Organic Chemistry: Nomenclature and Isomerism

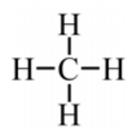
1. Hydrocarbons:

   a) Naming of hydrocarbons is done based on the number of carbons.

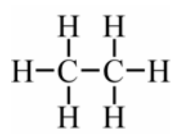
1 = meth	6 = hex
2 = eth	7 = hept
3 = prop	8 = oct
4 = but	9 = non
5 = pent	10 = dec

   b) **Alkanes** are hydrocarbons without any double or triple bonds. They have the formula $\mathbf{C_nH_{2n+2}}$. The suffix for alkanes is "ane". For instance, C_3H_8 ($CH_3CH_2CH_3$) is called propane.

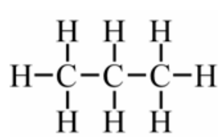
Methane CH_4



Ethane CH_3CH_3

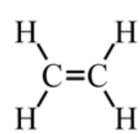


Propane $CH_3CH_2CH_3$

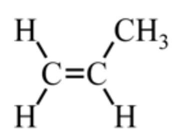


   c) **Alkenes** are hydrocarbons that have a double bond. They have the formula $\mathbf{C_nH_{2n}}$. The suffix for alkenes is "ene". For instance, C_3H_6 (CH_2=$CHCH_3$) is called propene. For alkenes longer than propene, it is necessary to designate the location of the double bond. For instance, CH_3CH=$CHCH_3$ is 2-butene. CH_2=$CHCH_2CH_3$ is 1-butene.

Ethene (ethylene) CH_2=CH_2



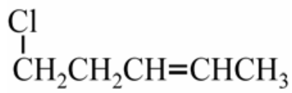
Propene CH_2=$CHCH_3$

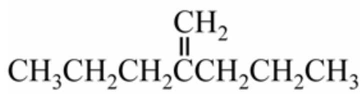


For alkenes past propene, you can have more than one possible location for the double bond. You therefore must indicate the location of the double bond by indicating the number of the carbon immediately preceding the double bond, always starting at the end closest to the double bond. Note: the long carbon chain MUST contain the double bond.

1-butene CH_2=$CHCH_2CH_3$

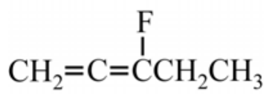
2-butene CH_3CH=$CHCH_3$

5-chloro-2-pentene 

2-propyl-1-pentene 

You can also have compounds with two double bonds, called dienes (and so on).

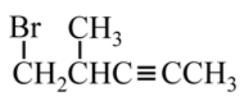
1,3-butadiene $CH_2=CHCH=CH_2$

3-fluoro-1,2-pentadiene 

d) **Alkynes** are hydrocarbons that have a triple bond. They have the formula $\mathbf{C_nH_{2n-2}}$. The suffix for alkynes is "yne". For instance, C_3H_4 ($CH\equiv CCH_3$) is called propyne. For alkynes longer than propyne, it is necessary to designate the location of the triple bond. For instance, $CH_3C\equiv CCH_3$ is 2-butyne. $CH\equiv CCH_2CH_3$ is 1-butyne.

Ethyne (acetylene) $CH\equiv CH$

Propyne $CH\equiv CCH_3$

5-bromo-4-methyl-2-pentyne 

e) **Cycloalkanes** are alkanes that form a loop. Because they need to form another C-C bond, two hydrogens are removed, making the formula $\mathbf{C_nH_{2n}}$. Cyclopropane is the smallest cycloalkane that can form.

f) **Cycloalkenes** are alkenes that form a loop. Because they need to form another C-C bond, two hydrogens are removed, making the formula $\mathbf{C_nH_{2n-2}}$. Cyclobutene is the smallest cycloalkene that can form.

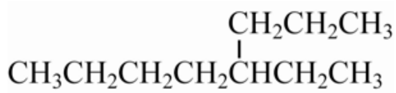
2. Substituted Hydrocarbons:

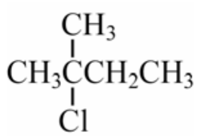
a) Any hydrogen on an alkane can be replaced by either a halogen or another hydrocarbon group. Prefixes for these substituted groups are as follows (note... the line is a bond, not a negative charge):

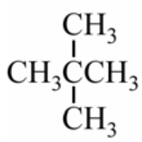
F– = fluoro	CH_3– = methyl
Cl– = chloro	CH_3CH_2– = ethyl
Br– = Bromo	$CH_3CH_2CH_2$– = propyl
I– = Iodo	$CH_3CH_2CH_2CH_2$– = butyl

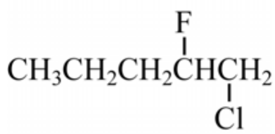
b) The key to naming substituted alkanes is to find the longest carbon chain and use it to form the base group. Then, find the largest (by mass) group dangling off of the chain. That is the end of the chain you start numbering on. Then list and number all the groups alphabetically. For instance, $BrCH_2CH(CH_3)CH_2F$ would be called 1-bromo-3-fluoro-2-methyl propane.

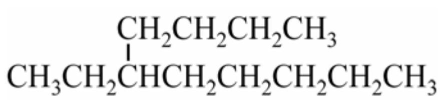
1-fluoropropane 

4-ethyloctane 

2-chloro-2-methylbutane 

2,2-dimethylpropane 

1-chloro-2-fluoropentane 

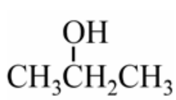
5-ethyldecane 

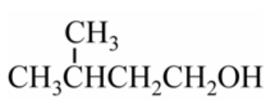
c) For alkenes and alkynes, you start the numbering of the carbons with the end of the chain closest to the double or triple bond. The chain must always encompass the double or triple bond. For some alkenes, there is an additional naming step in which the cis- and trans- isomers are determined.

4. Functional Groups:

a) **Alcohols** have the formula $\mathbf{C_nH_{2n+2}O}$. They are just alkanes that have an –OH instead of a –H. Alcohols can either be named by the proper alkane prefix and alcohol (like methyl alcohol) or can be named with the root word plus "ol" (like methanol). Alcohols have hydrogen bonding, are polar, and are structural isomers of ethers.

ethanol CH_3CH_2OH

2-propanol 

3-methyl-1-butanol 

b) **Ethers** also have the formula $\mathbf{C_nH_{2n+2}O}$. They are just alkanes that have an –O– sandwiched in between two carbons. Ethers are named by naming the two groups around the oxygen and adding the word "ether". For instance, $CH_3–O–CH_2CH_3$ has the name ethyl methyl ether. Ethers can accept hydrogen bonds from other molecules with OH, FH, and/or NH, are polar, and are structural isomers of alcohols.

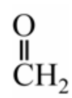
dimethyl ether $CH_3–O–CH_3$

ethyl methyl ether $CH_3–O–CH_2CH_3$

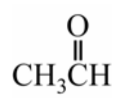
methyl propyl ether $CH_3–O–CH_2CH_2CH_3$

c) **Aldehydes** have the formula $\mathbf{C_nH_{2n}O}$. They are just alkanes that have an CH=O attached to the end. Aldehydes can be named with the root word for the hydrocarbon chain (including the carbon from the CH=O) plus "al". For instance, $CH_3CH_2CH=O$ is called propanal. Aldehydes are polar, and are structural isomers of ketones.

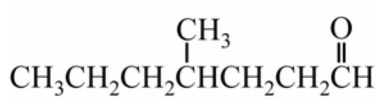
methanal (formaldehyde)



ethanal (acetaldehyde)

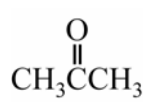


4-methylheptanal



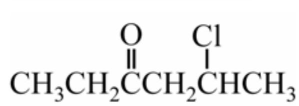
d) **Ketones** have the formula $\mathbf{C_nH_{2n}O}$. They are just alkanes that have an –CO– (the oxygen is double bonded to the carbon) sandwiched into the chain. Ketones are named by naming the two groups around the C=O and adding the word "ketone". For instance, $CH_3COCH_2CH_3$ is called ethyl methyl ketone. Ketones are polar, and are structural isomers of aldehydes.

propanone (acetone)



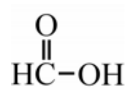
2-pentanone

5-chloro-3-hexanone

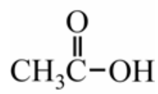


e) **Carboxylic acids** have the formula $\mathbf{C_nH_{2n}O_2}$. They are just alkanes that have an –COOH group on the end. Acids can be named with the root word for the hydrocarbon chain (including the carbon from the COOH) plus "oic acid". For instance, CH_3CH_2COOH is called propanoic acid. Acids have hydrogen bonding, are polar, and are structural isomers of esters. They also partially ionize in water, that is they are *acids*.

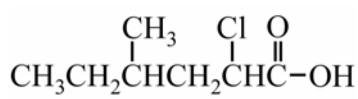
methanoic acid (formic acid)



ethanoic acid (acetic acid)

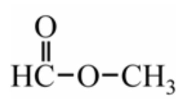


2-chloro-4-methylhexanoic acid

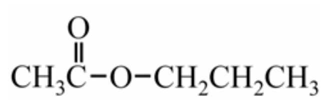


f) **Esters** have the formula $\mathbf{C_nH_{2n}O_2}$. They are just alkanes that have an –COO– (like a mix between a ketone and an ether) sandwiched into the chain. Esters are named by naming the group dangling off the oxygen plus the root word for the other carbon chain plus the suffix "ate". For instance, $CH_3CH_2COOCH_2CH_3$ is called ethyl propanate. Esters are polar, and are structural isomers of acids.

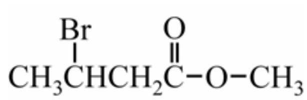
methyl methanate (methyl formate)



propyl ethanate (propyl acetate)



methyl 3-bromobutanate



g) **Amines** are formed when one or more hydrogens off of ammonia are substituted with alkane group. For instance, CH_3NH_2 is a primary (1 carbon group) amine called methylamine. $(CH_3)_2NH$ is a secondary amine (2 carbon groups) called dimethylamine. $(CH_3)_3N$ is a tertiary amine (3 carbon groups) called trimethylamine. All amines are bases, and all except tertiary amines can form hydrogen bonds. They are also all polar.

A. Primary Amines

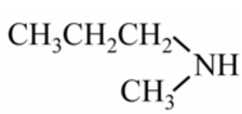
methylamine CH_3NH_2

propylamine $CH_3CH_2CH_2NH_2$

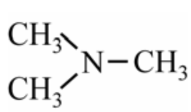
B. Secondary Amines

diethylamine $(CH_3CH_2)_2NH$

methylpropylamine



C. Tertiary Amines



3. Isomers:

   a) **Structural isomers** are two molecules that have the same formula but have different molecular structures. For instance, 1-butene and 2-butene are structural isomers.

   b) **Geometric isomers**, otherwise known as cis/trans isomers, occur with alkenes that have at least two different groups (out of 4) around the double bond). The cis isomer is formed when the two largest groups are on the same side but on different carbons. The trans isomer is formed when the two largest groups are diagonally across from each other. Remember, there is also always a structural isomer that goes along with these two in which the two largest groups are on the *same* carbon.

   c) **Optical isomers** or **chiral** molecules are molecules that have the same basic structure and formula, but are not superimposeable. This occurs only when there are 4 different groups around a single carbon (could be any different groups, even long carbon chains). That carbon is called a chiral center.