Nomenclature

International Union of Pure and Applied Chemistry (IUPAC)

I. Alkanes

A. Alkanes: Simple-Chain

Alkanes consist of only hydrogen and carbon molecules and are known to be the simplest type of organic molecules.

# of Carbons	1	2	3	4	5	6	7	8	9	10
Prefix	Meth	Eth	Prop	But	Pent	Hex	Hept	Oct	Non	Dec

CH_4 = **Meth**ane
CH_3CH_3 = **Eth**ane
$CH_3CH_2CH_3$ = **Prop**ane
$CH_3CH_2CH_2CH_3$ = **But**ane
C_5H_{12} = **Pent**ane
C_6H_{14} = **Hex**ane
C_7H_{16} = **Hept**ane
C_8H_{18} = **Oct**ane
C_9H_{20} = **Non**ane
$C_{10}H_{22}$ = **Dec**ane

*General Formula: C_nH_{2n+2}

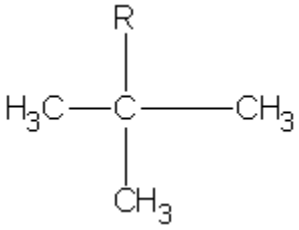
Table 1.1: Names of the ten simplest alkanes

B. Alkanes: Branched-Chains

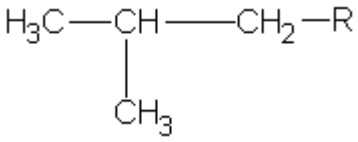
The straight simple-chain alkanes have simple names and can be easily memorized, but the branched-chain alkanes require a set of simple rules derived by the International Union of Pure and Applied Chemistry (IUPAC).

Basic Rules:

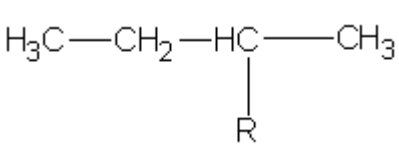
1. Identify the parent chain, longest carbon chain (backbone), in the molecule.
    a. If there is more then one carbon chain of equal length, then identify the chain that is more substituted.
2. Number the carbon atoms in the longest carbon chain, the parent chain, from the end that gives the substituents as low a number as possible.
3. Name all the substituents, groups, that are attached to the parent chain.
    a. The substituents are named by their respective prefix from the table above and end with **-yl**.
        i. Example: **CH_3- methyl, CH_3CH_2-ethyl**
    b. There are some common "special" names for branched alkane substituents which should be memorized. A few of them are:



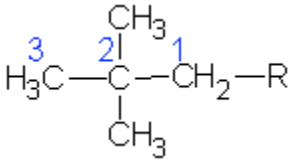
t-butyl



isobutyl



***sec*-butyl**



neopentyl

Figure 1.0: Common "Special" Names for branched alkane substituents[1]

4. Assign numbers to substituents to identify where the attachment of the substituent is to the parent chain.
    a. You must still assign a number to **each** substituent along with the prefixes **di-, tri-¸tetra-,** etc., even if there are the same substituents in the molecule.
        i. Example: **1,2-dimethyl, 1-methyl**

5. Add the prefixes, suffixes, infixes, together, remembering to alphabetize substituents in the complete name.
    a. You must list the substituents in alphabetical order along with their respective numbers.
        i. The prefixes **cyclo-, iso-,** and **neo-** are considered part of the group name so they are alphabetized.
        ii. Ignore the prefixes **di-, tri-¸tetra-, tert-, sec-,** etc., when alphabetizing.
        iii. Use commas between numbers and dashes between numbers and words.
            1. **Example: 1,3-dimethyl**
        iv. If you are required to describe the isomer, you may also need identify whether the molecule is R or S, *cis* or *trans*, E/Z, etc.

C. Cycloalkanes

Alkanes that form rings are named differently. They are named with the prefix **cyclo-** and then by the total number of carbon atoms in the ring. After adding the prefix **cyclo-**, it follows the same rules as simple-chain alkanes.
Example:

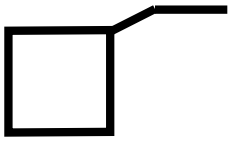
[1] Images taken from:
http://www.chem.queensu.ca/people/faculty/mombourquette/FirstYrChem/organic/index.htm

Cyclopropane

1. Substituted Cycloalkanes

   First name the substituent, then began numbering the carbon atoms in the ring from the beginning of where there is greater substitution. Don't forget that we want to assign the lowest number possible to the substituents.

Example:



Ethylcyclobutane

II. Alkenes (double bonds)

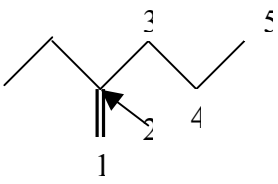
A. Alkenes are molecules that have a carbon-carbon double bond.

Basic Rules:

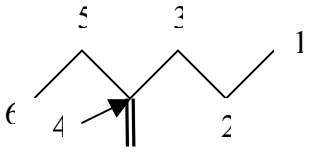
1. The rules are similar to that of naming the alkanes, except instead of ending with **-ane,** you use **-ene.**
   a. Example: **Methene**
2. When naming the compound, identify the longest carbon chain that contains the carbon-carbon double bond. If there is more then one carbon-carbon double bond, then identify the carbon chain with the greatest number of double bonds as the parent chain (backbone).
3. When numbering the carbon chain with the carbon-carbon double bond, be sure that the double bond receives the lowest number. Chains with multiple double bonds are named using the prefixes **di-, tri-, tetra,** etc along with a number.

Example:

Correct



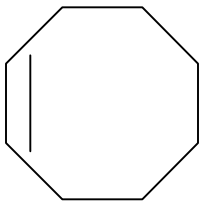
Incorrect



B. Cycloalkenes

Cycloalkanes are named just like cycloalkanes except that the ending is **-ene** instead of **-ane**.

Example:



Cyclooctene

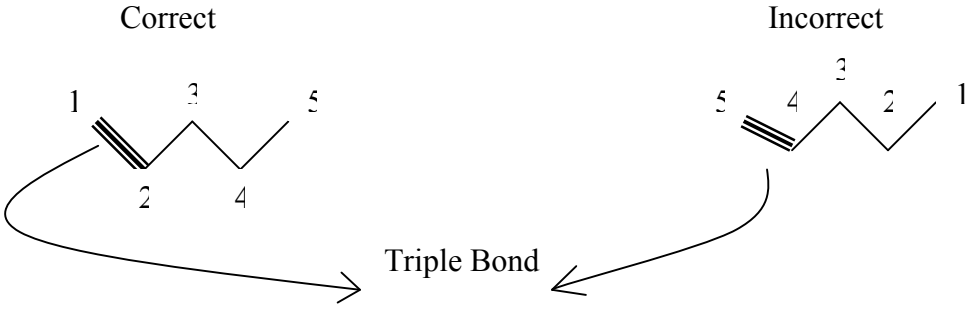
III. Alkynes (triple bonds)

A. Alkynes are molecules that have a carbon-carbon triple bond.

Basic Rules:

1. The rules are similar to that of naming the alkanes, except instead of ending with **-ane,** you use **-yne** in the parent chain.
    a. Example: **Ethyne** (common name: Acetylene)
2. When naming the compound, identify the longest carbon chain that contains the carbon-carbon triple bond. If there is more then one carbon-carbon triple bond, then identify the carbon chain with the greatest number of triple bonds as the parent chain (backbone).
3. When numbering the carbon chain with the carbon-carbon triple bond, be sure that the triple bond receives the lowest number. Chains with multiple triple bonds are named using the prefixes **di-, tri-, tetra,** etc along with a number.

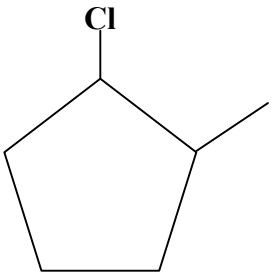
Example:



IV. Substituted Alkanes

A. **Haloalkanes** - molecules that include a substituent that is a halogen. Haloalkanes follow the same rules regarding numbering and alphabetizing as simple-chain alkanes.

Example:

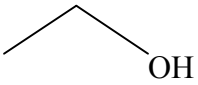


1-chloro-2-methylcyclopentane

B. **Alcohols** - alcohol containing molecules replace the **-e** at the end of an alkane name with **-ol**. The chain is numbered so that the hydroxyl group (**-OH**) obtains the lowest number <u>even if the molecule contains multiple bonds</u>.

   a. Molecules with two hydroxyl groups are called **diols** and are named with **-diol** at the end.
      i. If the two hydroxyl groups are on the same carbon are known as **geminal** and on adjacent carbons it is referred to as **vicinal**.

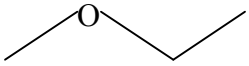
Example:



Ethanol

C. **Ethers** - The chain is numbered to give the ether the lowest number possible. The prefix to the molecule ether is smallest akyl group **meth-, eth-,** etc. followed by **-oxy-** and then ended with the appropriate carbon chain name.

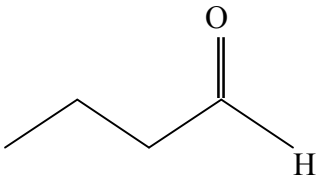
Example:



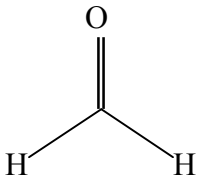
meth**oxy**ethane

D. Aldehydes - are named with the longest carbon chain that contains the aldehyde group. The carbonyl group is a terminal group in the molecule and is given priority when assigning numbers. Instead of **-e,** you use the suffix **-al**.

Examples:



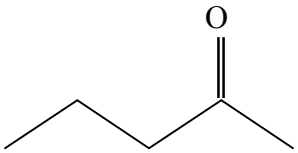
n-butanal



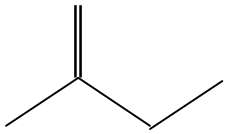
methanal

E. Ketones - are named liked aldehydes, except instead of the **-al**, you use the suffix **-one.** The carbonyl group in the molecule is given the lowest number possible.

Examples:



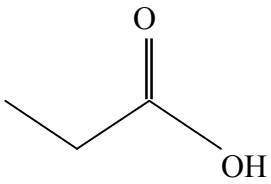
2-pentanone



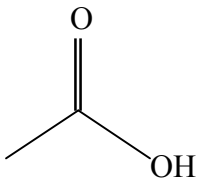
2-butanone

F. Carboxylic Acids - are named liked aldehydes, except instead of the **-al**, you use the suffix **-oic.** Carboxylic acids are terminal groups in the molecule and take priority when assigning numbers.

Examples:



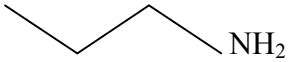
Propanoic Acid



Ethanoic Acid

G. Amines - the longest chain that has a nitrogen attached is used as the parent chain. In simple alkanes, the **-e** ending is dropped and replaced with -**amine**. In molecules with higher priority groups such as a hydroxyl group, we use the prefix **amino-** instead (Ex: 2-aminooct-en-1ol). The nitrogen is given the smallest number possible unless there it is restricted due to a higher priority group present in the molecule.

Example:



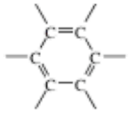
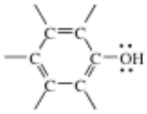
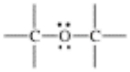
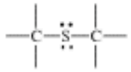
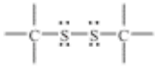
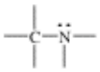
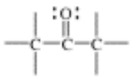
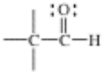
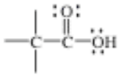
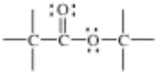
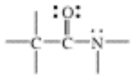
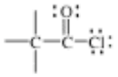
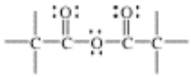
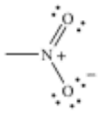
Propanamine

Functional Groups:

"A characteristically bonded group of atoms that determines molecular properties regardless of what molecule contains it."[2] It is recommended to memorize these functional groups because they are commonly found in molecules making it easier to recognize and name.

[2] Lecture Supplement 2008; Steven Hardinger, slide 21

Table 1.2: Common functional groups you will find in compounds[3]

Alkene 	**Alkyne**	**Benzene ring** 
Alkyl halide haloalkane; X = F, Cl, Br, I 	**Alcohol** 	**Phenol** 
Ether 	**Thiol** 	**Sulfide** 
Disulfide 	**Amine** 	**Ketone** 
Aldehyde 	**Carboxylic acid** carboxyl group; RCO_2H 	**Ester** RCO_2R 
Amide 	**Acid chloride** 	**Acid anhydride** 
Imine 	**Nitrile**	**Nitro** 

[3] Lecture Supplement 2008; Steven Hardinger, slide 21