

Organic Chemistry

The classification of chemical compounds into the general areas of organic and inorganic derives from the use of the "mineral, vegetable and animal" designation by the early workers in chemistry. Those compounds derived from living systems were termed **organic** (about 1777) whereas those derived from mineral sources were termed **inorganic**. In modern times, organic compounds are classified as compounds of carbon containing either carbon-carbon or carbon-hydrogen bonds or both. Originally, organic compounds were thought to be imbued with a "vital essence" attainable only from God. Thus, it was believed that organic compounds could be prepared from sources that had once lived, as this would be the only way that this vital essence could be obtained by man. In 1828, Friedrich Wöhler prepared the organic compound urea (found in human urine) from entirely nonliving sources, thereby destroying the theory of organic vitalism. Since Wöhler's time, approximately 5 million organic compounds have been synthesized and characterized, many of which are not found in nature.

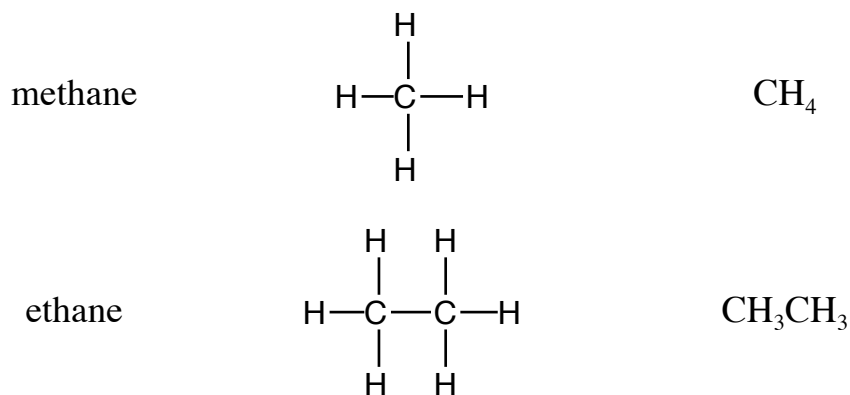
Why are there so many organic compounds? The reason is that carbon atoms have the ability to link to other carbon atoms (concatenate) to produce chains or rings of almost infinite size. Other elements do not concatenate nearly as well due to such factors as poor orbital overlap and lone pair-lone pair electronic repulsions. Other elements can also combine with carbon to form hetero-species, including hydrogen, oxygen, nitrogen, sulfur and the halogens.

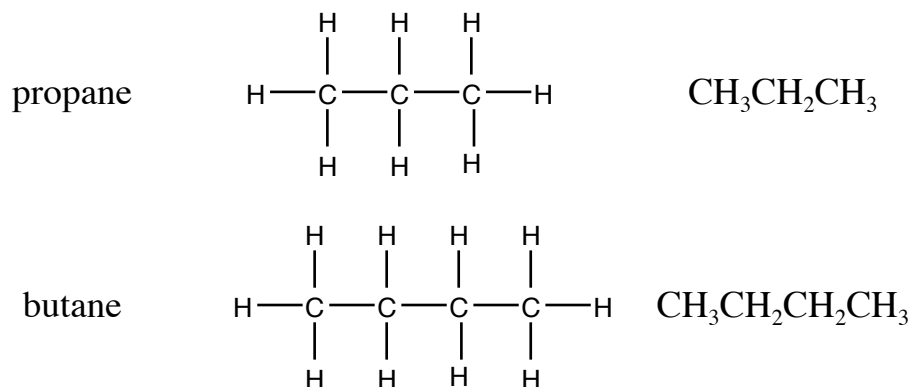
The distinction between the organic and inorganic disciplines is not very sharp. The bonding of metals to carbon has resulted in the large, important and fast growing area of **organometallic** chemistry. Organometallic compounds containing metals and metalloids such as lithium, magnesium, copper, iron, boron, silicon, and other elements play major roles as synthetic reagents.

The purpose of this experiment is to prepare models of the more common organic compound types to enhance their three dimensional nature. Bond angles between atom groupings will become apparent as you build the models.

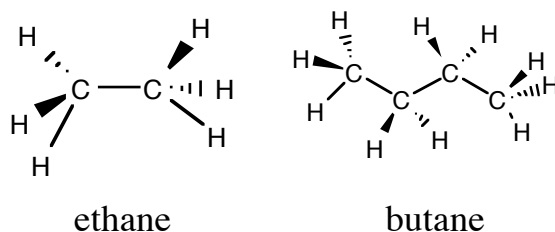
Saturated Hydrocarbons: The Alkanes

Alkanes are **hydrocarbons** (compounds with hydrogen and carbon atoms) linked with single bonds. All the carbon atoms are sp^3 hybridized and are tetrahedrally bonded to four other carbon or hydrogen atoms. Members of this class have the general formula C_nH_{2n+2} , where n is an integer. Examples of this class of organic compound include methane (CH_4 , $n=1$), ethane (C_2H_6 , $n=2$) and propane (C_3H_8 , $n=3$). Structures of the first four straight chain compounds are shown below.



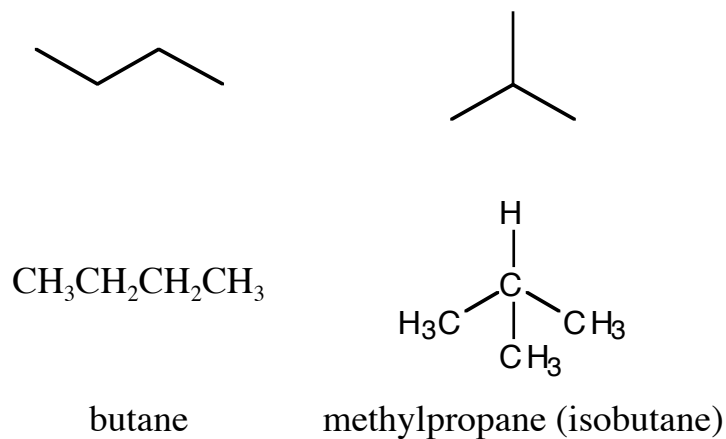


These representations do not show the actual geometrical structure of these compounds. Due to the sp^3 hybridization of the carbon atoms, all the bond angles in the molecules are close to 109.5° (tetrahedral) and thus, the carbon chain is nonlinear. The **wedge-dash** notation can be used to represent the nonlinear nature of these molecules. Examples of ethane and butane are given below using the wedge-dash notation.



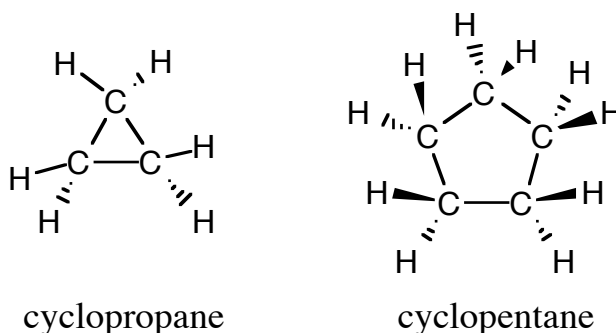
As you prepare models of the alkanes, note that each carbon atom can rotate about its respective carbon-carbon bond. Some conformations (arrangements of the bonds and groups relative to each other) are more stable than others, since in these arrangements there is less interference (steric repulsion) between the hydrogen atoms attached to nearby carbons.

An interesting aspect of the alkanes is that **structural isomers** can exist in compounds having more than three carbon atoms. Structural isomers are species that have the same molecular formula but possess different physical properties due to different arrangements of the carbon backbone. The two compounds below are an example of an isomeric pair of hydrocarbons. Both are butanes and have the formula C_4H_{10} , but their structures are different.



This figure relates several new points. First is the use of the **skeleton formula**. These structures represent the carbon backbone without the hydrogen atoms being shown and are often used as a shorthand method of representing the structures. The second point is the use of substituents in naming compounds. We can see that in methylpropane, one of the CH_3 groups is a "twig" off of the main "branch" of the compounds. Such twigs are called **alkyl groups**. In the figure, the **methyl group** (CH_3) name is derived from the hydrocarbon methane (CH_4) having lost a hydrogen. The number of possible isomers increases rapidly as the number of carbon atoms increases in a compound. For example, the pentane system (five carbons) has three isomers, the heptane system (seven carbons) has nine isomers, and the decane system (ten carbons) has seventy-five isomers!

Alkanes can also exist as **cyclic** hydrocarbons where the carbon atoms are arranged in rings. The general molecular formula is C_nH_{2n} , where n is an integer. These carbons are named identically to the alkanes except for the additional prefix *cyclo*. The structures for two cyclic hydrocarbons are given below.

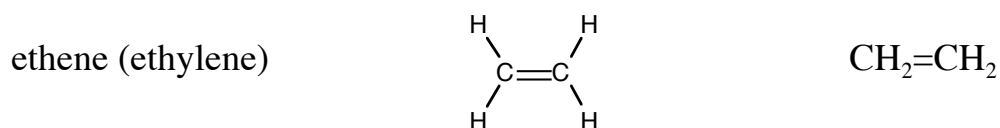


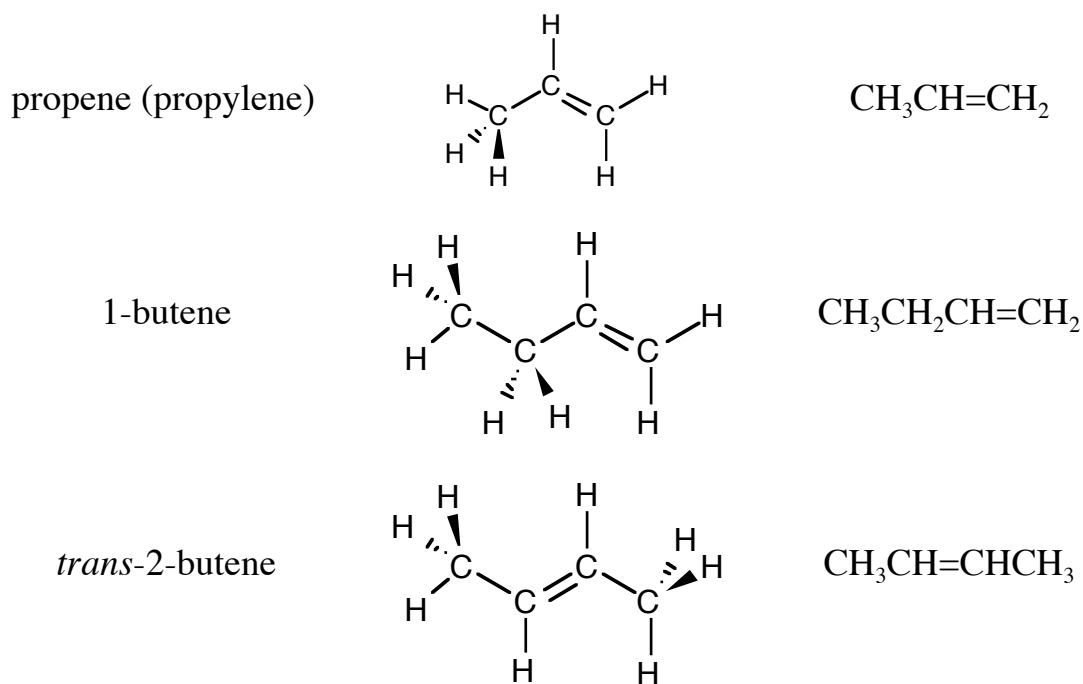
In the smaller rings such as cyclopropane and cyclobutane, smaller bond angles (60° and 90° , respectively) are evident. Such angles are seen as being strained from their normal tetrahedral angle, and these compounds have less stability than their larger counterparts. The most stable cyclic compounds contain rings of five and six carbons (cyclopentane and cyclohexane, respectively).

Unsaturated Hydrocarbons: The Alkenes

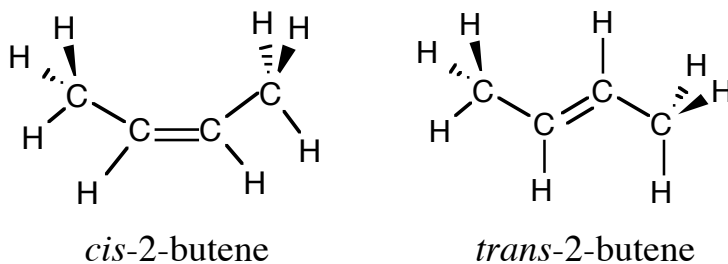
Alkenes are hydrocarbons in which there are one or more carbon-carbon double bonds, $\text{C}=\text{C}$. The carbon atoms attached to the double bond are sp^2 hybridized. One of the double bonds is a **sigma** bond (oriented along the internuclear axis) and the other is a **pi** bond (oriented perpendicular to the internuclear axis). Members of this class have the general formula C_nH_{2n} , where n is an integer (note that this is the same formula as for the cycloalkanes.) Examples of alkenes include ethene (C_2H_4 , $n=2$, also known as ethylene), propene (C_3H_6 , $n=3$, also known as propylene) and butene (C_4H_8 , $n=4$). Structures of several of the alkenes are shown below. Alkenes are named in the same fashion as the alkanes except that the ending *-ene* replaces the ending *-ane*. In cases where more than one structural isomer exists (such as butene, below), it is necessary to indicate the

location of the double bond by numbering the carbon atoms in the longest chain containing the double bond, and then giving it the lowest possible number.

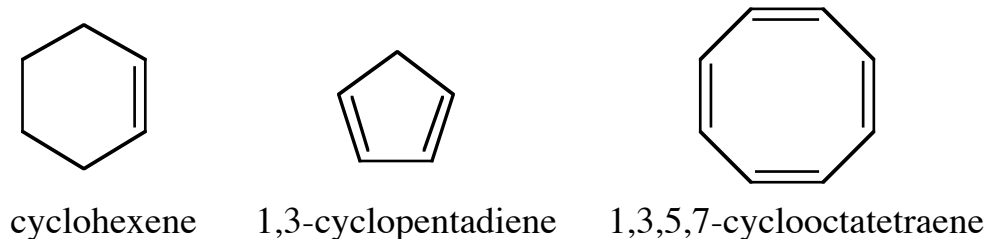




Many kinds of isomerism exist in organic compounds. Since carbon atoms are free to rotate around the C-C single bonds but not around a C=C double bond (this disrupts the overlap of the pi part of the double bond), it is possible to have two separate geometrical isomers of 2-butene. These are known as the *cis*- and *trans*- isomers and are shown below:

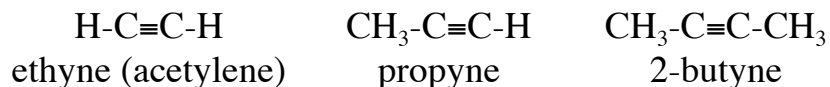


Cyclic structures containing C=C bonds are also possible, and three examples follow.



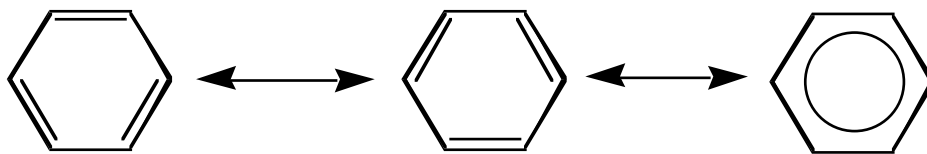
Unsaturated Hydrocarbons: The Alkynes

Hydrocarbons containing a carbon-carbon triple bond are named **alkynes**. The two carbon atoms forming the triple bond are joined by one sigma and two pi bonds and are sp hybridized. The alkynes have the general molecular formula C_nH_{2n-2} . Several representatives of this class are shown below. Alkynes are named in the same manner as alkenes except that the ending *-yne* replaces the ending *-ene*.

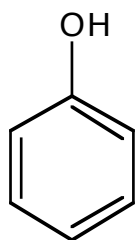


Aromatic Hydrocarbons

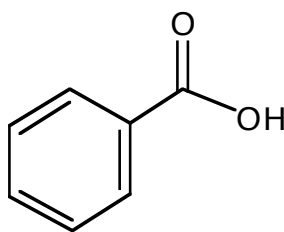
Benzene, C_6H_6 , is the most crucial member of this important class of hydrocarbons. The molecule contains a ring of six sp^2 hybridized carbon atoms with the unhybridized p orbitals perpendicular to the ring system. The six electrons in the pi parts of the bonds are **delocalized** (spread evenly over the six carbon nuclei). Such molecules are often unusually stable. There are two equally valid ways of representing the structure of benzene. These two ways are called resonance forms, and the molecule is a **resonance hybrid** with the "true structure" of benzene lying midway between the two resonance forms. As an example, a mule is a genetic hybrid descendant of a male donkey and a female horse. The mule does not change back and forth, being a donkey half the time and a horse the other half. Thus, the properties of a resonance hybrid (such as benzene) are fixed.



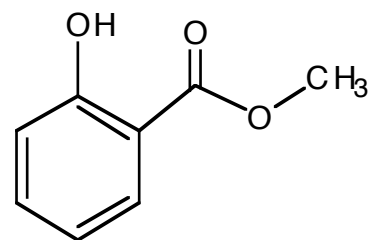
There are many familiar hydrocarbon species which are based on the benzene structure that contain various functional groups. A few representative examples are given below. Note that the delocalized pi electrons can be represented by a circle in the ring. This is an alternate representation of the ring often used by chemists.



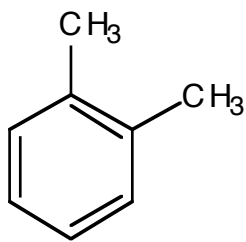
phenol



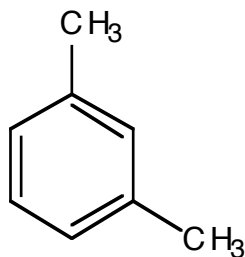
benzoic acid



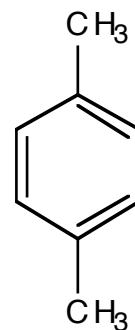
oil of wintergreen



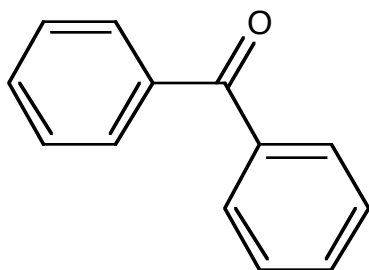
1,2-dimethylbenzene
(ortho-xylene)



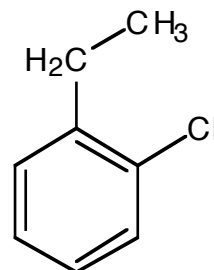
1,3-dimethylbenzene
(meta-xylene)



1,4-dimethylbenzene
(para-xylene)

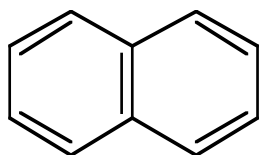


benzophenone

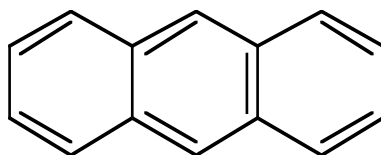


2-chloroethylbenzene

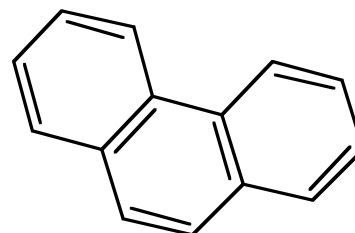
There are also many important aromatic hydrocarbons that contain more than one fused benzene ring. Several are illustrated here.



naphthalene



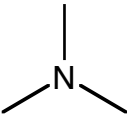
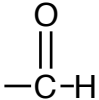
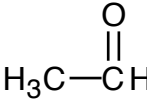
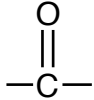
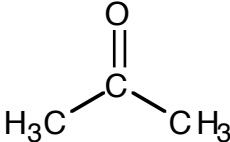
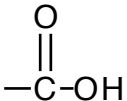
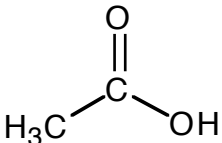
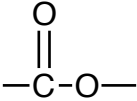
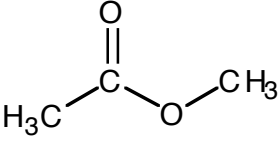
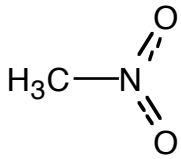
anthracene



phenanthrene

Hydrocarbons Containing Functional Groups

The basic types of hydrocarbon compounds outlined above may have one or more of their hydrogen atoms replaced by a **functional group**. The substituted benzenes earlier illustrated a number of functionalities (-CH₃, -OH, etc.) attached to the aromatic ring. Additional examples are shown in the table below.

Functional Group	Class of Compound	Example	Name
-OH	alcohol	H ₃ C—CH ₂ —OH	ethanol (ethyl alcohol)
-O-	ether	H ₃ C—O—CH ₃	dimethyl ether
	amine	H ₂ N—CH ₃	methylamine
	aldehyde		ethanal (acetaldehyde)
	ketone		propanone (acetone)
	carboxylic acid		ethanoic acid (acetic acid)
	ester		methyl acetate
-NO ₂	nitro		nitromethane
-X (X = F, Cl, Br, I)	haloalkane	H ₃ C—CH ₂ —Cl	chloroethane (ethyl chloride)

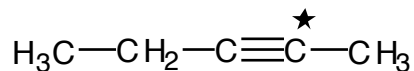
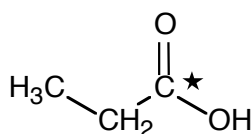
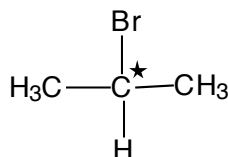
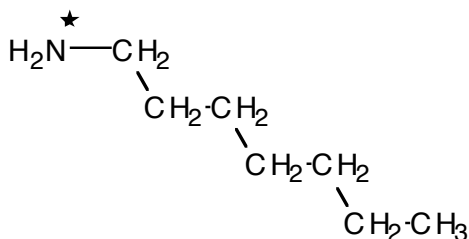
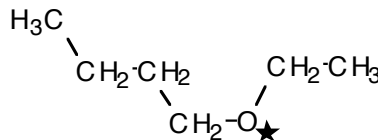
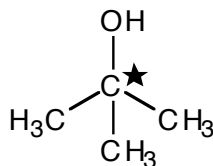
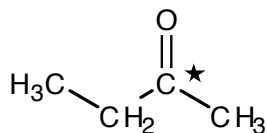
Organic Chemistry Worksheet - Continued

3. Aromatic Compounds

- a. Prepare a model and sketch the line structure of the aromatic compound benzene, C_6H_6 . Comment on the fact that measurement of the C-C bond distances in benzene shows that all are the same length (1.397 Angstroms) and that the C-C bond angles are all 120° . Is benzene a flat molecule?
- b. Benzene was at one time used extensively as a solvent. However, since it has been found to be carcinogenic, it has largely been replaced by toluene. Toluene, which is formally known as methylbenzene, contains an aromatic ring substituted with a methyl group and has a molecular formula of C_7H_8 . Sketch a possible structure for toluene. Do you think toluene would have a higher or lower boiling point than benzene? Explain.
- c. Draw two resonance structures for naphthalene.
- d. There are three dichlorobenzene isomers. Draw them. Which one would you expect not to have a dipole moment? Explain.

Organic Chemistry Worksheet - Continued

4. Identify the functional group and/or class of compound in each of the following molecules. List the hybridization around the marked atom in each compound. Finally, name the compound.



5. Draw structures for acetone, formaldehyde and acetic acid. What are the bond angles around the C=O carbon atom in each of these compounds?

Organic Chemistry Worksheet - Continued

6. Draw the structures for the following compounds:

a. 2,3-difluorohexane

g. *cis,trans*-2,6-octadiene

b. dimethyl ether

h. 2-hexyne

c. butanone

i. 3-nitrotoluene

d. dimethylamine

j. 4-bromobenzoic acid

e. 2-pentanol

k. 2,4,6-trinitrotoluene

f. 2,3-diethyltoluene

l. 2-chlorophenol

