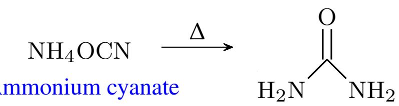
Ch. 1. Organic Chemistry

ORGANIC chemistry is a vast subject that studies the properties of carbon-based compounds, and organic compounds are chemicals based mostly on carbon as well as hydrogen. On one hand, organic chemistry plays a key role in the understanding of the functioning and composition of living cells. On the other hand, many products of industrial organic chemistry such as plastics, fuels, perfumes, or prescription drugs are an accepted part of our everyday lives. These types of compounds have common organic properties, from their smells to their powerful action. Key organic chemistry concepts are the naming of organic compounds and the properties of functional groups that give unique properties to molecules such as caffeine or even addictive drugs such as cocaine.

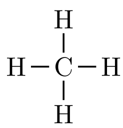
1.1 Organic and non-organic compounds

Organic compounds are chemicals mostly made of carbon and hydrogen, containing chains or rings of carbon atoms. Here a few examples of organic compounds: CH_4, C_2H_6, or C_6H_6. Differently, inorganic compounds contain elements other than carbon and hydrogen. Examples of inorganic compounds are: NaCl, CO_2, HCl, FeO or NaOH. Mind that carbonates (Na_2CO_3), carbon monoxide (CO) or carbon dioxide (CO_2) are not organic compounds. Originally the distinction between organic and inorganic compounds was made based on whether the chemical comes from a living system. Indeed organic compounds were thought of as synthesized only from living organisms. This belief was disregarded after Friedrich Wöhler was able to synthesize urea–a component of urine–from ammonium cyanate, an inorganic salt:



Urea

Alkanes are simple organic compounds made of carbon and hydrogen with all carbons connected using simple bonds–these are single lines representing the connections between atoms. The simplest alkane and the simplest organic compound is methane: CH_4, a fuel and the main constituent of natural gas.

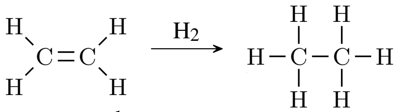


Methane, CH_4

Its structure is representative of organic compounds in general as it shows that each carbon atom in an organic molecule is connected to four different atoms.

1.2 Alkanes

Hydrocarbons composed of single C-C bonds are called saturated hydrocarbons, whereas hydrocarbons containing multiple C-C bonds are described as being unsaturated. All carbons in a saturated hydrocarbon are bound to four atoms. You can produce saturated hydrocarbons by reacting an unsaturated hydrocarbon with hydrogen:



unsaturated saturated

This first section will introduce organic chemistry, covering the simplest organic compounds: alkanes. Alkanes–also called hydrocarbons–are simply made of carbon and hydrogen with all C-C bonds being single bonds. First, you will be introduced to a few organic chemicals, and you will learn about a series of different organic formulas that can represent the same compound. Then, you will learn the basic naming rule of alkanes, which extends to other–more complex–organic chemicals.

▼Methane (CH_4) is used as a fuel for ovens, homes, water heaters.

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`Molecular formula for alkanes` The naming of alkanes results from the combination of a prefix and a suffix. On one hand, the suffix is always *ane*. On the other hand, the prefix depends on the number of carbons in the molecule. Table **??** shows a list of the different prefixes. For example, the alkane with a single carbon is called methane (CH_4). Other examples of alkanes are ethane which contains two carbons (C_2H_6) or propane with three carbons (C_3H_8). The molecular formula for an alkane with n carbon atoms is:

$$C_nH_{2n+2} \tag{1.1}$$

Hence, we have that the molecular formula for methane ($n = 1$) is CH_4 and the molecular formula for octane ($n = 8$) is C_8H_{18}. *Molecular formulas* represent only the molecular compositions, showing only the elements in the molecule.

▼Hydrocarbons, made of carbon and hydrogen, tend to be gaseous molecules.

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Sample Problem 1

Write down the molecular formula for decane and pentane.

SOLUTION

Using Equation **??** we have that the molecular formula for decane ($n = 10$) would be: $C_{10}H_{22}$. Similarly, the molecular formula for pentane ($n = 5$) would be: C_5H_{12}.

▶Answer: (decane) $C_{10}H_{22}$; (pentane) C_5H_{12}

STUDY CHECK

Name the alkane with formula C_7H_{16} and give the molecular formula for nonane.

▶Answer: heptane, C_9H_{20}.

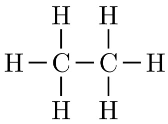
▼The octane rating of gas is a standard measure of the performance of engine fuels, originally determined by mixing a gasoline made entirely of heptane and 2,2,4-trimethylpentane (a highly branched octane).

© wikipedia

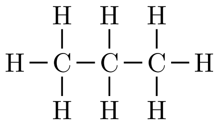
Table ?? Prefixed for alkane naming

# Carbons	prefix	# Carbons	prefix
1	Meth	6	Hex
2	Eth	7	Hepta
3	Prop	8	Octa
4	But	9	Nona
5	Pent	10	Deca

`Expanded structural formula for alkanes` At this point, we have addressed the molecular formulas of three simple alkanes: methane (CH_4), ethane (C_2H_6), and propane (C_3H_8). However, these formulas do not inform about the molecular connetions. The structure of ethane and propane is shown below:



Ethane, C_2H_6



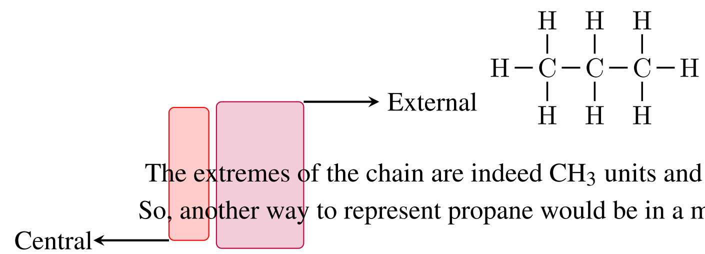
Propane, C_3H_8

These structures show that each carbon connects to four different atoms, and each hydrogen connects to only one atom. The formulas presented above are called *expanded structural formulas* as all atoms and all bonds connecting these atoms are shown, representing the molecular structure.

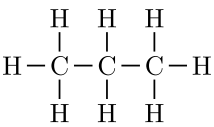
Table ?? Alkane names based on the number of carbons in the chain

Number of Carbons	Name	Condensed Structural formula	Molecular formula
1	Methane	CH_4	CH_4
2	Ethane	CH_3-CH_3	C_2H_6
3	Propane	$CH_3-CH_2-CH_3$	C_3H_8
4	Butane	$CH_3-CH_2-CH_2-CH_3$	C_4H_{10}
5	Pentane	$CH_3-CH_2-CH_2-CH_2-CH_3$	C_5H_{12}
6	Hexane	$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$	C_6H_{14}
7	Heptane	$CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3$	C_7H_{16}
8	Octane	$CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3$	C_8H_{18}
9	Nonane	$CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3$	C_9H_{20}

`Condensed structural formula` Let us analyze the formula of propane shown below. In this molecule, there are two different types of carbons: the end of the chain carbon, in the left and the right of the structure, and a central carbon. The external carbons are bound to three hydrogens (and one carbon), whereas the central carbons are bonded to two hydrogens (and two carbons).



The extremes of the chain are indeed CH_3 units and the central carbon is a CH_2 unit. So, another way to represent propane would be in a more condensed way:

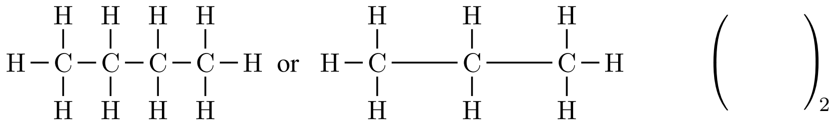


Expanded propane, C_3H_8

$CH_3-CH_2-CH_3$

Condensed propane, C_3H_8

This new representation is called *condensed structural formula* or simple condensed structure, as the units of carbon and hydrogen are condensed into CH_2 and CH_3 units. Table **??** displays molecular formulas and condensed structures for different alkanes. For larger alkenes it is often convenient to use parenthesis to simplify the structure. For example, the expanded structure of butane can be written as:



Similarly, the condensed structure of butane can be written as:

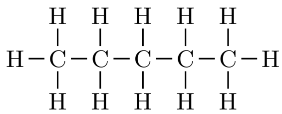
$$CH_3-CH_2-CH_2-CH_3 \text{ or } CH_3-CH_2-CH_3 \quad (\qquad)_2$$

Sample Problem 2

Write down the condensed and expanded formulas for pentane.

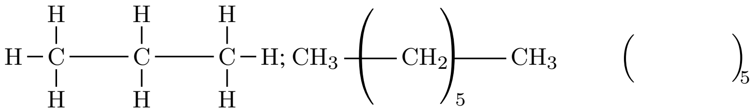
SOLUTION

Pentane has five carbons, hence its condensed formula will have two CH_3 units and three CH_2 units. On the other hand, the expanded formula for pentane should display all carbons and hydrogens:

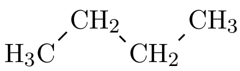
▸ Answer: $CH_3-CH_2-CH_2-CH_2-CH_3$ and 

STUDY CHECK

Write down the condensed and expanded formulas for heptane.

▸Answer: 

Skeletal structural formula Let us analyze the structure of butane again. This molecule has four carbons in the form of a C-C chain such as C-C-C-C.

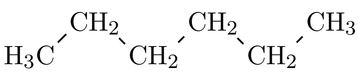


Butane, C_4H_{10}

However, in reality, C-C chains with more than two carbons are not linear, and their structure resembles more a zig-zag rather than a line, since the tetrahedral C-C-C angle is 109.5°. So instead of representing butane as a line, it should be represented as:

Butane, C_4H_{10}

This type of structural representation is called *skeletal structural formula* as you only represent the C-C skeleton of the molecule. Another example would be:

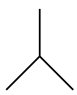


condensed formula of hexane

skeletal formula of hexane

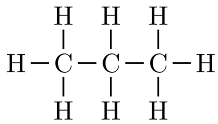
The ending of a skeletal formula represents a CH_3, and the points in between represent CH_2. Hydrocarbons in which carbon atoms form a long, continous string are called straight-chain (e.g. butane) or unbranched hydrocarbons, in contrast to branched hydrocarbons (e.g. isobutane).

butane



isobutane

`A review of the different structural formulas` At this point, you have seen four different ways to represent organic molecules, as shown below. We have that the *molecular formula* (e.g. C_3H_8 for propane) is mainly used to indicate the composition of the molecule in the form of carbon and hydrogen atoms. A second way to represent propane is using its *expanded structural formula*, that is by representing all atoms and atomic connections. A third molecular representation is the *condensed structural formula* that uses CH_3 and CH_2 units, only representing the C-C bonds. Finally, the *skeletal formula* is perhaps the most simplistic representation as only the C-C bonds are represented in the form of simple lines. It is important to understand that *all formulas are just different ways to represent the same molecule*.

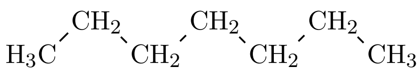
C_3H_8	$CH_3-CH_2-CH_3$		
Molecular formula	Condensed structural formula	Expanded structural formula	Skeletal structural formula

Sample Problem 3

Write down the condensed and skeletal formulas for heptane.

SOLUTION

Heptane has seven carbons, hence its condensed formula will have two CH_3 units and five CH_2 units:



The skeletal formula for would be:

▶Answer: 

STUDY CHECK

Draw the skeletal formula of decane.

▶Answer: 

1.3 Alkanes with substituents

Oftentimes alkanes have other groups of atoms called substituents attached to the hydrocarbon chain. This section covers the naming of alkanes with substituents. Here is an example of an alkane and a substitued alkane:

$$\underset{\displaystyle CH_2-CH_2-CH_3}{\overset{H}{|}} \qquad \underset{\displaystyle CH_2-CH_2-CH_3}{\overset{NO_2}{|}}$$

Propane 1-Nitropropane

In the substituted molecule, a nitro group has replaced a hydrogen atom.

`Substituents` There are many different substituents–also called groups–that can be found attached to an alkane chain. Their names are indicated in Table **??**. The easiest substituents are halogens; atoms of chorine (Cl —), bromine (Br —) or iodine (I —) can replace hydrogen atoms in an alkane. The name of these substituents–chloro, bromo, and iodo– resembles the name of the corresponding atom. Other substituents can contain carbon, like a methyl (CH_3 —) or a ethyl (CH_3CH_2 —). There are even more complex substituents such as tert-butyl in which a central carbon atom is connected to three different methyl groups. The name of substituents (methyl) comes from the name of the alkane (methane) by replacing the *-ane* suffix with *-yl*.

`Alkanes with a single substituent` Let us consider the following example. The condensed formula for propane is

$$CH_3-CH_2-CH_3 \qquad \text{Propane}$$

Now, this would be propane with a substituent:

$$\overset{\displaystyle Br}{\overset{|}{CH_2}}-CH_2-CH_3 \qquad \text{1-Bromopropane}$$

As you can see, a bromine atom substitutes one of the hydrogen atoms of the second first of the molecule (starting from the left). The name simply results from the combination of the substituent group and the alkane name

Table ?? Substituent name

Substituents	name	Substituents	name		
CH_3 —	Methyl	F —	Fluoro	$CH_2=CH$ —	Vinyl
CH_3CH_2 —	Ethyl	Cl —	Chloro	NO_2 —	Nitro
$CH_3CH_2CH_2$ —	Propyl	Br —	Bromo	NH_2 —	Amino
$CH_3CH_2CH_2CH_2$ —	Butyl	I —	Iodo	$H_3C-\overset{|}{C}H-CH_2CH_3$	sec-Butyl
$H_3C-\overset{|}{\underset{\underset{\displaystyle CH_3}{|}}{C}}-CH_3$	t-butyl	$H_3C-\overset{|}{C}H-CH_3$	Isopropyl	$CH_3CH_2CH_2$ —	Propyl

`Alkanes with two or more equal substituents` In the same way, as when you have a single bromo substituent attached to propane, you can also have two Br —. In this case, you need to use the prefix *di* to indicate there are two identical bromos. For example, the name of the following molecule would be:

$$\overset{\displaystyle Br}{\overset{|}{\underset{\underset{\displaystyle Br}{|}}{CH}}}-CH_2-CH_3 \qquad \text{1,2-Dibromopropane}$$

Similarly, you should use the prefix *tri* and *tetra* for three equal substituents.

Sample Problem 4

Name the following hydrocarbon:

$$CH_3-CH_2-CH_2-\overset{\displaystyle I}{\overset{|}{\underset{\underset{\displaystyle I}{|}}{CH}}}$$

SOLUTION

The carbon chain has four carbons and hence the ending of the name would be: butane. Also there are two iodines (iodo substituents) attached to the carbon chain. As there are two of the same iodo atoms, we need to use the prefix *di*. The full name would be:

▶Answer: 1,1-Diiodobutane.

STUDY CHECK

Name the following hydrocarbon:

$$\begin{array}{c} \qquad\qquad\qquad\qquad\qquad\qquad\quad \mathrm{F} \\ \qquad\qquad\qquad\qquad\qquad\qquad\quad | \\ \mathrm{CH_3-CH_2-CH_2-CH_2-C-F} \\ \qquad\qquad\qquad\qquad\qquad\qquad\quad | \\ \qquad\qquad\qquad\qquad\qquad\qquad\quad \mathrm{F} \end{array}$$

▶Answer: 1,1,1-trifluoropentane.

Alkanes with different substituents Now imagine you have two different halogens as substituents: Br — and I — like in next example

$$\begin{array}{l} \mathrm{Br} \\ \; | \\ \mathrm{CH-CH_2-CH_3} \\ \; | \\ \; \mathrm{I} \end{array}$$

As both substituents have different names you cannot use the prefix *di*. Still, when you indicate the names of the substituents you need to order them alphabetically. So Bromo goes first in the name and Iodo after. You also need to separate the different substituents with a hyphen ('-'). The final name of the hydrocarbon above would be 1-bromo-1-iodopropane.

Naming rules for alkanes Overall, the rules for naming alkanes are:

1. **Step one:** The number of carbon atoms in the chain will give the ending name of the molecule (e.g. four carbons would be butane).
2. **Step two:** Number the main chain starting at the end closest to the substituents so that the numbers for the substituents are small.
3. **Step three:** Name the substituents with their position and order them alphabetically (di, tri, etc. do not count in the alphabetic order).

Sample Problem 5

Name the following hydrocarbon:

$$\begin{array}{c} \qquad\quad \mathrm{F} \\ \qquad\quad | \\ \mathrm{CH_3-C-Br} \\ \qquad\quad | \\ \qquad\quad \mathrm{I} \end{array}$$

SOLUTION

The carbon chain has two carbons and hence the ending of the name would be: ethane. Also there are three different substituents: iodine (iodo substituents), bromine (bromo substituents) and fluorine (fluoro substituents). We need to order them according to the *abc* rule, hence the order would be: bromo, then fluoro and finally iodo. The full name of the alkane would be:

▶Answer: 1-bromo-1-fluoro-1-iodoethane.

STUDY CHECK

Name the following hydrocarbon:

$$\begin{array}{c} \qquad\qquad\qquad F \\ \qquad\qquad\qquad | \\ CH_3CH_2CH_2-C-Br \\ \qquad\qquad\qquad | \\ \qquad\qquad\qquad F \end{array}$$

▶Answer: Bromodifluorobutane.

Numbering the chain Substituents are atoms or groups of atoms that replace hydrogens in alkane chains. You could envision attaching substituents at different points of the chain. For example:

$$\begin{array}{ccc} \begin{array}{c} \quad Br \\ \quad | \\ CH_3-CH-CH_3 \end{array} & \text{or} & \begin{array}{l} Br \\ | \\ CH_2-CH_2-CH_3 \end{array} \end{array}$$

In the right example, Br is plugged into the left C atom, whereas in the left example, C is plugged into the middle carbon. Hence, it is important first, to learn how to number a hydrocarbon chain. Let us use propane–a molecule with three atoms–as an example. To number the chain, you start by selecting the extreme that is the closest to the substituent using this carbon as number one. Next carbon would be carbon number two and so on until you arrive at carbon number three.

$$\begin{array}{ccccc} Br & & & & \\ | & & & & \\ CH & - & CH_2 & - & CH_3 \\ 1 & & 2 & & 3 \end{array}$$

As the Br atom in the carbon number one, the name of the molecule would be 1-bromopropane or simply bromopropane. Differently, when the substituent is in a carbon different than one, you need to indicate that location. For example:

$$\begin{array}{c} \quad Br \\ \quad | \\ CH_3-CH-CH_3 \end{array} \qquad \text{2-Bromopropane}$$

Sample Problem 6

Name the following hydrocarbon:

$$\begin{array}{ccccccc} & & CH_3 & & & & \\ & & | & & & & \\ CH_3 & - & CH & - & CH & - & Br \\ & & & & | & & \\ & & & & I & & \end{array}$$

SOLUTION

First we find the ending of the name: as the molecule has three carbons in the main chain, the ending of the name would be: propane. Then we need to number the chain so that the number one carbon is the closest to the substituents:

$$\begin{array}{ccccccc} & & CH_3 & & & & \\ & & | & & 1 & & \\ CH_3 & - & CH & - & CH & - & Br \\ 3 & & 2 & & | & & \\ & & & & I & & \end{array}$$

A methyl is connected to carbon two, and two halogens, a iodo and a bromo are connected to carbon number one. The substituents are: 2-methyl, 1-bromo, 1-iodo. If we order them: 1-bromo-1-iodo-2-methyl. And the final name would be:

▶Answer: 1-bromo-1-iodo-2-methylpropane.

STUDY CHECK

Name the following hydrocarbon:

$$\begin{array}{c} CH_3 \\ | \\ CH_3-C-CH_2-I \\ | \\ F \end{array}$$

▶Answer: 1-iodo-2-fluoro-2-methylpropane.

Finding the longest chain Alkanes are complex molecules often containing more than one hydrocarbon chain. Therefore, one can envision several ways to number the chain. However, the rule is to first locate the longest chain. Let us use the following hydrocarbon. How many chains can you find, and which is the longest chain?

$$\begin{array}{l} CH_2-CH_2-CH_2-CH_3 \\ | \\ CH_3-CH_2-CH-CH_3 \end{array}$$

The answer should be three chains. Let me highlight the three different possibilities and the number of atoms in each chain:

$$\begin{array}{l} CH_2-CH_2-CH_2-CH_3 \\ | \\ CH_3-CH_2-CH-CH_3 \end{array}$$

4 Carbons

$$\begin{array}{l} CH_2-CH_2-CH_2-CH_3 \\ | \\ CH_3-CH_2-CH-CH_3 \end{array}$$

7 Carbons

$$\begin{array}{l} CH_2-CH_2-CH_2-CH_3 \\ | \\ CH_3-CH_2-CH-CH_3 \end{array}$$

6 Carbons

As the longest chain has seven carbons, the name of the molecule would be heptane. Still, you need to add the substituents to the name. Hence, after you locate the longest chain, you need to number the chain so that the substituents are located the closest to the carbon number one possible:

$$\begin{array}{l} \overset{4}{CH_2}-\overset{5}{CH_2}-\overset{6}{CH_2}-\overset{7}{CH_3} \\ | \\ \underset{1}{CH_3}-\underset{2}{CH_2}-\underset{3}{CH}-CH_3 \end{array}$$

As there is a methyl in carbon number three the final name of the molecule would be: 3-methylheptane.

Naming rules for branched alkanes Overall, the rules to name branched alkanes are:

1. **Step one:** Look for the longest carbon-carbon chain that will give the ending name of the molecule (e.g. four carbons would be butane).
2. **Step two:** Number the main chain starting at the end closest to the substituents so that the numbers for the substituents are small.
3. **Step three:** Name the substituents with their position and order them alphabetically.

Sample Problem 7

Name the following hydrocarbon:

$$\begin{array}{l} \qquad\qquad\qquad\quad CH_3 \\ \qquad\qquad\qquad\quad\ | \\ CH_3-CH_2-C-CH_3 \\ \qquad\qquad\qquad\quad\ | \\ \qquad\qquad\qquad\quad CH_2-CH_2-CH_3 \end{array}$$

SOLUTION

First we locate the longest chain. We have five possible chains, and the longest one has six carbons. Hence the name of the hydrocarbon would be hexane. Now we need to number the carbons so that we start numbering the closes to the substituents the possible.

$$\begin{array}{l} \qquad\qquad\qquad\quad CH_3 \\ \qquad\qquad\qquad\quad\ | \\ CH_3-CH_2-C-CH_3 \\ \ \ 1 \qquad\quad 2 \qquad\ |3 \\ \qquad\qquad\qquad\quad CH_2-CH_2-CH_3 \\ \qquad\qquad\qquad\qquad 4 \qquad\quad 5 \qquad\quad 6 \end{array}$$

We have two methyl connected to carbon number three. Hence the final name will be:

▶Answer: 3-dimethylhexane.

STUDY CHECK

Name the following hydrocarbon:

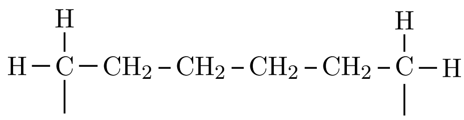
$$\begin{array}{l} \qquad\qquad\qquad\quad CH_2-CH_2-CH_2-CH_3 \\ \qquad\qquad\qquad\quad\ | \\ CH_3-CH_2-C-CH_3 \\ \qquad\qquad\qquad\quad\ | \\ \qquad\qquad\qquad\quad CH_2-CH_2-CH_3 \end{array}$$

▶Answer: 4-ethyl-4-methyloctane.

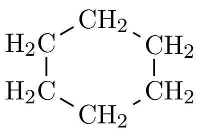
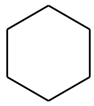
1.4 Cycloalkanes

Alkanes are perfect examples of hydrocarbons, with C-C chains and all carbon atoms saturated with hydrogen. Cycloalkanes are simply alkanes with a cyclic structure. We will cover the molecular, condensed, and skeletal formulas for these chemicals.

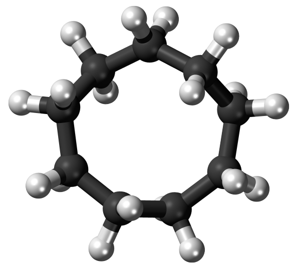
`Cyclic alkanes` Consider the expanded structure of hexane. A cycloalkane results from removing the left and right hydrogen while connecting the molecule in the form of a cycle:



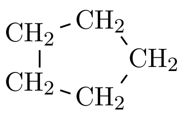
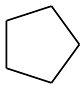
As the most stable structure for six lines is the hexagon, the resulting structure of cyclohexane would be:

 or  cyclohexane

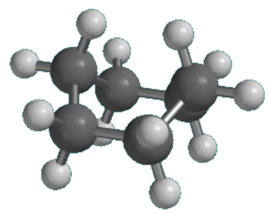
▼3D representation of Cyclononane



Naming cycloalkanes The naming of alkanes and cycloalkanes is very similar. You just need to add the cyclo prefix to the name. For example, the alkane with five carbons is called pentane, whereas the corresponding cycloalkane is called cyclopentane:

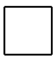
 or  Cyclopentane

▼3D representation of Cyclohexane with the shape of a chair.



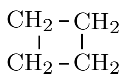
Sample Problem 8

Write down the condensed structure and name the following cycloalkane:



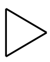
SOLUTION

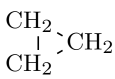
The cycloalkane has four carbons and its name is cylcobutane. Its condensed structure is

▶Answer: 

STUDY CHECK

Write down the condensed structure and name the following cycloalkane:



▶Answer: cyclopropane, 

Molecular formulas for cycloalkanes The molecular formula for a general cycloalkane with n carbon atoms is:

$$C_nH_{2n} \tag{1.2}$$

As an example, the formula for cyclobutane ($n = 4$) is C_4H_8 and the formula for cyclooctane ($n = 8$) is C_8H_{16}.

Sample Problem 9

Write down the molecular formula for cyclodecane and cyclopentane.

SOLUTION

Using Equation **??** we have that the molecular formula for cyclodecane ($n = 10$) would be: $C_{10}H_{20}$. Similarly, the molecular formula for cyclopentane ($n = 5$) would be:

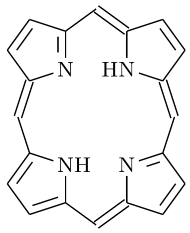
▶Answer: C_5H_{10}.

STUDY CHECK

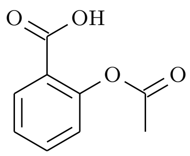
Name the alkane with formula C_7H_{14} and give the formula for cyclononane.

▶Answer: cycloheptane, C_9H_{18}.

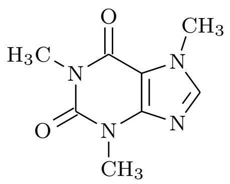
▼Porphyrin has several amine groups.



▼Aspirin contains an aromatic cycle, a carboxylic acid and a ester.



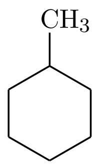
▼Caffeine contains amides and amines



1.5 Cycloalkanes with substituents

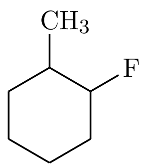
The naming rules for cycloalkanes are the same as the rules for naming linear alkanes. This means first you will find the ending of the name by counting the number of carbons in the cycle. Then you will locate each substituent and number the carbon chain so that the position numbers are small. Finally, all substituents should be ordered alphabetically.

`Cycloalkanes with one substituent` Let us take a look at the following cycloalkane:

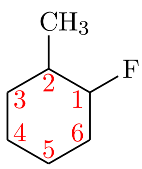


this is a cyclohexane connected to a methyl substituent. As there is only one substituent, there is no need to number the carbon chain. Hence the name would be simply methylcyclohexane.

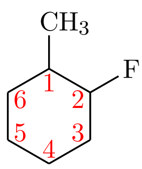
`Cycloalkanes with two substituents` Let us look at the following cycloalkane:



this is a cyclopentane connected to two different substituents: a methyl and a fluoro. In order to name this molecule, we need to number the carbons first, and there are two different ways to number the cyclohexane ring:



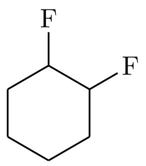
1-Fluoro-2-methylcyclohexane



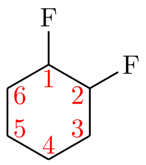
~~Fluoro-1-methylcyclohexane~~

we will choose the name that gives the lowest numbers: 1-Fluoro-2-methylcyclohexane.

`Cycloalkanes with repeated substituents` Let us look at the following cycloalkane, which has two repeated fluorine substituents:



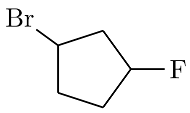
After numbering the chain:



The name would be: 1,2-difluorocyclohexane.

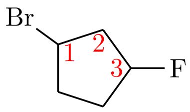
Sample Problem 10

Name the following hydrocarbon:



SOLUTION

The molecule is a cyclopentane with two substituents: fluoro and bromo. I will start numbering in bromo and continue until bromo. This way I will have small numbers and follow the abc rule:

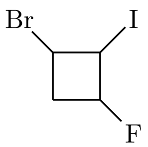


And the name of the molecule would be:

▶Answer: 1-bromo-3-fluorocyclopentane.

STUDY CHECK

Name the following hydrocarbon:

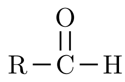


▶Answer: 1,2-dibromo-3-fluorocyclobutane.

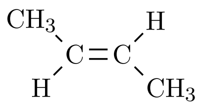
1.6 Molecular diversity

You have certainly taken painkillers for a headache or over-the-counter drugs to get over a cold. Maybe you drink coffee and perhaps you like tea. All these substances contain active organic molecules. These active molecules are hydrocarbon derivatives and differ from plain hydrocarbons, which are simply made of carbon and hydrogen. Active molecules contain functional groups such as alcohol, ethers, carboxylic acids, amines, amides, or aromatic groups. These groups of atoms have a specific function and give activity to the molecule. The goal of this section is simply to identify the different groups.

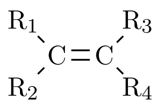
`Multiple bonds` Ketones and aldehydes both contain a C=O group called carboxyl group. Still, these are two different groups, and ketones have a C=O group bounded to two different carbon atoms


Aldehyde

whereas aldehydes have the same C=O group but this time bound to a carbon and a hydrogen. Alkenes contain at least one double bond between carbons. An example would be:

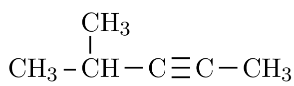

or $CH_3CH_2-HC=CH-CH_3$

Double bonds are also called unsaturations. Hence, we say alkenes are unsaturated. Both extremes of an alkene chain can be connected to different hydrocarbons. We normally represent this as:


Alkene

where R and R' represent any hydrocarbon chain. For Example R and R' can be CH_3- or CH_3CH_2-. Alkynes contain at least one triple bond between carbons. An example would be:

$CH_3-C\equiv C-C(CH_3)_3$ or

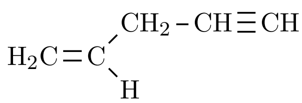


Again, we could use R and R' to represent any hydrocarbon chain:

$R-C\equiv C-R'$ Alkyne

Sample Problem 11

Identify the alkene and alkyne groups in the molecule:



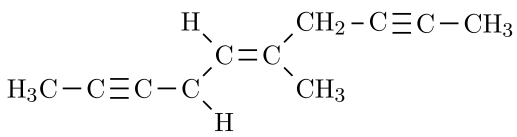
SOLUTION

A double bond is carbon atoms sharing two pairs of electrons, whereas a triple bond is a pair of atoms sharing three pairs of electrons. They are represented with a double and triple line, respectively.

▸Answer: (left) alkene; (right) alkyne

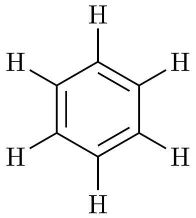
STUDY CHECK

Identify the alkene and alkyne groups in the molecule:

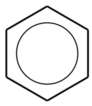


▶Answer: (center) alkene; (right, left) alkyne

`Aromatic group` Aromatic groups are based on benzene, a carcinogenic cyclohexane-like molecule with a series of alternates double bonds, which is often represented as a circle for simplicity:

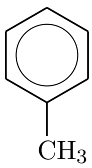


Benzene

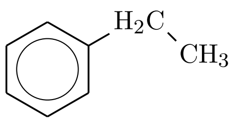


Benzene

Examples of molecules containing aromatic groups are:



or



and

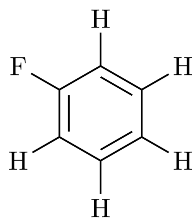
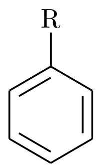


Table ?? Names of several functional groups

Functional group	Name	Functional group	Name	Functional group	Name
$(R_1)(R_2)C=C(R_3)(R_4)$	Alkene	$R-C(=O)-R'$	Ketone	$R-OH$	Alcohol
$R-C\equiv C-R'$	Alkyne	$R-C(=O)-H$	Aldehyde	$R-SH$	Thiol
$R-C(=O)-OH$	Carboxylic acid	$R-N(R')-R''$	Amine	$R-O-R'$	Ether
$R-C(=O)-O-R'$	Ester	$R-C(=O)-N(R'')-R'$	Amide		Phenyl

`Alcohol, ether and thiol group` Alcohols contain an $-OH$ group called hydroxyl group attached to a carbon.

$$R-OH \quad \text{Alcohol}$$

Whereas ethers have oxygen atoms attached to two carbon atoms:

$$R-O-R' \quad \text{Ether}$$

Examples of alcohols and ether are:

$$\mathrm{CH_3-CH_2-OH} \qquad \mathrm{CH_3-O-CH_2-CH_3}$$

alcohol ether

Alcohols can be classified as primary (one hydrocarbon fragment), secondary (two hydrocarbon fragments), and tertiary (three hydrocarbon fragments) alcohols, based on the number of hydrocarbon fragments connected to the carbon attatched to the hydroxyl group.

$$\begin{array}{ccc} \begin{array}{c} \mathrm{H} \\ | \\ \mathrm{CH_3-C-OH} \\ | \\ \mathrm{H} \end{array} & \begin{array}{c} \mathrm{CH_3} \\ | \\ \mathrm{CH_3-C-OH} \\ | \\ \mathrm{H} \end{array} & \begin{array}{c} \mathrm{CH_3} \\ | \\ \mathrm{CH_3-C-OH} \\ | \\ \mathrm{CH_3} \end{array} \\ \text{Primary} & \text{Secondary} & \text{Tertiary} \end{array}$$

Thiols contain a $-\mathrm{SH}$ group called mercapto group attached to a carbon. They are equivalent to alcohols but based on sulfur:

$$\mathrm{R-SH} \quad \text{thiol}$$

Examples of thiols are:

$$\mathrm{CH_3-CH_2-SH} \qquad \begin{array}{c} \mathrm{SH} \\ | \\ \mathrm{CH_3-CH-CH_3} \end{array}$$

Thiols are responsible for the characteristic smell of rotten eggs and burned hair.

Sample Problem 12

Classify the following molecules as alcohol or ether.

$$\mathrm{CH_3-CH_2-CH_2-OH} \qquad \mathrm{CH_3-O-CH_2-CH_3}$$

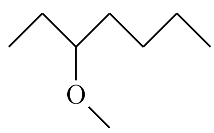
SOLUTION

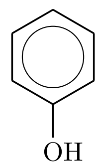
The OH groups is an alcohol, and we find this group in the left molecule. Differently, the right molecule is an ether as it contains the $\mathrm{R-O-R'}$ group.

▶Answer: (left) alcohol; (right) ether.

STUDY CHECK

Classify the following molecules as alcohol or ether.

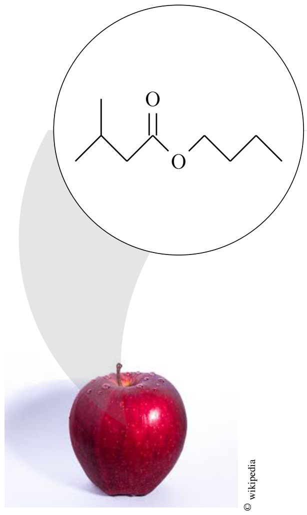




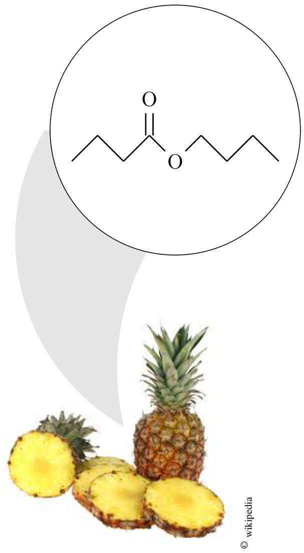
▶Answer: (left) ether; (right) alcohol.

▼Acetone, the smallest ketone, is also known as nail polish remover.

▼Ethyl isovalerate is an ester that flavors apples.

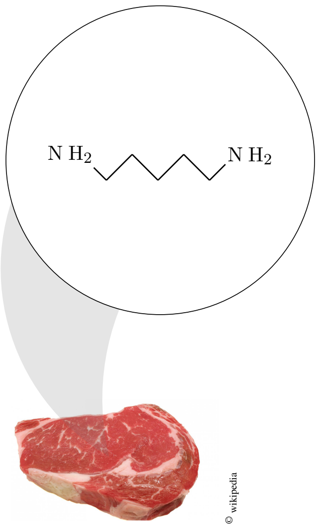


▼Butyl butyrate is an ester that flavors pineapple.

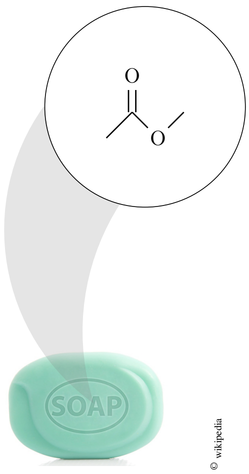


▼Diethyl ether was formerly used as a general anesthetic, until non-flammable drugs were developed.

▼Amines are responsible of the bad smell of decaying meat.



▼Esters are found in soaps



▼Vinegar contains acetic acid, the smallest carboxylic acid.

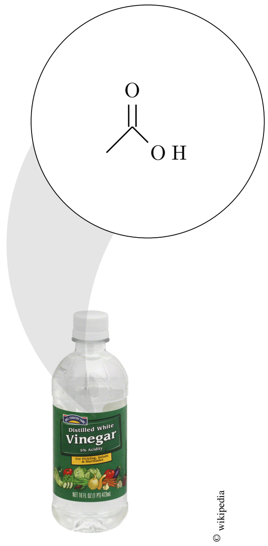


Figure ?? Some examples of functional groups with applications to real life.

`Aldehydes and ketones` Ketones and aldehydes both contain a C=O group. Still, these are two different groups, and ketones have a C=O group bounded to two different carbon atoms

$$\mathrm{R-\overset{\overset{\displaystyle O}{\|}}{C}-H} \qquad \text{Aldehyde}$$

whereas aldehydes have the same C=O group but this time bound to a carbon and a hydrogen.

$$\mathrm{R-\overset{\overset{\displaystyle O}{\|}}{C}-R'} \qquad \text{Ketone}$$

Examples of aldehydes and ketones are:

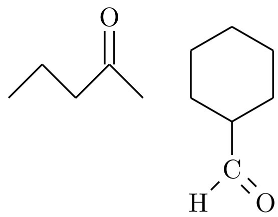
$$\mathrm{CH_3CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-H} \qquad \text{or} \qquad \mathrm{CH_3-\overset{\displaystyle O}{\overset{\|}{C}}-CH_3}$$

Aldehyde   Ether

Ketones are good solvents. For example, acetone is commonly found in nail polish removes for example. Aldehydes have strong smells. For example, vanillin is an aldehyde responsible for the vanilla smell. Cinnamaldehyde is responsible for the cinnamon odor.

Sample Problem 13

Classify the following molecules as an aldehyde or ketone



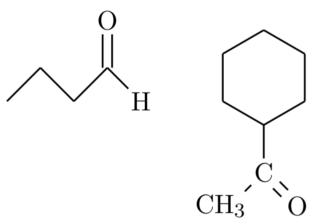
SOLUTION

The left molecule is a ketone as the carbonyl group (C=O) is connected to a CH_3 and a CH_2. Differently, the right molecule is an aldehyde as the carbonyl group is connected to a cycloalkane but also to a hydrogen.

▶Answer: (left) ketone; (right) aldehyde.

STUDY CHECK

Classify the following molecules as an aldehyde or ketone



Carboxylic acids and esters Carboxylic acids contain a carbonyl group (C=O) connected to both a hydrocarbon chain and an alcohol group:

$$\mathrm{R-\overset{\displaystyle O}{\overset{\|}{C}}-OH} \qquad \text{Carboxylic acid}$$

Esters have the same C=O group but this time bounded to a carbon (R) and an ether group (–O–R').

$$\mathrm{R-\overset{\displaystyle O}{\overset{\|}{C}}-O-R'} \qquad \text{Ester}$$

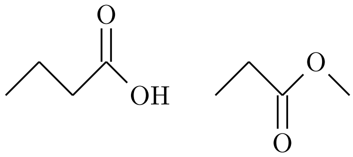
Examples of carboxylic acids and esters are:

$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-OH \qquad \text{or} \qquad CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-O-CH_3$$

Carboxylic acid Esters

Sample Problem 14

Classify the following molecules as an carboxylic acid or ester:

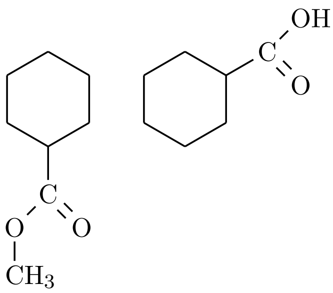


SOLUTION

The molecule in the left is a carboxylic acid as the carbonyl group (C=O) is connected to an alcohol $-OH$. Differently, the molecule in the right is a ester as the carbonyl group is connected to a $-O-CH_3$ group.

STUDY CHECK

Classify the following molecules as an carboxylic acid or ester:



▶Answer: (left) ester; (right) acid.

Amines and amides Amines and amides are groups containing nitrogen. Amines are derivative of ammonia (NH_3) with one or more of the hydrogen atoms being replaced by a hydrocarbon

$$R-\overset{\overset{\displaystyle R'}{|}}{N}-R'' \qquad \text{Amine}$$

Examples of amines are:

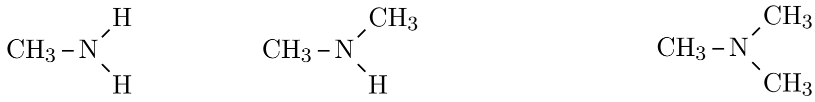
$$CH_3-\overset{\overset{\displaystyle CH_3}{|}}{N}-H \qquad CH_3-NH_2 \qquad CH_3-\overset{\overset{\displaystyle CH_3}{|}}{N}-CH_2CH_3$$

Amines have very strong and unpleasant odors–fishy like–often associated with the smell of decaying flesh:

$NH_2 — CH_2 — NH_2$ (NH_2)$_3$ — CH_2 — NH_2 ( )$_5$

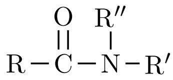
putrescine cadaverine

Simmilar to alcohols, amines can be classified as primary (one hydrocarbon fragment), secondary (two hydrocarbon fragments), and tertiary (three hydrocarbon fragments) amines, based on the number of hydrocarbon fragments connected to the nitrogen atom:



Primary Secondary Tertiary

Amides, on the other hand, contain a carbonyl group (C=O) connected to an amine group (—N—)



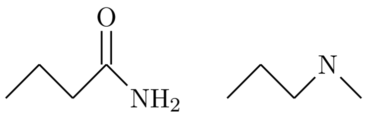
Amide

Examples of amides are:

Amides are primarily used in the pharmaceutical industry as drugs, including pain killers like morphine and Demerol, anesthetics like Novocain, and are also found in many important structural materials like nylon.

Sample Problem 15

Classify the following molecules as an amide or amine:



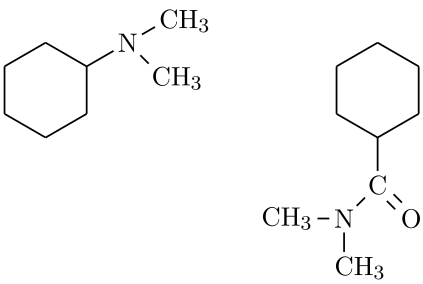
SOLUTION

The molecule in the left is a amide as the carbonyl group (C=O) is connected to a nitrogen atom. Differently, the molecule in the right is an amine as the nitrogen group is not connected to any carbonyl group.

▶Answer: (left) amide; (right) amine.

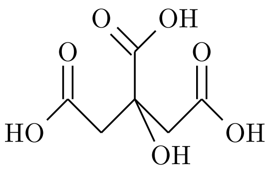
STUDY CHECK

Classify the following molecules as an amide or amine:

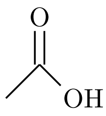


▶Answer: (left) amine; (right) amide.

`Identifying organic acids and bases` Acid organic molecules, in general, contain one or more carboxylic acid groups. An example would be vinegar and citric acid, the acid found in citrus.

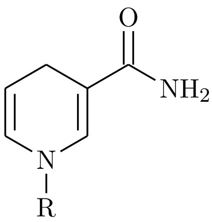


Citric acid

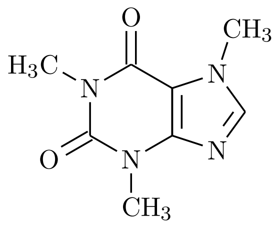


Acetic Acid

Bases contain one or more amine groups. Examples of bases are NADH, a coenzyme found in all living cells, or caffeine, a base found in coffee.



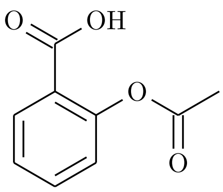
NADH



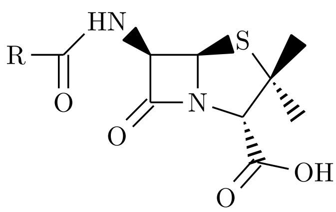
Caffeine

Sample Problem 16

Classify the following molecules as an acid or base:



Aspirin



Penicillin

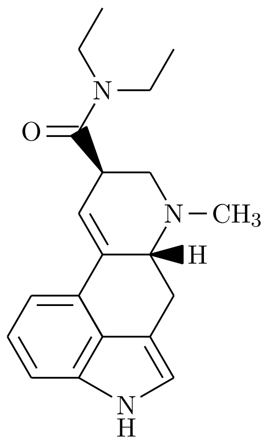
SOLUTION

Aspirin contains an acid group and hence it will be acidic. Penicillin contains both acidic and amine groups and hence it can either act as an acid or a base.

▶Answer: (left) acid; (right) both.

STUDY CHECK

Classify the following molecules as an carboxylic acid or base:



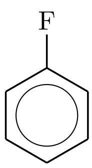
LDS

Answer: base

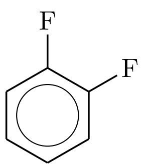
1.7 Aromatic hydrocarbons

Aromatic compounds are unsaturated hydrocarbons with increased stability and unique chemical properties. Benzene represents the simplest of all aromatic compounds. In this molecule, all carbon atoms are equivalent. A combination of the localized electron model and hybrid orbitals predicts this equivalency. The localized electron model supports this equivalence through two equivalent resonant structures. The orbitals model describes each carbon using three sp^2 orbitals that form three σ bonds (one C-H and two C-C bonds), while a remaining $2p$ atomic orbital creates a π delocalized orbital. The circle inside benzene's ring represents a combination of all delocalized π orbitals. This electronic delocalization gives benzene unique chemical properties. This section will address the reactivity and nomenclature of aromatic hydrocarbons.

`Nomenclature` The standard nomenclature for benzene derivatives resembles the ones for substituted alkanes. For benzenes with more than one substituent, we follow the *abc* ordering rule and we use numbers to indicate the location of each substituent. See examples below:

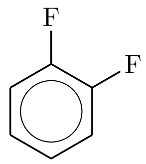


Fluorobenzene

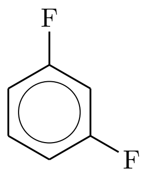


1,2-difluorobenzene

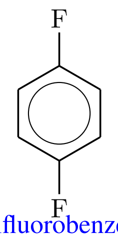
There is an alternative, but extensively used, nomenclature that uses the prefixes *ortho*, *meta*, and *para* to describe the location of double-substituted benzene. Ortho *o-* is used when the substituents are adjacents (1,2 location), whereas meta *m-* is used when there is a carbon in between the two substituents (1,3 location). Para *p-* is used when there are two carbons in between the two substituents (1,4 location). Below you can see this alternative nomenclature in use:



o-difluorobenzene
(1,2-difluorobenzene)



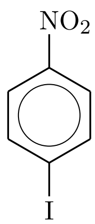
m-difluorobenzene
(1,3-difluorobenzene)



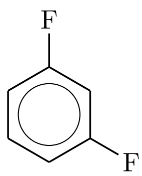
p-difluorobenzene
(1,4-difluorobenzene)

Sample Problem 17

Name or formulate the following aromatic compounds:



(a)



(b)

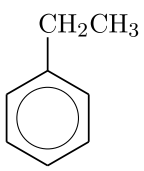
SOLUTION

(a) This chemical is *p*-iodonitrobenzene also called 1,4-iodonitrobenzene. (b) This chemical is *m*-difluorobenzene also called 1,3-difluorobenzene.

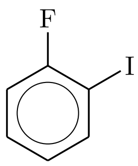
▶Answer: (a) *p*-iodonitrobenzene; (b) *m*-difluorobenzene (1,3-difluorobenzene).

STUDY CHECK

Name or formulate the following aromatic compounds:



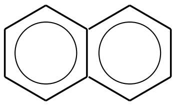
(a)



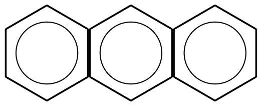
(b)

▶Answer: (a) ethylbenzene; (b) *o*-fluoroiodobenzene (1,2-fluoroiodobenzene).

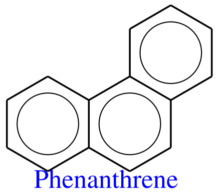
`Complex aromatic systems` Benzene rings can fuse forming complex aromatic rings as shown below. Naphthalene was used for the manufacturing of mothballs, whereas anthracene is used for the production of dyes. Phenanthrene is a precursor of synthetic drugs. 3,4-benzpyrene is an active carcinogen found in smoke and smog.



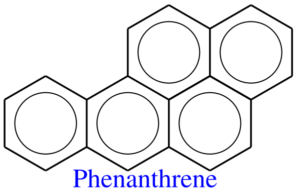
Naphthalene



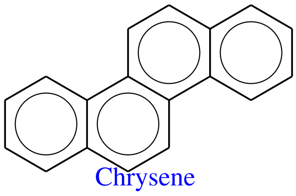
Anthacene



Phenanthrene

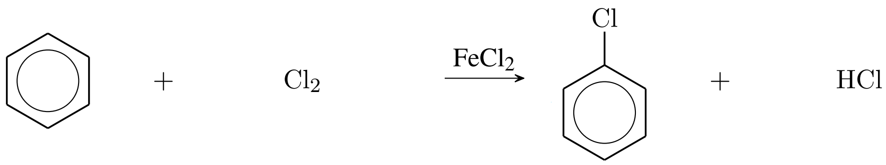


Phenanthrene



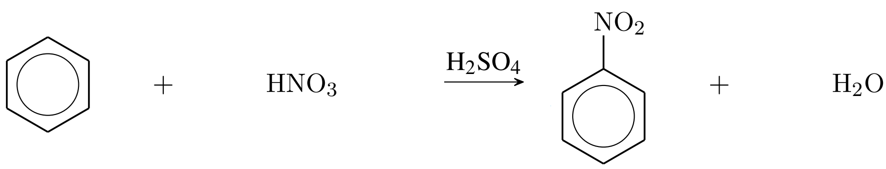
Chrysene

`Reactivity` Aromatic hydrocarbons undergo *substitution reactions* in which hydrogen atoms are replaced by other atoms. For example, chlorine replaces a hydrogen atom in benzene, hence producing chlorobenzene, when iron(II) chloride is used as a catalyst:



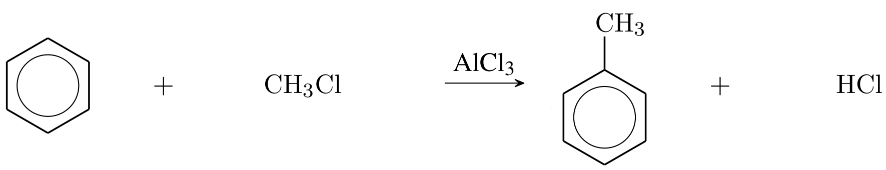
chlorobenzene

Also, benzene reacts with nitric acid in the presence of sulfuric acid producing nitrobenzene.



nitrobenzene

Finally, chloromethane reacts with benzene to produce toluene (methylbenzene).



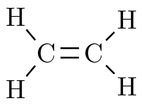
toluene

The reactivity of aromatic compounds is very different than that of unsaturated hydrocarbons which undergo *addition reactions* in which external atoms add to double bonds.

1.8 Alkenes and alkynes

Alkenes and alkynes are hydrocarbons with multiple C-C bonds, particularly double and triple bonds. They result from removing hydrogens from the hydrocarbon's structure. This section addresses the naming and structure of these important chemicals.

`Bonding` Alkenes contain at least one double bond. Ethylene is the smallest of all alkenes with just two carbon atoms. Let us analyze its structure and bonding:



$(5\sigma, 1\pi)$

Every carbon center in the double bond has three sp^2 orbitals and two empty $2p$ orbitals. The three sp^2 orbitals combine, giving three σ bonds. Two of these are used to bond carbon atoms with two hydrogens, whereas the remaining bond is used in the C-C double bond. One of the empty $2p$ orbitals forms a π orbital in the double bond. Therefore, for every double bond, we have a σ and a π orbitals.

Alkyles contain at least one triple bond. Ethylene, also called acetylene, is the smallest of all alkynes with just two carbon atoms. Let us analyze its structure and bonding:

$$\mathrm{H-C{\equiv}C-H} \qquad (3\sigma, 2\pi)$$

The triple bond in acetylene can be understood as a σ bond with two π bonds between the carbon atoms. σ and π bonds have very different movility. π bonds are rigid, as the p orbitals involved in the bond need to be lined up parallel to the three σ bonds (see Figure **??**). Differently, σ bonds are mobile and as such, free rotation is possible. Therefore, double and triple bonds are rigid, whereas single bonds are mobile.

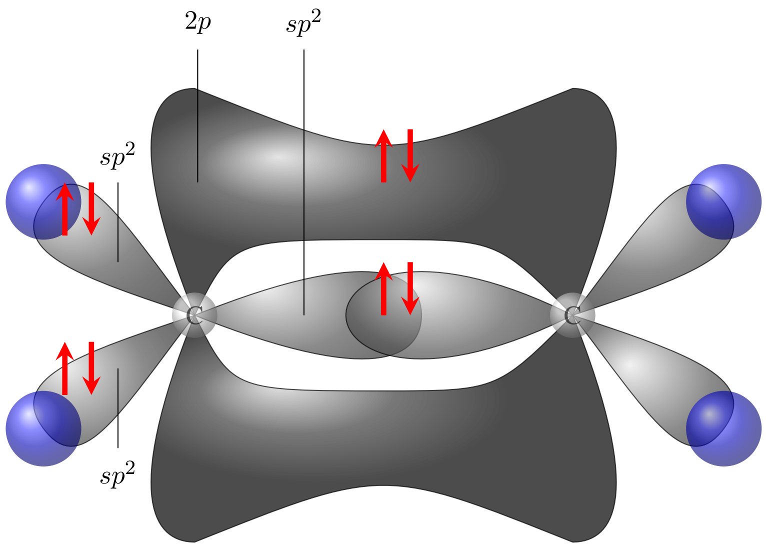
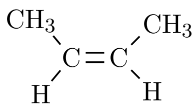
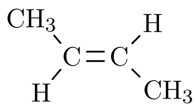


Figure ?? Bonding of ethylene in which three sp^2 hybrid orbitals and one $2p$ orbital populated with paired electrons. The orbitals of C (H) are represented with grey (blue) shading.

`Stereoisomerism` As the carbon atoms bonded through a double bond have restricted rotation, their mobility is limited, which enables cis-trans stereoisomerism. Remember isomers are molecules with the same molecular formula but different properties. In particular, stereoisomers are molecules with the same molecular formula but different spatial arrangements of the bonds. Let us address the two possible isomers of butene: cis-butene and trans-butene. Cis isomers have the same substituents located on the same side of the double bond, whereas trans isomers have the same substituents placed on opposite sides of the double bond.



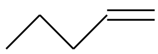
cis-butene



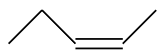
trans-butene

Alkynes do not present cis-trans stereoisomerism as every carbon atom in the triple bond is only bonded to a single substituent.

`Nomenclature` For the case of alkenes, its nomenclature is similar to that of alkanes, but switching the *-ane* ending into *-ene*. For example, the smallest alkene CH_2CH_2 is called ethene (its common name is ethylene). When the molecule has more than three carbons, one needs to specify the location of the double bond with a number as the lowest-numbered carbon arom involved in the double bond. For example, 1-pentene and 2-pentene are represented below.

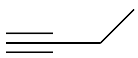


1-pentene

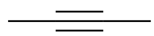


2-pentene

The nomenclature of alkynes involves the use of *-yne* and for example $HC{\equiv}CHCH_2CH_3$ is called 1-butyne and $HC{\equiv}CHCH(CH_3)_2$ is called 3-methyl-1-butyne.



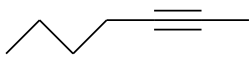
1-butyne



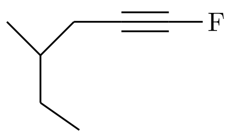
2-butyne

Sample Problem 18

Name or formulate the following organic compounds:



(a)



(b)

SOLUTION

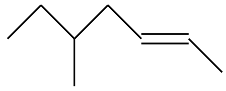
(a) This alkyne has seven carbons, and its triple bond is located on carbon number two. Hence its name would be: 2-heptyne; (b) This alkyne has six carbons, with a fluorine and the triple bond on carbon number one, and a methyl on carbon number four. Hence, its name is 1-fluoro-4-methyl-1-hexyne

▶Answer: (a) 2-heptyne; (b) 1-fluoro-4-methyl-1-hexyne.

STUDY CHECK

Name or formulate the following organic compounds:

(a)



(b)

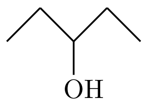
▶Answer: (a) *cis*-2-heptene; (b) 5-methyl-*trans*-2-heptene.

1.9 Naming of hydrocarbon derivatives

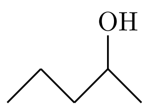
Hydrocarbon derivatives are organic molecules with a hydrocarbon base and extra functional groups. Examples are alcohols, ketones, aldehydes, or carboxylic acids. All those contain a hydrocarbon skeleton with some functional group. This section covers the naming rules for these chemicals.

`Alcohols` Alcohols are systematically named from the parent hydrocarbon by replacing the *-e* (methane) ending with an *-ol* ending (methanol). A number should indicate the location of the alcohol group for alcohols with more than one carbon. For example, CH_3OH is called methanol and $CH_3CH_2CH_2OH$ is called 1-propanol. Examples of five-carbon alcohols are:

pentanol

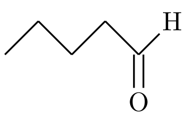


3-pentanol

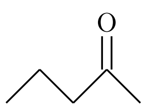


2-pentanol

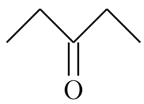
`Ketones and aldehydes` Aldeydes are systematically named from the parent hydrocarbon by replacing the *-e* (methane) ending with the *-al* ending (methanal). For example, CH_3COH is called ethanal. Ketones are systematically named from the parent hydrocarbon by replacing the *-e* (propane) ending with the *-one* ending (propanone). A number should indicate the location of the carboxyl group. For example, $CH_3COCH_2CH_3$ is called 2-butanone. Examples of aldehydes and ketones are:



pentanal



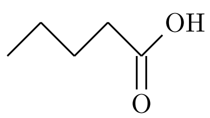
2-pentanone



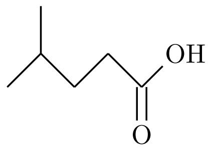
3-pentanone

`Carboxylic acids and esters` Carboxylic acids are systematically named from the parent hydrocarbon by replacing the *-e* (methane) ending with an *-oic* ending and ending the name with the word acid (methanoic or formic acid). For example, CH_3COOH is called ethanoic (acetic) acid.

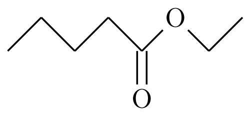
Esters, which result from the combination of an alcohol and a carboxylic acid, are systematically named from the parent hydrocarbon by replacing the *-ol* (methane) ending of the alcohol part with an *-yl* ending and the -oic ending the acid with an -oate ending, with a space between both words. For example, the ester resulting from the combination of methanol (CH_3OH) and methanoic acid (CH_3COOH) is called methylmethanoate (CH_3COOCH_3). Esters have also common names. As (CH_3COOH) is also called acetic acid, the corresponding ester from the combination with methanol can be called methyl acetate. Examples of carboxylic acids and esters are:



pentanoic acid

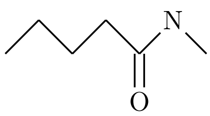


4-methylpentanoic acid

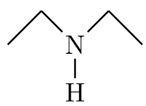


ethyl pentanoate

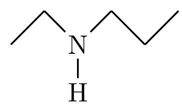
`Amines and amides` Amines are named used the name *amino* for the funcional group and for example CH_3NH_2 is called aminomethane. Common name of amines end with the word amine. For example, CH_3NH_2 is commonly called methylamine and $(CH_3)_2NH$ is called dimethylamine. Amides, which result from the combination of an amine and a carboxylic acid, are systematically named from the parent hydrocarbon by replacing the -amine (methylamine) ending of the amine part with an -yl ending and the -oic ending the acid with an -amide ending, without space between both words. For example, the amide resulting from the combination of methylamine (CH_3NH_2) and methanoic acid (CH_3COOH) is called methylmethanamide ($CH_3CONH_2CH_3$). Examples of amines and amides are:



methylpentanamide



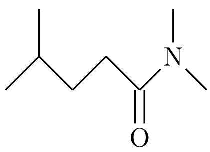
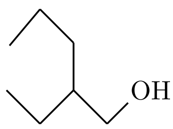
diethylamine



ethylpropylamine

Sample Problem 19

Name the following hydrocarbon derivatives:

(a)  (b) 

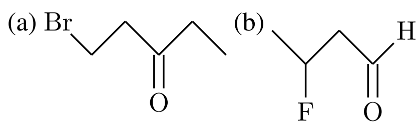
SOLUTION

(a) This amide results from combining dimethylamine and 4-methylpentanoic acid. Hence, the amide is called: dimethyl-4-methylpentanamide; (b) This is an alcohol with five carbons on its longest hydrocarbon chain. It has an ethyl substituent in carbon number two. Hence its name is 4-ethylpentanol.

▶Answer: (a) dimethyl-4-methylpentanamide; (b) 4-ethylpentanol

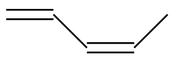
STUDY CHECK

Name the following hydrocarbon derivatives:

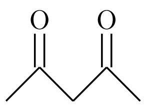


▶Answer: (a) 1-bromo-3-pentanone; (b) 3-fluorobutanal

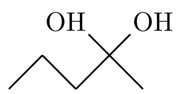
`Double functional groups` Yyou must use the *di* prefix before the *ol* ending if a chemical has two alcohol groups, while preserving the *-ane* ending. For example, a pentane hydrocarbon with two alcohol groups on carbon 2 would be named 2,2-pentanediol. The same rule applies for other functional groups and even double or triple bonds:



cis-2,4-pentanediene



2,4-pentanedione



2,2-pentanediol

1.10 Reactivity of organic compounds

This section addressed some of the reactions undergone by organic compounds. For example, carboxylic acids can also react with alcohols producing esters, which are indeed organic salts, commonly known as soaps or gels. In this chapter, reducing or oxidation conditions will be represented as $\xrightarrow{\text{[reduc]}}$ and $\xrightarrow{\text{[ox]}}$, respectively, as many reagents can carry out oxidations or reductions.

`Hydrocarbons` Alkanes are almost inert materials under normal conditions. They do not react with acids, bases, or oxidizing agents. This is because of the C-C and C-H strength. As such, alkanes are used in the manufacturing industry to produce plastics and lubricants. At high temperatures (Δ), they can undergo *combustion reactions* with oxygen.

$$CH_4 + 2\,O_2 \xrightarrow{\Delta} CO_2 + 2\,H_2O$$

Alkanes can also react with halogens undergoing *substitution reactions*, in which one or more hydrogen atoms of the alkane are replaced with a halogen. In this reaction, ultraviolet light hν is needed to break down the halogen (e.g. Cl_2) producing very reactive halogen radical (e.g. $Cl^\bullet$): an atom with an unpaired electron.

$$CH_4 + Cl_2 \xrightarrow{h\nu} CH_3Cl + HCl$$

Halogenated alkanes have many uses. For example, CF_xCl_{4-x} are chlorofluorocarbons or freons. These chemicals were historically used in air conditioning systems and can present a threat to the ozone layer. Alkanes can also undergo *dehydrogenation reaction* producing alkenes as hydrogen atoms are removed by a reducing agent at high temperature:

$$CH_3{-}CH_3 \xrightarrow[500\,^\circ C]{Cr_2O_3} CH_2{=}CH_2 + H_2$$

Alkenes and alkynes undergo *addition reactions* as hydrogen, or halogens can add to the multiple bonds, replacing a π bons with a σ bond. Alkenes can hydrogenate at normal temperature with the use of a Ni or Pt catalyst.

$$CH_2{=}CH_2 + H_2 \xrightarrow{Pt} CH_3{-}CH_3$$

This reaction is involved in the manufacturing of solid shortenings from liquid, unsaturated fats. Similarly, halogens can add to a triple bond:

$$CH{\equiv}CH + Cl_2 \longrightarrow CHCl{=}CHCl$$

Alcohols There are a few relevant alcohols, both simple and complex alcohols. The simplest alcohol is called methanol, CH_3OH. It was originally called wood alcohol as it can be produced by heating wood in the absence of air. It is produced from the hydrogenation of carbon monoxide catalyzed by supported chromium(III) oxide:

$$CO + 2\,H_2 \xrightarrow[Cr_2O_3/ZnO]{400\,°C} CH_3OH$$

Another important alcohol is ethanol CH_3CH_2OH, which is produced in the fermentation of glucose ($C_6H_{12}O_6$) catalyzed by yeast

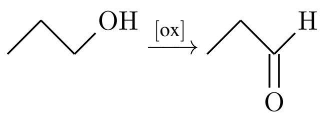
$$C_6H_{12}O_6 \xrightarrow{yeast} CH_3CH_2OH + 2\,CO_2$$

This reaction only proceeds until the alcohol concentration is 13%. After that point, yeast can not survive the high alcohol level and distilling is necessary to produce high-alcohol beverages. Ethanol (rubbing alcohol) can also be produced by means of the hydration of ethane catalyzed by phosphoric acid:

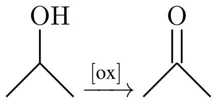
$$CH_2{=}CH_2 + H_2O \xrightarrow{H_3PO_4} CH_3CH_2OH$$

Finally, 1,2-ethanediol known as ethylene glycol is a toxic chemical used as car antifreeze.

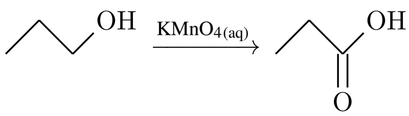
Aldehydes and ketones Ketones and aldehydes are products of the partial oxidation of complex alcohols with mild oxidants (e.g. Pyridinium chlorochromate (PCC), Dess-Martin periodinane (DMP), Swern oxidation reagent). In particular, primary alchols produce aldehydes



and secondary alcohols produce ketones:



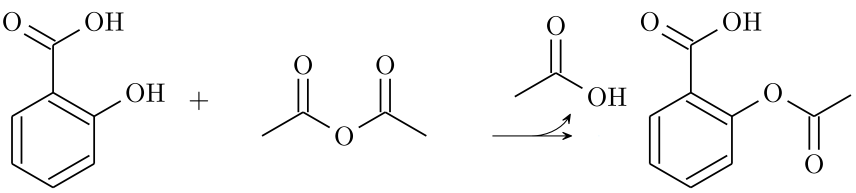
Carboxylic acids and esters Carboxylic acids are produced from the total oxidation of primary alcohols. One can use a strong oxidant such as potassium permanganate to carry out the oxidation:



Carboxylic acids also react with alcohols to produce esters, for example:

$$\underset{\text{carboxylic acid}}{CH_3-\overset{\overset{\displaystyle O}{||}}{C}-OH} + \underset{\text{alcohol}}{OH-CH_2CH_3} \xrightarrow{H_2O} \underset{\text{ester}}{CH_3-\overset{\overset{\displaystyle O}{||}}{C}-O-CH_2CH_3}$$

The synthesis of acetylsalicylic acid is a very important reaction between an acid and an alcohol as acetylsalicylic acid is also known as aspirin. Aspirin is currently the most widely used drug worldwide, being one of the most important pharmacological achievements of the twentieth century. Unfortunately, the acidic nature of acetylsalicylic acid makes it damaging for the stomach, where it is absorbed.



salicylic acid   acetic anhydride   acetylsalicylic acid

Sample Problem 20

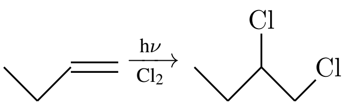
Predict the product of the following reactions:

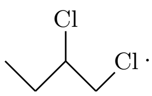
SOLUTION

(a) This is the combution of butane reaction and the products are:

 $4\,CO_2 + 5\,H_2O$;

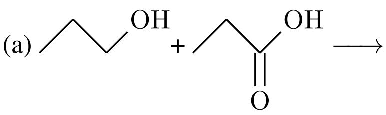
(b) This is the chlorination of butene that produces 1,2-dichlorobutane:

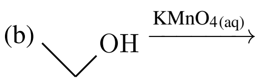


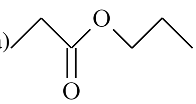
▸Answer: (a) $4\,CO_2 + 5\,H_2O$; (b)  .

STUDY CHECK

Predict the product of the following reactions:





▸Answer: (a)  ; (b)