



## Readings for this section

Oxtoby: Chapter 17, all sections.

## Organic Chemistry 2006-01-17

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### Introduction

Organic chemistry involves the study of the chemistry of carbon-containing compounds (organic compounds). At first glance, one may think this to be a relatively small area of chemistry. In fact, Carbon-containing compounds comprise over 90% of all known compounds. This could be due in part to the fact that there are many areas of research in organic chemistry and thus, many compounds have been discovered. It is, however, largely due to the vast number of compounds that carbon and hydrogen (and a few other elements) form.

Organic compounds contain mostly hydrogen and carbon. Those compounds containing only these two elements are called **hydrocarbons**. Hydrocarbons can have single-, double-, and triple- CC bonds, they can form many branches and ring structures and form a large part of chemistry. More interesting in their reactivity, however are compounds that contain atoms other than these two. We call these other atoms **heteroatoms** to refer to the fact that they are other than hydrogen and carbon. Heteroatoms cause changes in the reactivity (or function) of the organic compound and the locations in the molecules where these groups exist are called functional groups. For example, a very common functional group that contains a single oxygen-hydrogen pair is the alcohol group. for example, methanol is  $\text{CH}_3\text{OH}$  and ethanol is  $\text{CH}_3\text{CH}_2\text{OH}$ . Other functional groups include carboxylic acids -  $\text{COOH}$ , ethers Amines  $-\text{NH}_3$ , etc. These actually make up the compounds of most interest to organic chemists.

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### Alkanes

The simplest class of organic compounds (but not limited to simple molecules) is called alkanes. An **alkane** is a compound made up of only hydrogen and carbon (**hydrocarbon**) that has only single bonds in it. Of these, the straight-chain hydrocarbons are the easiest to deal with. These compounds are called straight-chain not because the line of carbons forms a straight line but because they form a continuous line. The following table lists a few straight-chain hydrocarbons and gives names and properties

n	Name	BP	MP	Structural formula	Formula
1	methane	-162	-193	CH <sub>4</sub>	CH <sub>4</sub>
2	ethane	-89	-183	CH <sub>3</sub> CH <sub>3</sub>	C <sub>2</sub> H <sub>6</sub>
3	propane	-42	-188	CH <sub>3</sub> (CH <sub>2</sub> )CH <sub>3</sub>	C <sub>3</sub> H <sub>8</sub>
4	butane	0	-138	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	C <sub>4</sub> H <sub>10</sub>
5	pentane	36	-130	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>	C <sub>5</sub> H <sub>12</sub>
6	hexane	69	-95	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub>	C <sub>6</sub> H <sub>14</sub>
7	heptane	98	-91	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>	C <sub>7</sub> H <sub>16</sub>
8	octane	126	-57	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> CH <sub>3</sub>	C <sub>8</sub> H <sub>18</sub>
9	nonane	151	-54	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> CH <sub>3</sub>	C <sub>9</sub> H <sub>20</sub>
10	decane	174	-30	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> CH <sub>3</sub>	C <sub>10</sub> H <sub>22</sub>
20	eicosane	343	37	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> CH <sub>3</sub>	C <sub>20</sub> H <sub>42</sub>
30	triacontane	446	66	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>28</sub> CH <sub>3</sub>	C <sub>30</sub> H <sub>62</sub>

The general formula for alkanes is C<sub>n</sub>H<sub>2n+2</sub>. It is interesting to note that as the alkanes get larger, their boiling and melting points get higher. This makes sense on two counts: the heavier the molecule, a) the more energy it needs to be "lifted" out of the liquid phase, etc. and b) the larger chains get tangled in each other, making the un-tangling process nearly impossible.

- ◆ molecules of n = 1 - 5 are gas at room temperature (like methane, *alias*, natural gas)
- ◆ molecules of n = 6-16 are liquids at RT (like hexane, a major component of gasoline)
- ◆ if n >16 we see a waxy solid (like parowax)

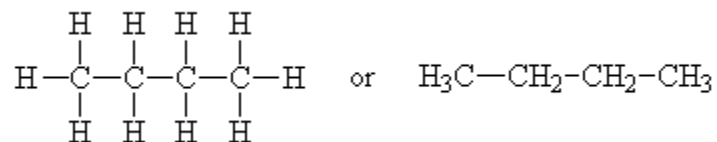
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## Structural isomers

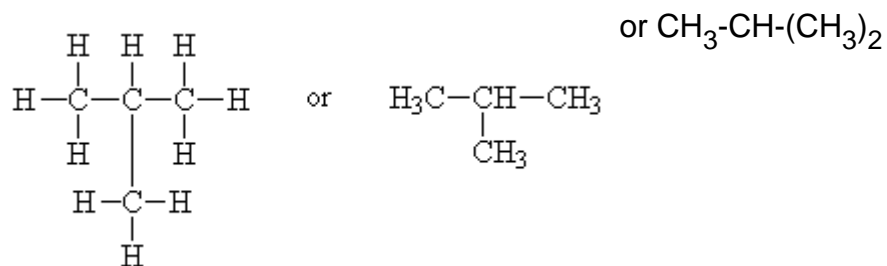
Alkanes can form many compounds, often, several compounds with the same chemical formula can have different structures. Compounds with this relationship are called structural isomers of each other.

For example, consider a hydrocarbon with four carbons,  $C_4H_{10}$ . This molecule can be represented as a straight-chain



(common name: n-butane, IUPAC\* name: butane)

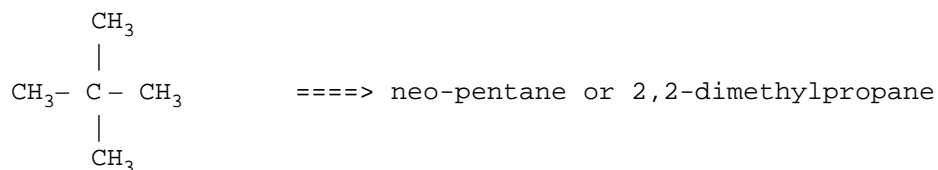
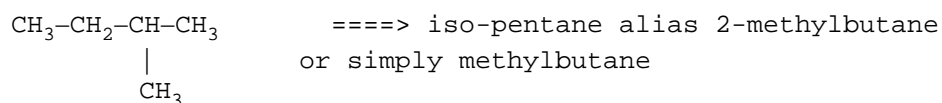
or as a branched molecule



(common name: isobutane, IUPAC name: 2-methylpropane or just methylpropane; *the 2 is redundant since there is no other place for a branch to go.*)

These molecules both have the same chemical formula but are obviously different in their connectivity (structure). They are structural isomers of each other.

If we consider a five-carbon alkane, we can have three different isomers.



These three molecules are all structural isomers of each other, *i.e.*, they all have the formula  $C_5H_{12}$  but they have different connectivities (structures).

Remember, these structural formulas are not real three-dimensional representations of the shape of the molecules themselves. They merely map out the way the atoms are connected. No information is implied regarding the orientation of these molecules based solely on structural drawings like these, except in special cases which we'll get to later.

Thus, for example, the molecule methylbutane can equally well be represented as any one of the following structures (hydrogens not shown for simplicity).



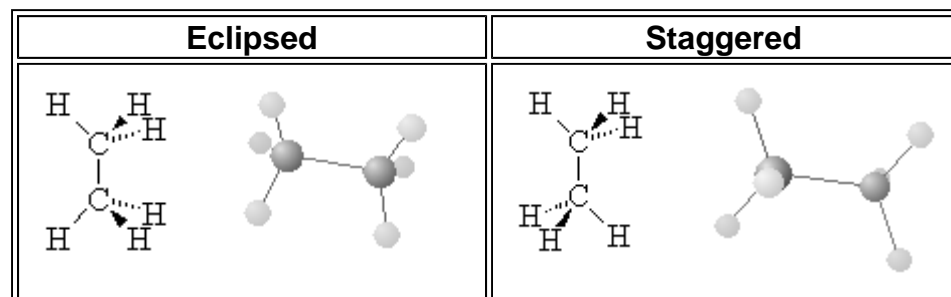
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## CHEM112 Class Notes

### Conformers

In the previous discussion of structural isomers, we stated that the 3-D representation of the molecules was nearly completely neglected in the structural drawings we normally create to represent the various molecules. If we study for a moment the 3-D arrangement of atoms in a simple molecule, we see that this adds to the level of complexity that we need consider to completely understand a given molecule.

In the case of alkanes (no double bonds or ring structures) there is (in principle) free rotation around any of the single bonds in the structure (as around single bonds in any chemical structure). Thus, it is not correct to write down a single picture of the molecule and expect that that is how it always looks. If we consider the two-carbon alkane ethane we see that the Methyl groups can rotate around each other such that at one instant, the hydrogens of one methyl group are exactly aligned with those of the other group. This arrangement is called the eclipsed conformation since the hydrogens eclipse each other when viewed down the axis of the molecule. On the other hand, a slight rotation of one methyl group compared to another brings the hydrogens out of alignment to a conformation called staggered. In this case, all six hydrogens are visible when viewed down the molecular axis. Study the drawings and manipulate the 3D models below to satisfy yourself that you understand this.



These two images show us instantaneous pictures of the geometry of this molecule, in reality, it is rotating so fast about the C-C bond that the two orientations swap more than  $10^6$

times per second. Some molecules with bulkier groups instead of hydrogens can find themselves trapped in one conformation or another. This can lead to observed differences in the properties of the two conformers (isomerism), as if they were in fact isomers.

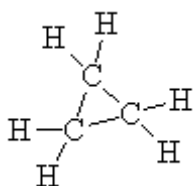
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## CHEM112 Class Notes

### Cycloalkanes

A further step in the complications of structures of alkanes involve the possibility that a ring structure may be formed. If no C=C double bonds exist these compounds are called cycloalkanes. They have the general formula  $(CH_2)_n$ . Let us consider just the first few cycloalkanes.

#### $C_3H_6$ : cyclopropane

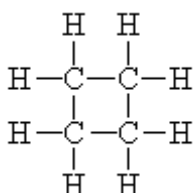


This molecule has bond angles of  $60^\circ$  even though the carbons are all  $sp^3$  hybridized. Thus, the atomic orbitals cannot overlap as well as they would if the molecule were unconstrained. We would thus expect that the energy of such a bond is higher than that of a normal C-C single bond not constrained by geometry. This is



experienced in the exothermic reaction whereby the ring is opened with the addition of two hydrogen atoms.

#### $C_4H_8$ : cyclobutane

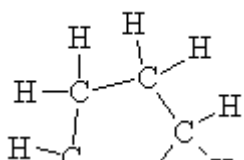


This molecule, like cyclopropane is strained since the bond angles must be, on average, only  $90^\circ$  as compared to the tetrahedral angle of  $109.5^\circ$ . Thus, the C-C bond in cyclopropane is also higher in energy than the C-C bond in a non-constrained alkane. Actually, for other reasons, this molecule is not exactly flat. One of the carbons is



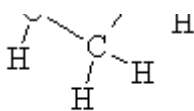
raised out of the plane of the molecule a few degrees.

#### $C_5H_{10}$ : cyclopentane



The bond angle in this molecule is on average  $108^\circ$ , very close to the ideal tetrahedral angle. There is little strain on the bonds here. Cyclopentane is a relatively stable molecule. Due to steric interactions of

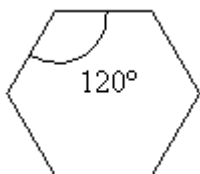




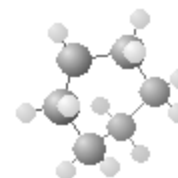
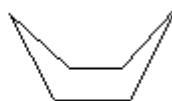
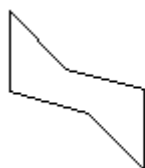
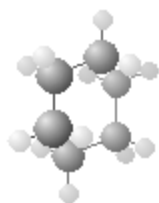
hydrogens with other hydrogens, this molecule is actually slightly puckered. See the three-dimensional model to visualize this.

All the above molecules are nearly flat molecules on the time average at room temperature (not counting the hydrogens). Actually, cyclopentane is slightly puckered at absolute zero, as shown (exaggerated) in the 3d model. No other cycloalkanes are flat. Let's look at the next in the series to see why.

### $C_6H_{12}$ : cyclohexane



The "flat" molecule would have a bond angle larger than the tetrahedral angle. This angle could easily be reduced to the tetrahedral by merely bending the molecule out of its flat configuration. The two possible conformers of the non-flat cyclohexane are the chair and the boat as indicated in the drawing below.



In these conformations, the carbon atoms can assume more closely the ideal tetrahedral geometry of the  $sp^3$ - hybridized atoms they are.

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## CHEM112 Class Notes

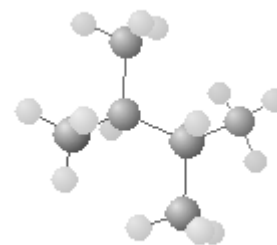
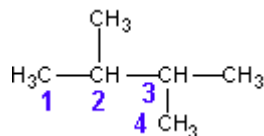
### Naming (Nomenclature)

It is obvious that using the chemical formula alone is not sufficient to uniquely identify the vast majority of organic compounds. Structural formulas too are difficult to use and impractical to put in spoken language. Originally, names for compounds were not well coordinated and there were often compounds that had been named by different people completely different things. It was very hard to determine exactly what chemical the names were referring to without first researching the history of each individual name. A structured naming regime called IUPAC is now in place to help us both name new compounds and rebuild the structure of named compounds. This set of rules helps us to uniquely identify each chemical compound by its name alone. One drawback to this scheme is that the names can become quite long. For a more complete listing of the IUPAC rules than I can give in these lecture notes, [click here](#),

Let's look at the some of the rules to help you learn how to use this nomenclature scheme.

## 1. Parent Chain

**Select the longest continuous 'chain'.** It is the *parent* chain. Its name is used as the last part of the compounds name. If there are several "longest" chains within the molecule of the same length then the parent chain will have the most possible branches and will have the lowest possible branch numbers of all the choices. Take, for example, the molecule pictured below ( $C_6H_{14}$ ).



The longest straight chain is a four carbon chain (Numbered in blue). There are several possible choices for the four-carbon chain. It makes no difference which you pick. I chose the four carbons (blue numbered). Avoid the erroneous thinking that the 'chain' must be linear along the paper. This is not the case. Check out the 3D model and prove this for yourself.

Hence, the last part of the name for this example is *butane*

## 2) Numbers

**Number the carbons** in the parent chain (and in the branches) such that the branches (and any other non-alkane features like double bonds, hetero-atoms, etc) occur at the lowest possible number carbon. Start with the first branch, if there are two ways to number the parent such that the first branch occurs on the same number then chose the one which gives the smallest numbered second branch, etc. In the above example, the numbering sequence could have been reversed with no difference in the location of the branches.

## 3) Branches

The branch names are those of the normal alkane of the same length but with the -ane suffix replaced by -yl (indicating a molecular fragment) thus, methane becomes methyl for a one-carbon chain, etc.

You now prefix the parent name with the chain names, indicating their location on the parent chain. In the above example, there are two methyl chains, located at carbons 2 and 3 on the parent chain. Hence, we use the prefix 2,3-dimethyl to describe the location and type of branches on the parent.

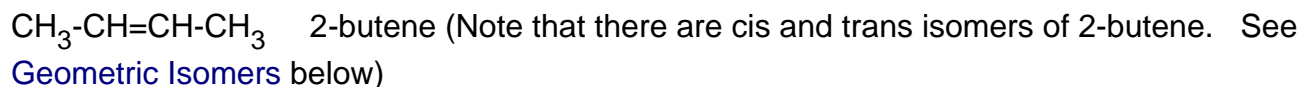
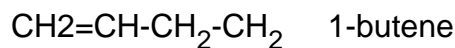
In this example, the completed name is 2,3-dimethylbutane. NOTE: no spaces in the name.

## 4) Double bonds and triple bonds

**Double bonds and triple bonds** are indicated by changing the -ane to -ene and -yne, respectively, in the name of the chain. They should be included as part of the parent chain,

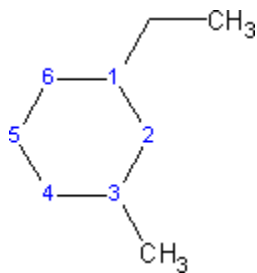
even if a longer chain is possible but which excludes this functional group. The location of the functional group (double or triple bond) is indicated as the first carbon in the chain that has that type of bond.

Thus, the following 4-carbon compounds are named accordingly



## 5) Cycloalkanes

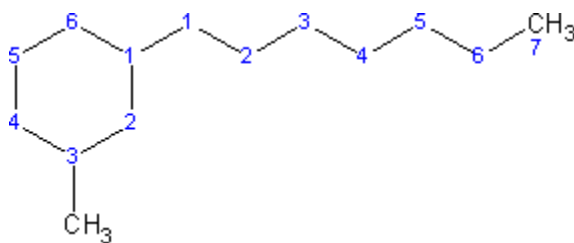
**Cyclic alkanes** should be the parent chain in a compound (unless there is a "straight-chain" part that is larger or which contains an important [functional group](#)). If more than one cycle, then the largest one is the parent. Prefix the normal alkane name with "cyclo-" to make the name. Thus, a three-carbon ring is cyclopropane ([see above](#)) and a four-carbon ring is cyclobutane ([see above](#)). If there are substituents or branches on the ring, then numbering of the carbons is done such that they occur at the lowest possible numbered carbons. See the drawing below as example.



### 1-ethyl-3-methylcyclohexane

(Note: always put the substituents in alphabetical order and name it so. Also note that there is an alternate naming scheme where the largest substituents is first. I prefer the former method)

In the case where the acyclic part is longer than the cyclo part then the cyclo part is named as a cycloalkyl branch.

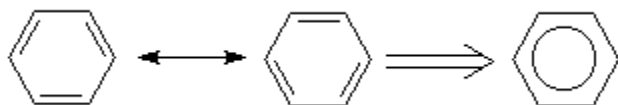


In this case, the cycloalkyl is called 3-methylcyclohexyl and it's on carbon 1 of a heptane parent chain. Thus the name is 1-(3-methylcyclohexyl)heptane.

© Mombourquette

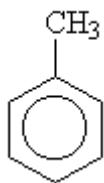
## o) Arenes

Arenes are a special class of organic compounds. They have what is called a conjugated  $\pi$ -bond system that rapidly resonates, creating a large delocalized orbital. This large delocalization creates an especially stable molecule towards certain types of reactions. The most common arene is a six-member ring of carbons where each carbon has one hydrogen on it, called benzene.

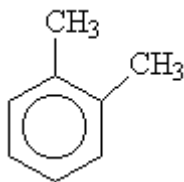


The alternating double and single bonds seen in the two resonance structures to the left of the double arrow  $\rightleftharpoons$  helps us to see the number of bonds but don't properly indicate that all carbon-carbon bonds are in fact equal in all respects. The overall resonance can be represented by the right-hand diagram where the double/single bonds are replaced by the circle indicating that the ring is aromatic. This, however is not a "Lewis Structure" in the classical sense since you cannot tell how many bonds each carbon has.

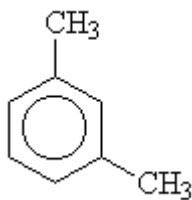
Substituent groups can exist on these rings, numbering is such that they occur at the lowest possible numbers. Let's look at some specific examples:



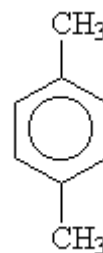
methylbenzene (1-methylbenzene is redundant)  
(Common name toluene)



1,2-dimethylbenzene  
(orthodimethylbenzene)

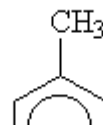
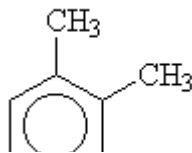
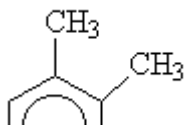


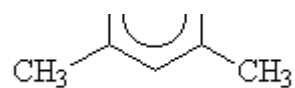
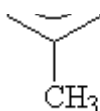
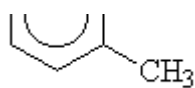
1,3-dimethylbenzene  
(metadimethylbenzene)



1,4-dimethylbenzene  
(paradimethylbenzene)

Note that there is an alternate form of naming the location of the substituents on a benzene ring. This is not strictly IUPAC but is very commonly used. The prefix *ortho* indicates the adjacent position, *meta* indicates two positions away and *para* indicates directly across from (3 positions away).





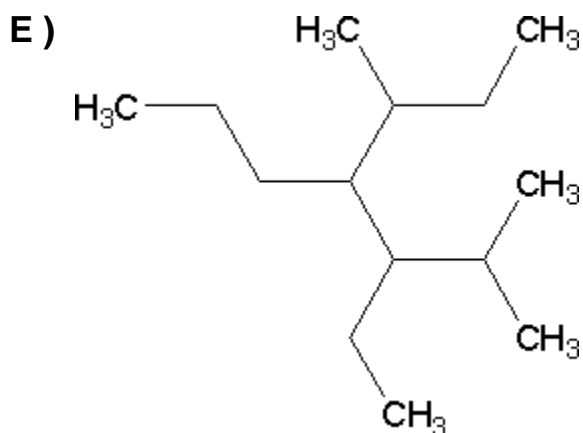
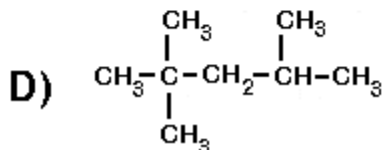
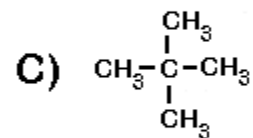
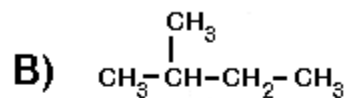
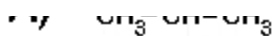
1,2,3-trimethylbenzene 1,2,4-trimethylbenzene 1,3,5-trimethylbenzene

There are also molecules with multiple aromatic rings. Look at these few.

	naphthalene
	anthracene
	pentacene (blue)
	coronene (yellow)
	graphite (black)

Here are a few examples, Name the following: (click on the drawing for the name)



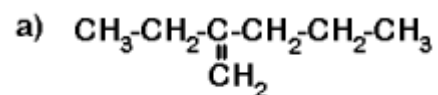


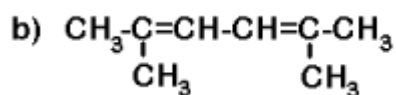
Now, draw the structures corresponding to the following names (click on the names to see the answer).

- a) [hexane](#)
- b) [2-methylpentane](#)
- c) [3-methylpentane](#)
- d) [2,2-dimethylbutane](#)
- d) [2,3-dimethylbutane](#)

Note that these are all structural isomers of each other.

Now try a few with multiple bonds. Click on the diagram to see the name.





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## Branched Alkyls.

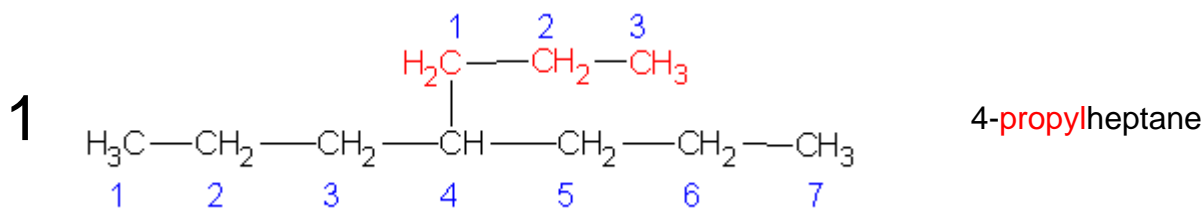
As we have seen above, it is possible to get branches on the branches of our alkanes. These branched alkyls must also be named using the same rules we've seen above for the main-chain alkanes.

1. Identify the longest part of the branch and use it as the root of the branch.
2. Number the carbons on the branch (this time you must always start from the carbon attached to the main chain).
3. Identify and number each branch off this branch using rules 1 and 2 recursively.
4. name the entire branch using the identified alkyl components and then attach the whole branch using the rules above.

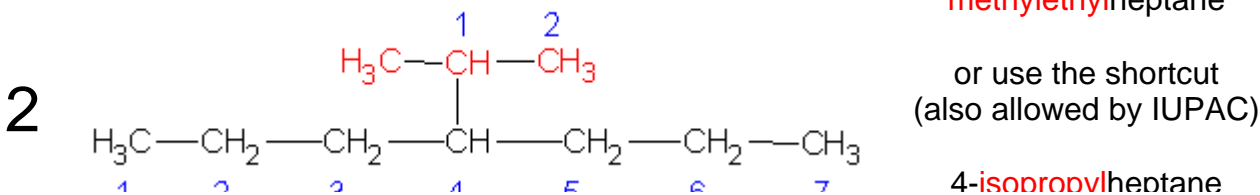
Take for example, the two formulas below.

There are a few common names that are often used as a part of a "IUPAC" name. If you recall the molecule isobutane ([see above](#)) which consisted of a three-carbon chain with a methyl group on the 2 position. It is more correctly named 2-methylpropane or just methylpropane (the 2- is redundant). There are many molecules that contain a group that could be classified as a three-carbon chain attached at position 2 rather than position 1. Take for example, the following two molecules.

Molecule 1 has a three carbon branch joined at the end to carbon 4 of the main chain. Since a three carbon chain has the root "prop" and this chain is a branch (suffix of yl) it is a propyl group. although it serves no purpose this time, the carbons on this group are numbered as shown, starting with the propyl carbon that's bonded to the main chain.



IUPAC: 4-1-methylethylheptane



1 2 3 4 5 6 7  
 (isopropyl group is shown here in red)

We can also look at the name of the three-carbon group in molecule 2. In this case, the propyl group is not attached at the end. It's attached in the middle. We must start numbering from the carbon attached to the main chain, thus, we find a two-carbon chain with a methyl branch on carbon 1. Hence the IUPAC name is 4-1-methylethylheptane. In this case, we can use the shortcut prefix "iso" to give this branch a simpler name. Rather than a 1-methylethyl group, we can call it an isopropyl group and thus the name of the molecule is shortened to 4-isopropylheptane.

If we have a 4-carbon alkyl group, rather than the three carbon one above, there are more possibilities.

Recall that there are 2 structural isomers of the 4-carbon alkane. These two can each attach to a larger main chain in two ways. They can use a terminal carbon or a middle carbon. Thus we can find 4 different 4-carbon alkyl groups are possible. In the following molecules, I will not draw the main chain. I will represent it merely as R (the Rest of the molecule)

#C	Alkane	Alkyl	name
4	butane $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_3$	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{R}$	butyl
		$\text{H}_3\text{C}-\text{CH}_2-\underset{\text{R}}{\text{HC}}-\text{CH}_3$	1-methylpropyl or sec-butyl s-butyl*
	isobutane (2-methylpropane) $\text{H}_3\text{C}-\underset{\text{CH}_3}{\text{CH}}-\text{CH}_3$	$\text{H}_3\text{C}-\underset{\text{CH}_3}{\text{CH}}-\text{CH}_2-\text{R}$	2-methylpropyl or isobutyl
		$\text{H}_3\text{C}-\underset{\text{CH}_3}{\overset{\text{R}}{\text{C}}}-\text{CH}_3$	1,1-dimethylethyl or tert-butyl t-butyl t-butyl*
pentane $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_3$	$\text{H}_3\text{C}-\underset{\text{CH}_2-\text{CH}_2}{\text{CH}_2}-\text{CH}_2-\text{R}$	pentyl	
	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\underset{\text{R}}{\text{CH}}-\text{CH}_3$ 4 3 2 1	1-methylbutyl	
	4 3 2 1		

<b>5</b>	2-methylbutane	$\begin{array}{c} \text{H}_3\text{C}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{R} \\   \\ \text{CH}_3 \end{array}$	2-methylbutyl
	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}-\text{CH}_3 \\   \\ \text{CH}_3$	$\begin{array}{c} \text{R} \\   \\ \text{H}_3\text{C}-\text{CH}_2-\text{C}-\text{CH}_3 \\   \\ \text{CH}_3 \end{array}$	1,1-dimethylpropyl
		$\begin{array}{c} \text{H}_3\text{C}-\text{CH}-\text{CH}-\text{CH}_3 \\   \quad   \\ \text{R} \quad \text{CH}_3 \end{array}$	1,2-dimethylpropyl
	2,2-dimethylpropane or neopentane	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_3\text{C}-\text{C}-\text{CH}_2-\text{R} \\   \\ \text{CH}_3 \end{array}$	2,2-dimethylpropyl or neopentyl

\* In a couple of cases, we have some prefixes we've never seen before. Prefixes sec- and tert- (or sometimes t-) refer to secondary and tertiary, respectively. These terms refer specifically to the number of carbons in the branch attached directly to the root (carbon 1)

A carbon is considered a primary carbon if it has only 1 other carbon attached to it on the branch. In this case, the carbon is at the end of a chain. For example the ethyl group  $\text{H}_3\text{C}-\text{CH}_2-\text{R}$  can only have a primary carbon (in red). The propyl group could have a

primary  $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{R}$  or a secondary  $\begin{array}{c} \text{H}_3\text{C}-\text{CH}-\text{R} \\ | \\ \text{H}_3\text{C} \end{array}$  carbon, depending on where the

R is attached. In the case of the secondary carbon (in the branch called 1-methylethyl), there are 2 other carbons bonded to that carbon. (we don't use the name sec-butyl for this alkyl group since a more common shortcut is isobutyl as is indicated above).

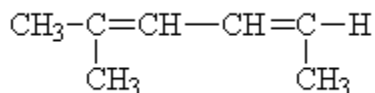
The butyl group can have a primary,  $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{R}$ , a secondary,

$\begin{array}{c} \text{CH}_3 \\ | \\ \text{H}_3\text{C}-\text{CH}_2-\text{CH}-\text{R} \end{array}$ , or a tertiary carbon,  $\begin{array}{c} \text{CH}_3 \\ | \\ \text{H}_3\text{C}-\text{C}-\text{R} \\ | \\ \text{CH}_3 \end{array}$ , depending on the structure. The tertiary carbon is one with three *other* carbons attached.

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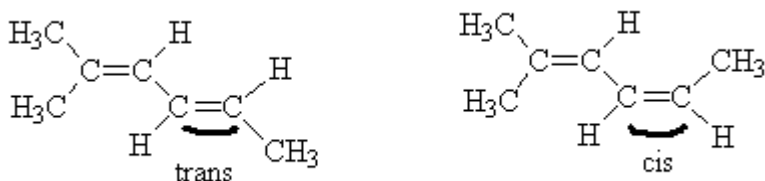
## Geometric isomers.

Let's try another example. What is the name of this molecule?



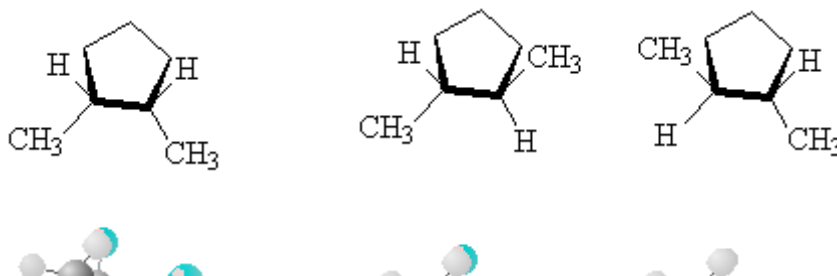
Actually, this example is more complex than it seems. The molecule, at first glance seems simpler than [example b](#) a few pages back. This is not the case. Because there is not free rotation about the double (or triple) bonds it is possible to have different isomers where the structure of the isomers is identical but where the geometric arrangement is not the same. Thus, we create **geometric isomers**. This is different from the conformers that we saw earlier where free rotation easily (some times) converts one geometric arrangement into another. Here, the geometric arrangements are not changeable without breaking a bond.

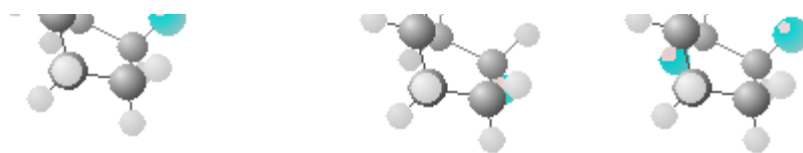
Thus, example b) above should actually be better drawn as follows:



We can see two distinct isomers because the position of the  $\text{CH}_3$  group relative to the ethylene group on the other side of the (right-hand) double bond is different from one case to another. In one case, the non-hydrogen constituents are on opposite sides of the double bond. This is the *trans* configuration. In the other case, the non-hydrogen constituents are on the same side of the double bond. This is the *cis* configuration. thus, the names for these two molecules are ***trans-2-methyl-2,4-hexadiene*** and ***cis-2-methyl-2,4-hexadiene***, respectively. Of course, there are always more complex cases where these simple rules break down and need refinement. We can't cover all the rules in just a few hours worth of lectures.

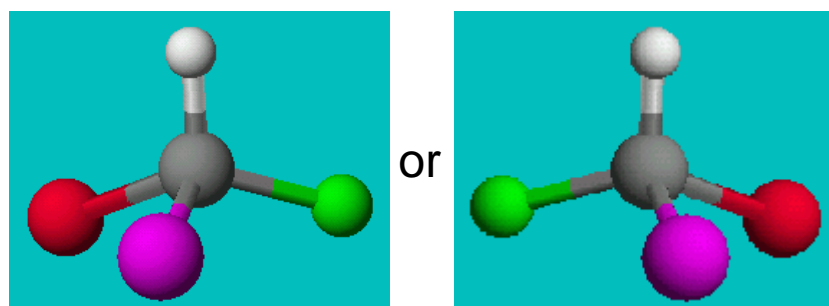
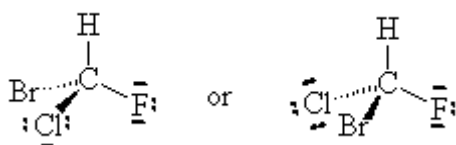
It is also possible to get cis-trans isomers from other molecular structures where rotation about a bond is not possible, for example, in cyclo- compounds, the ring prevents free rotation as follows.



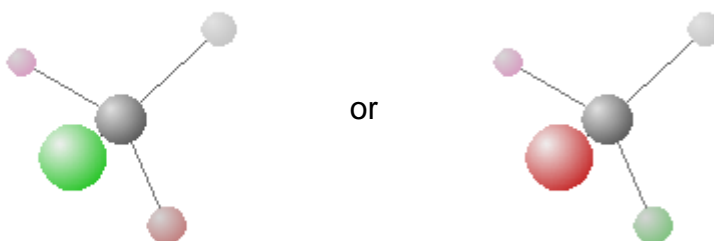


cis-1,2-dimethylcyclopentane      trans-1,2-dimethylcyclopentane

NOTE: The two drawings on the right are both the same structure and geometry and therefore with the same name. However, they are not quite identical. They are in fact optical isomers (enantiomers) of each other. Chemically, they are identical (except to enantiomeric reactants and catalysts like enzymes) but optically they are different. Optical isomers can only form if there is 3-d structure in the mode (for example tetrahedral carbons). If the molecule has planar symmetry (trigonal planar carbons) then any mirror image is also super imposable. A simpler set of enantiomers can be found in the VSEPR chapter where I discussed a tetrahedral carbon with 4 different substituents on it.



Can you superimpose these mirror images?



video: [non-super imposable mirror images](#)

video: [superimposable mirror images](#)

These molecules are optically active (they plane-rotate polarized light). The pair are enantiomers (optical isomers) of each other. Individually, any molecule that displays optical activity is called **chiral** and the amount and direction of it's optical activity is termed it's chirality.

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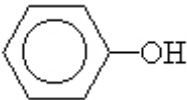
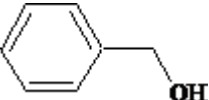


## Functional groups

Functional groups (other than double and triple bonds) occur whenever a heteroatom (not carbon or hydrogen) is incorporated into the structure. The following is a quick list of functional groups and some quick information on naming them.

### Alcohols

Alcohols are identified by presence of an OH group on a hydrocarbon chain (R-OH). These compounds are usually named by appending *-ol* to the end of the name and sometimes, indicating the location of the functional group using numbers as previously described. Below are a few examples of alcohols and their names.

$\text{CH}_3\text{-CH}_2\text{-OH}$	ethanol (note: remove the 'e' of 'ane')
$\begin{array}{c} \text{CH}_3\text{-CH-OH} \\   \\ \text{CH}_3 \end{array}$	2-propanol (the OH is on carbon 2 of the propane chain) <i>also called isopropanol</i> .
	benzenol <i>also called phenol</i>
	benzyl is a benzene with a methyl group. This is benzyl alcohol.

There are several types of alcohols, ethanol and methanol have their functional group on a terminal carbon and are called primary alcohols (the carbon to which the OH is attached has at most one other carbon attached to it. R-COH).

Secondary alcohols occur when the functional group occurs in the middle of the chain, as in 2-butanol. Here, the alcoholic carbon has two other carbons bonded to it, hence the terminology *secondary*.

2-propanol could also be named accordingly as *sec*-propanol. (*sec* means secondary).

Tertiary alcohols involve alcoholic carbons with three other carbons bonded to them. In this case, the OH occurs just at the junction between two alkane chains as in:

$\begin{array}{c} \text{OH} \\   \\ \text{CH}_3 - \text{C} - \text{CH}_3 \\   \\ \text{CH}_3 \end{array}$	2-methyl-2-propanol or <i>t</i> -butanol ( <i>t</i> is for tertiary)
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There are also diols and triols (and more), where more than one OH group exists on a single carbon chain.

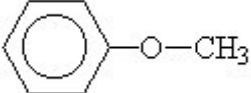
$\begin{array}{c} \text{CH}_2 - \text{CH}_2 \\   \quad   \\ \text{OH} \quad \text{OH} \end{array}$	1,2-ethanediol or ethylene glycol (antifreeze)
$\begin{array}{c} \text{CH}_2 - \text{CH} - \text{CH}_2 \\   \quad   \quad   \\ \text{OH} \quad \text{OH} \quad \text{OH} \end{array}$	1,2,3-propanetriol or glycerol or glycerine

## Ethers

An ether group contains two hydrocarbon chains connect by an oxygen atom (R–O–R').

Simple ethers can be names by simply naming the two branches first and then prepending them to the word ether. Alternatively, more complex molecules can be named by considering the R–O group to be the *alkoxy* group and simply treating it like a branch on the larger molecule. Below are a few examples, some use both naming conventions.

Numbering if necessary is done in the normal fashion.

$\text{CH}_3 - \text{CH}_2 - \text{O} - \text{CH}_2 - \text{CH}_3$	diethylether
$\text{CH}_3 - \text{CH}_2 - \text{O} - \text{CH}_3$	ethylmethylether or methoxyethane
	methylphenylether or methoxybenzene

## Aldehydes

An aldehyd has a terminal C with a double bonded oxygen (  $\begin{array}{c} \text{O} \\ // \\ \text{---C} \\ | \\ \text{H} \end{array}$  ).

such compounds are named by adding the suffix *-al*. Numbering is not necessary since the functional group must be (by definition) at the end of the carbon chain, therefore, it is always attached to carbon #1.

	methanal
	ethanal
	propanal

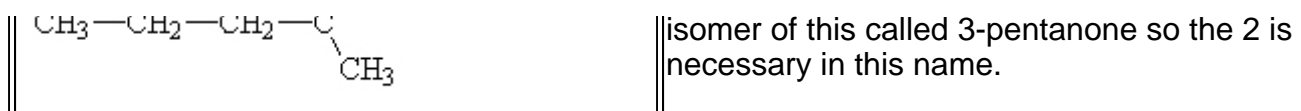
Notice that these molecules are all drawn with the aldehyde carbon looking to have bond angles of about 120°. That's because the C=O unit means the carbon is SP<sup>2</sup> hybridized and is therefore trigonal planar with bond angles of approximately 120°. It's best to represent the true geometry of at least the planar portions of molecules when you can and we do here.

## Ketones

Ketones occur when a non-terminal carbon contains a double bonded oxygen ( $\text{R}-\text{C}(\text{O})-\text{R}'$ ).

Here, the R chains may or may not be identical, hence the prime on one of them. Here, however, we treat the entire chain (R-C-R') as a single unit when naming and simply indicate the carbon number where the double bonded oxygen occurs (if necessary).

	propanone (the 2 is redundant since 1-propanone is, in fact propanal.) This is a structural isomer of propanal  commonly called acetone (nail-polish remover).
	butanone. (again, the 2 would be redundant since 3-butanone is merely 2-butanone improperly numbered and 1-butanone is really butanal).
	2-pentanone. There is also a structural



## Carboxylic acid

In this functional group, we combine the OH and the C=O on one carbon and the new

functional group is a carboxylic acid(  $\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—OH}$  ). This group is obviously always located on

the terminal carbon of a hydrocarbon chain. It is named using the name of the hydrocarbon parent chain and the suffix *-oic acid*. Below, find some examples, alternative common names are give in parentheses.

$\text{H}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	methanoic acid (formic acid)
$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	ethanoic acid (acetic acid)
$\text{CH}_3-\text{CH}_2-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	butanoic acid (butric acid)
$\begin{array}{c} \text{CH}_3-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	2-methylpropanoic acid (isobutric acid) <i>This is a structural isomer of butanoic acid.</i>

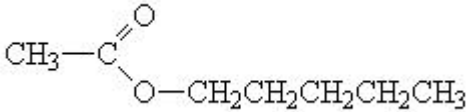
## Esters

An ester is made when a carboxylic acid and an alcohol react as follows



When naming an ester, we use the names of the component alcohol and of the carboxylic acid and append the suffix *-oate*.

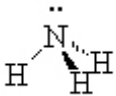
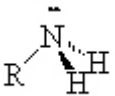
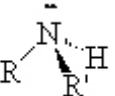
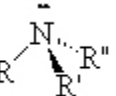


	pentylethanoate (banana smell)
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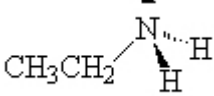
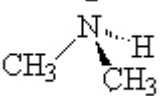
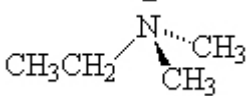
## Amines

Amines are compounds containing nitrogen, *cf.*, ammonia (NH<sub>3</sub>). There are three types of amines.

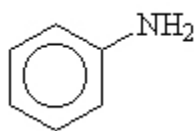
Primary amines have only 1 carbon attached to the nitrogen. Secondary amines have two carbons attached to the nitrogen and tertiary amines have three carbons attached to the one nitrogen atom.

			
ammonia	primary amine	secondary amine	tertiary amine

We name the amines by simply naming each of the R groups alphabetically as we do branched on an alkane and ending the name in *amine*.

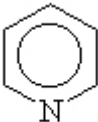
		
ethylamine	dimethylamine	ethyldimethylamine

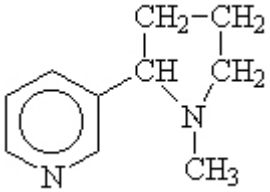
In some cases, the groups attached to the nitrogen are more important (or complex) than the amine and naming is simplified by treating the amine as the branch rather than the parent. In this case, we name the amine and append the letter *o* to the end and then name the parent.



aminobenzene (could also be phenylamine but this is not customary).

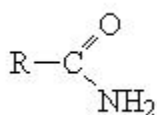
Other amines simply use the common name since other conventions become too complicated.

	pyridine
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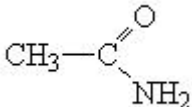
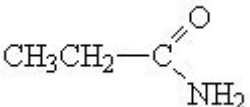
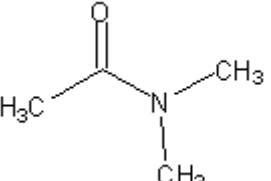
	<p style="text-align: center;">nicotine</p>
---	---

## Amides

These are the compounds that hold your DNA and RNA in their double helix shape. An amide is like a carboxylic acid but where the OH group is replaced by an amine group, for example, NH<sub>2</sub> or NHR or NRR'.



These molecules are easier to name. Simply name the carbon chain and then add the suffix *amide*.

	<p>ethanamide also called acetamide (like acetic acid)</p>
	<p>propanamide</p>
	<p>N,N-dimethylethanamide also called N,N-dimethylacetamide</p> <p>Note: we specify that the alkyl groups are on the Nitrogen using N.</p>

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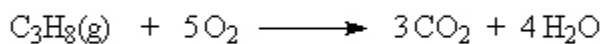


## Reactions

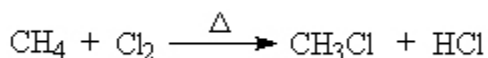
Here are a few common reaction types:

### Reactions of Alkanes

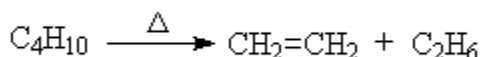
Burn in air to give carbon dioxide and water. This is the ultimate in a series of oxidation reactions of hydrocarbons. Lesser oxidation reactions would form alcohols, aldehydes, ketones and acids. We won't delve into those in this course.



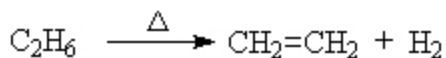
Reacts with halogen at high T.



Cracking (in oil refining, used to reduce the molar mass of the compounds so they can be used as gasoline, etc.) [Cracking Explained Details](#)



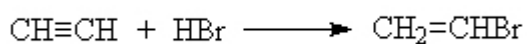
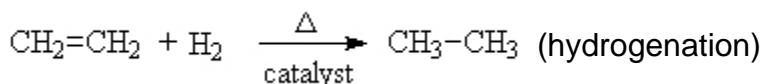
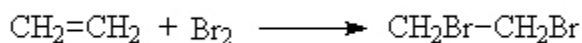
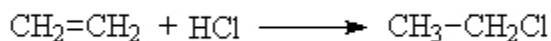
dehydrogenation (removal of a hydrogen molecule  $\text{H}_2$ )



## Reactions of alkenes and alkynes

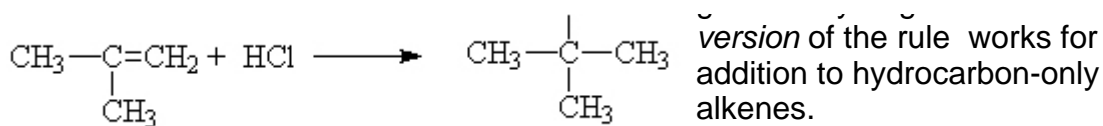
Double or triple bonds are more reactive.

### Addition reactions



**Markovnikov's rule Old Form:**  
when adding acids to an alkene,  
the side with the most hydrogens  
gets the hydrogen. This *old*

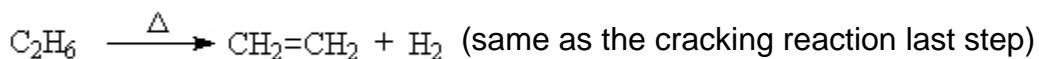
Cl



[For a detailed explanation, click here.](#)

### Elimination Reaction (opposite of addition)

A saturated hydrocarbon (as many hydrogens as possible) is converted to an unsaturated hydrocarbon by 'eliminating' a hydrogen molecule. This is also called dehydrogenation.

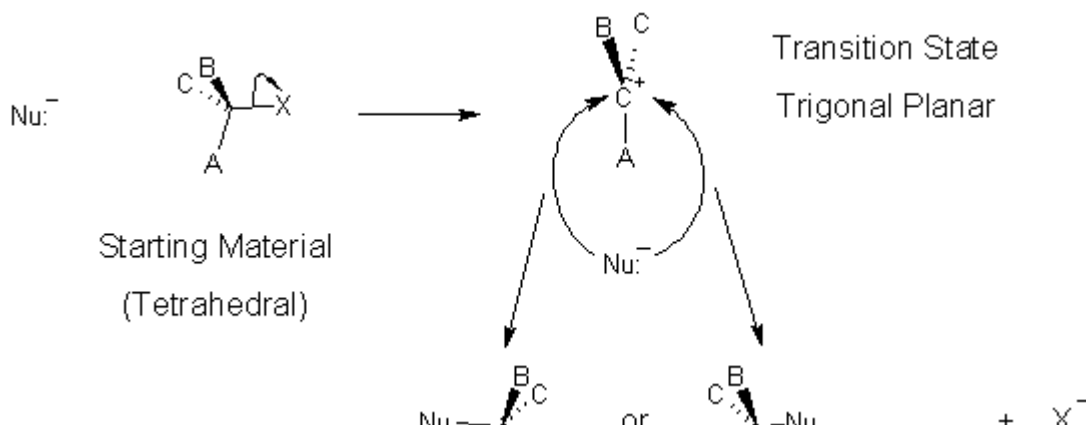


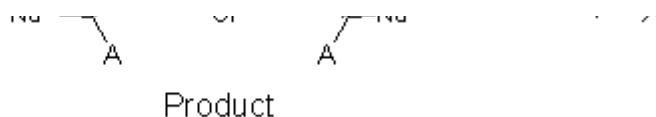
### Substitution Reactions

In a substitution reaction one substituent is substituted for another. A very common type of substitution involves the replacement of a leaving group X (X is something that can leave the molecule relatively easily) by a nucleophile Nu (~phile implies "attraction to" so a nucleophile is attracted to the positive charge of a nucleus). I will use Nu to stand for the generic nucleophile. Normally, a nucleophile is negatively charged or polar with lone pairs of electrons. These can be used to form new a new bond with the nucleus (carbon atom) involved. There are two types of Nucleophilic Substitution, S<sub>N</sub>1 and S<sub>N</sub>2:

### S<sub>N</sub>1

In an S<sub>N</sub>1 process, there are two steps involved. The first step (the slow step) involves only the starting molecule, the nucleophile is not involved. Hence the 1 of S<sub>N</sub>1 means 1 molecule is involved (*unimolecular*). In this step, the leaving group takes its pair of electrons and leaves behind a positively charged trigonal-planar carbon (alias *carbocation*). Then the nucleophile bonds to the carbocation. In this case, because the intermediate is symmetrical, before the nucleophilic attack, there are two possibly products, depending on the side from which the nucleophile attacks.

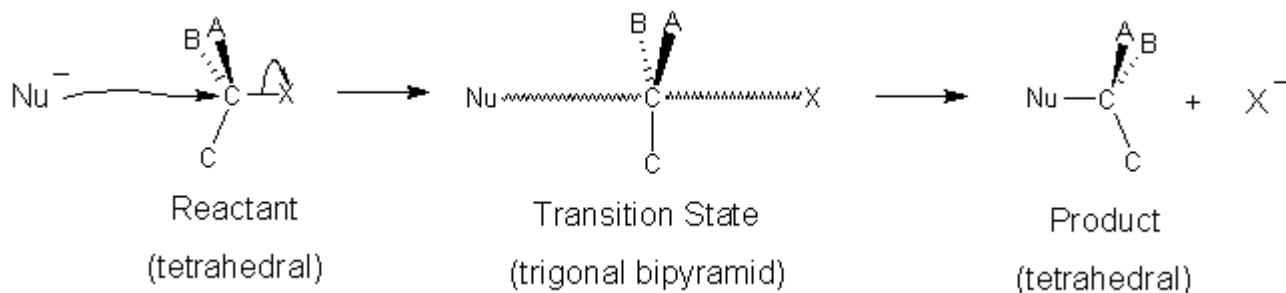




In this reaction mechanism, because the nucleophile is just as likely to attack from the left as from the right, we will get a 50:50 mixture of the two products. If the reactant was chiral (optically active) then the two products are both chiral but of opposite chirality. The mixture will display no optical activity since the two products optical activities cancel each other out. This is a *racemic mixture*.

## $S_N2$

In the  $S_N2$  process, the nucleophile bonds to the carbon while the leaving group breaks its bond in a concerted step. This first step (slow) involves 2 molecules simultaneously (*bimolecular*), the starting material and the nucleophile, hence the 2 in  $S_N2$ . At the intermediate (or transition state), the positions of constituents ABC move to a planar orientation with the Nu on one side and the leaving group X on the other to form a trigonal bipyramidal intermediate (transition state). As the nucleophile moves closer with its lone pair, the leaving group departs, taking its bonding pair as a lone pair and taking the excess charge in the process. The spatial orientation of the groups ABC is reversed in the process. In the case of an optical isomer (chiral molecule) the chirality (direction that light is rotated) is reversed.



Note that in the case of  $S_N2$  reactions, the carbon is tetrahedral when the Nucleophilic attack occurs. This means that there is greater possibility of steric hindrance. If the carbon on which the reaction should occur is tertiary then an  $S_N2$  reaction is unlikely and an alternate reaction processes may then dominate. One such possibility is an Elimination reaction (see second year Organic Chemistry courses/texts for details).

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\* IUPAC stands for International Union of Pure and Applied Chemistry