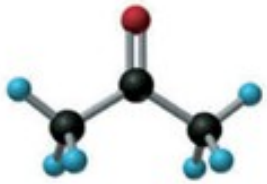
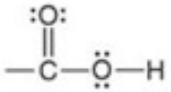
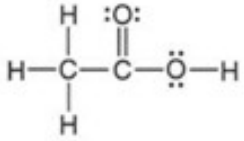
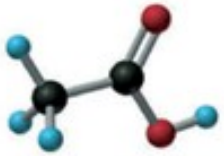
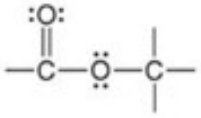
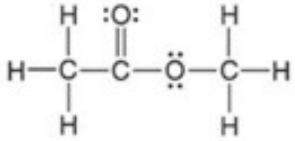
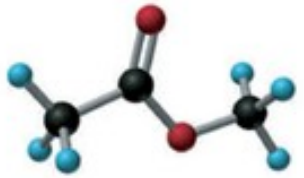
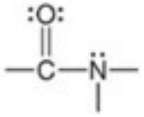
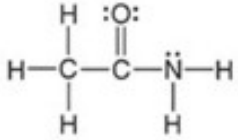
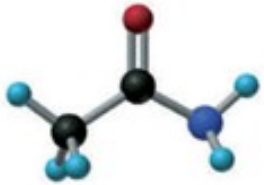
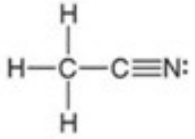
formamide
(methylamide)



ethanamide
(ethylamide or acetamide)

A summary of the functional group compounds, their structures and names is listed in tables on the next two pages.

Functional Group	Compound Type	Suffix or Prefix of Name	Example		Systematic Name (Common Name)
	alkene	-ene			ethene (ethylene)
	alkyne	-yne			ethyne (acetylene)
	alcohol	-ol			methanol (methyl alcohol)
	haloalkane	halo-			chloromethane (methyl chloride)
	amine	-amine			ethylamine
	aldehyde	-al			ethanal (acetaldehyde)

Functional Group	Compound Type	Suffix or Prefix of Name	Example		Systematic Name (Common Name)
	ketone	-one			2-propanone (acetone)
	carboxylic acid	-oic acid			ethanoic acid (acetic acid)
	ester	-oate			methyl ethanoate (methyl acetate)
	amide	-amide			ethanamide (acetamide)
	nitrile	-nitrile			ethanenitrile (acetonitrile, methyl cyanide)