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. Here a few examples of organic compounds: CH_4, C_2H_6, or C_6H_6. Differently, inorganic compounds contain other elements different 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. Alkanes are simple organic compounds made of Carbon and Hydrogen with all carbons connected using simple bonds–these are single lines to represent 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.

$$\begin{array}{ccccc} & & \mathrm{H} & & \\ & & | & & \\ \mathrm{H} & - & \mathrm{C} & - & \mathrm{H} \\ & & | & & \\ & & \mathrm{H} & & \end{array} \qquad \text{Methane, } CH_4$$

Its structure is very 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

This first section will introduce organic chemistry, covering the most simple organic compounds: the 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 extend to other–more complex–organic chemicals.

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

© www.wallpaperflare.com

`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 that 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.

© www.wallpaperflare.com

Sample Problem 1

Write down the molecular formula for decane and pentane.

SOLUTION

Using Equation 1.1 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.

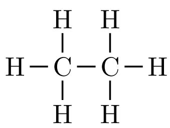
▼The octane rating of gas is a standard measure of the performance of engine fuels, originally determined by mixing a gasoline made entirely of heptane and 2,2,4-trimethylpentane (a highly branched octane).

© wikipedia

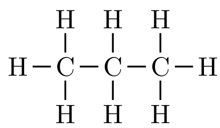
Table 1.1 Prefixed for alkane naming

# 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 have addressed the molecular formulas of three simple alkanes: methane (CH_4), ethane (C_2H_6) and propane (C_3H_8). However, these type of formulas does not inform about the structure of the molecule, that is how the atoms are connected. The structure of ethane and propane is shown below:



Ethane, C_2H_6



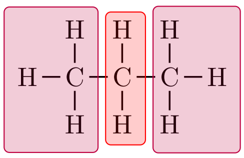
Propane, C_3H_8

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

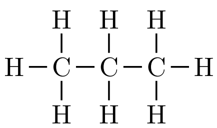
Table 1.2 Alkane names based on the number of carbons in the chain

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 extremes are bounded to three hydrogens (and one carbon), whereas the central atoms 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:

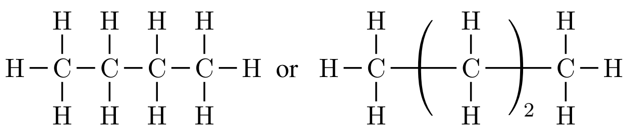


Expanded propane, C_3H_8

$$CH_3-CH_2-CH_3$$

Condensed propane, C_3H_8

This 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 1.2 displays some molecular formula as well as condensed structures for different alkanes. For larger alkenes 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:

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

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 $\begin{array}{c} \text{H}\quad\text{H}\quad\text{H}\quad\text{H}\quad\text{H} \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \text{H}\quad\text{H}\quad\text{H}\quad\text{H}\quad\text{H} \end{array}$

STUDY CHECK

Write down the condensed and expanded formulas for heptane.

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.

$H_3C-CH_2-CH_2-CH_3$ 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. 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:

$H_3C-CH_2-CH_2-CH_2-CH_2-CH_3$

condensed formula of hexane

skeletal formula of hexane

The ending of a skeletal formula represents a CH_3 and the points in between represents CH_2.

A review of the different structural formulas At this point, you have seen four different ways to represent organic molecules. Using propane as example, here all the formulas: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 in the molecule and all 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*.

Sample Problem 3

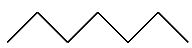
Write down the condensed and skeletal formulas for heptane.

SOLUTION

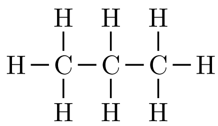
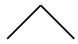
Heptane has seven carbons, hence its condensed formula will have two CH_3 units and five CH_2 units:

$H_3C-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3$

The skeletal formula for would be:

▶Answer: 

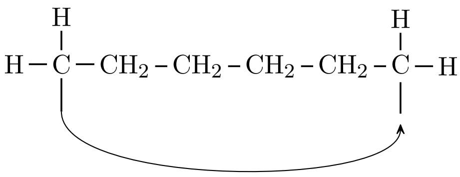
> **STUDY CHECK**
> Draw the skeletal formula of decane.

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

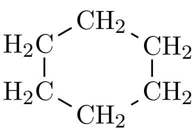
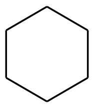
1.3 Cycloalkanes

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.

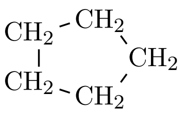
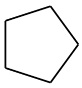
`Cyclic alkanes` Consider the expanded structure of hexane. A cycloalkane results from removing the left and right hydrogen while connecting the molecule in the form of a cycle:



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

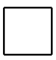
 or  cyclohexane

`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

Sample Problem 4

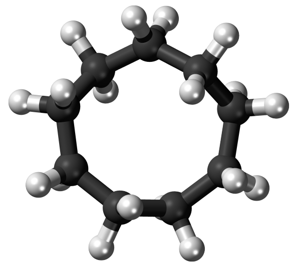
Write down the condensed structure and name the following cycloalkane:



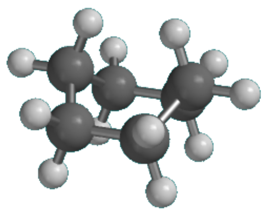
SOLUTION

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

▼3D representation of Cyclononane



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



structure is

$$\begin{array}{c}CH_2-CH_2\\ | \qquad | \\ CH_2-CH_2\end{array}$$

▶Answer: see the ring structure above.

STUDY CHECK

Write down the condensed structure and name the following cycloalkane:

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 cyclopropane ($n = 4$) is C_4H_8 and the formula for cycloctane ($n = 8$) is C_8H_{16}.

Sample Problem 5

Write down the molecular formula for cyclodecane and cyclopentane.

SOLUTION

Using Equation 1.2 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.

1.4 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 an alkane with a substituent:

$$\begin{array}{l}H\\ |\\ CH_2-CH_2-CH_3\end{array} \qquad \begin{array}{l}NO_2\\ |\\ CH_2-CH_2-CH_3\end{array}$$

Propane 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 1.2. 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:

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

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 of the combination of the substituent group and the alkane name.

Table 1.3 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	$H_3C-\overset{|}{CH}-CH_2CH_3$	sec-Butyl
$H_3C-\underset{\underset{\displaystyle CH_3}{|}}{\overset{|}{C}}-CH_3$	t-butyl	$H_3C-\overset{|}{CH}-CH_3$	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:

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

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

Sample Problem 6

Name the following hydrocarbon:

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

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: Dioiodobutane.

STUDY CHECK

Name the following hydrocarbon:

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

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

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

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 Bromo-Iodopropane.

`Naming rules for alkanes` Overall, the rules to name 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 7

Name the following hydrocarbon:

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

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*, hence the order would be: bromo, then fluoro and finally iodo. The full name of the alkane would be:

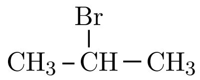
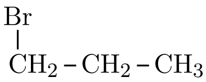
▶Answer: Bromo-Fluoro-Iodoethane.

STUDY CHECK

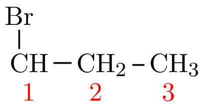
Name the following hydrocarbon:

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

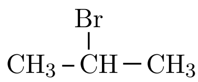
`Numbering the chain` Substituents are atoms or groups of atoms replace hydrogens in alkane chains. You could envision attaching substituents at different points of the chain. For example:

 or 

In the right example, Br is plugged to 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. In order 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.

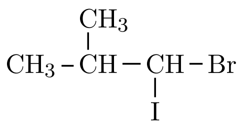


As the Br atom in the carbon number one, the name of the molecule would be: 1-bromopropane or simply bromopropane. Differently, when the substituent is in a carbon different than one, you need to indicate that location. For example:

 2-Bromopropane

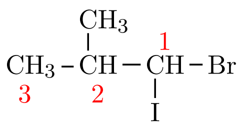
Sample Problem 8

Name the following hydrocarbon:



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:

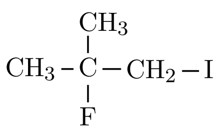


A methyl is connected to carbon two, and two halogens, a iodo and a bromo are connected to carbon number one. The substituents are: 2-methyl, 1-bromo, 1-iodo. If we order them: 1-bromo-1-iodo-2-methyl. And the final name would be:

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

STUDY CHECK

Name the following hydrocarbon:



`Finding the longest chain` Alkanes are complex molecules and often time they contain 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?

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

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

$$\begin{array}{llll} & & CH_2-CH_2-CH_2-CH_3 \\ & & | \\ CH_3-CH_2- & & CH-CH_3 \end{array} \qquad \text{4 Carbons}$$

$$\begin{array}{llll} & & CH_2-CH_2-CH_2-CH_3 \\ & & | \\ CH_3-CH_2- & & CH-CH_3 \end{array} \qquad \text{7 Carbons}$$

$$\begin{array}{llll} & & CH_2-CH_2-CH_2-CH_3 \\ & & | \\ CH_3-CH_2- & & CH-CH_3 \end{array} \qquad \text{6 Carbons}$$

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 the possible:

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

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 9

Name the following hydrocarbon:

$$\begin{array}{ll} & CH_3 \\ & | \\ CH_3-CH_2- & C-CH_3 \\ & | \\ & CH_2-CH_2-CH_3 \end{array}$$

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.

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

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

▶Answer: 3-dimethylhexane.

STUDY CHECK

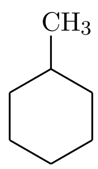
Name the following hydrocarbon:

$$\begin{array}{ccccccc} & & & & CH_2 & - & CH_2 - CH_2 - CH_3 \\ & & & & | & & \\ CH_3 & - & CH_2 & - & C & - & CH_3 \\ & & & & | & & \\ & & & & CH_2 & - & CH_2 - CH_3 \end{array}$$

1.5 Cycloalkanes with substituents

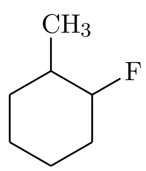
The naming rules for cycloalkanes are the same as the rules for naming linear alkanes. This means first you will find the ending of the name by counting the number of carbons in the cycle. Then you will locate each substituent and number the carbon chain so that the position numbers are small. Finally,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

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



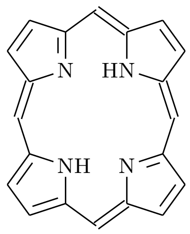
this is a cyclohexane connected to a methyl substituent. As there is only one substituent, there is no need to number the carbon chain. Hence the name would be simply methylcyclohexane.

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

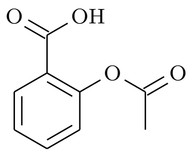


this is a cyclopentane connected to two different substituents: a methyl and a fluoro. In order to name this molecule we need to number the carbons first, and there are two different ways to number the cyclohexane ring:

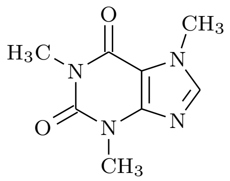
▼Porphyrin has several amine groups.

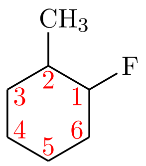


▼Aspirin contains an aromatic cycle, a carboxylic acid and a ester.

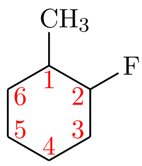


▼Caffeine contains amides and amines





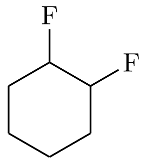
1-Fluoro-2-methylcyclohexane



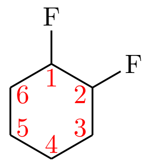
~~Fluoro-1-methylcyclohexane~~

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

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



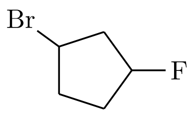
After numbering the chain:



The name would be: 1,2-difluorocyclohexane.

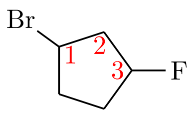
Sample Problem 10

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:

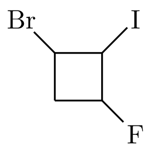


And the name of the molecule would be:

▶Answer: 1-bromo-3-fluorocyclopentane.

STUDY CHECK

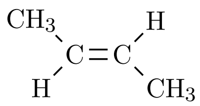
Name the following hydrocarbon:



1.6 Molecular diversity

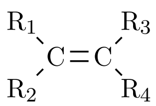
You have certainly taken painkillers for a headache or over-the-counter drugs to get over a cold. Maybe you drink coffee and perhaps you like tea. All these substances contain active organic molecules. These active molecules are hydrocarbon derivatives and differ from plain hydrocarbons, which are simply 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.

`Alkene group: double bonds` Alkenes contain at least one double bond between carbons. An example would be:



or $CH_3CH_2-HC=CH-CH_3$

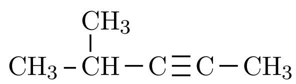
Double bonds are also called unsaturations. Hence, we say alkenes are unsaturated. As both sides of an alkene can be connected to different hydrocarbon chains we normally represent this as:



Alkene

where R and R' represent any hydrocarbon chain. For Example R and R' can be CH_3- or CH_3CH2-. Alkynes contain at least one triple bond between carbons. An example would be:

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

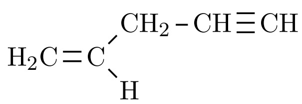


Again, we could use R and R' to represent any hydrocarbon chain:

$$R-C\equiv C-R' \quad \text{Alkyne}$$

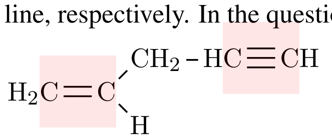
Sample Problem 11

Identify the alkene and alkyne groups in the molecule:



SOLUTION

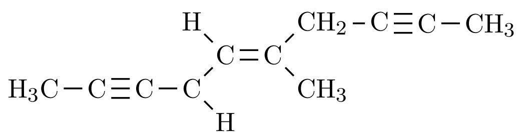
A double bond is carbon atoms sharing two pairs of electrons, whereas a triple bond is a pair of atoms sharing three pairs of electrons. They are represented with a double and triple line, respectively. In the question:



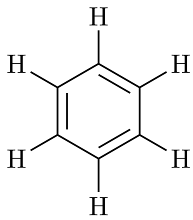
▶Answer: (left) alkene; (right) alkyne

STUDY CHECK

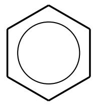
Identify the alkene and alkyne groups in the molecule:



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

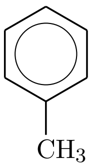


Benzene

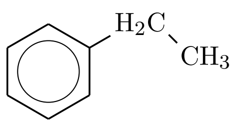


Benzene

Examples of molecules containing aromatic groups are:



or



and

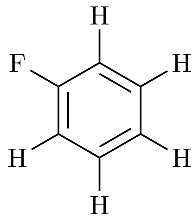
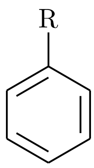


Table 1.4 Names of several functional groups

Functional group	Name	Functional group	Name	Functional group	Name
$R_1R_2C{=}CR_3R_4$	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 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:

$$CH_3-CH_2-OH \qquad CH_3-O-CH_2-CH_3$$

alcohol ether

Thiols contain a $-SH$ group attached to a carbon. They are equivalent to alcohols but based in sulfur:

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

Examples of thiols are:

$$CH_3-CH_2-SH \qquad CH_3-\overset{\overset{\displaystyle SH}{|}}{CH}-CH_3$$

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

Sample Problem 12

Classify the following molecules as alcohol or ether.

$$CH_3-CH_2-CH_2-OH \qquad CH_3-O-CH_2-CH_3$$

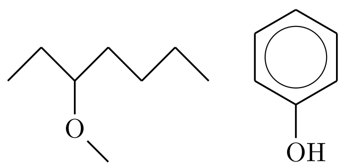
SOLUTION

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 $R-O-R'$ group.

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

STUDY CHECK

Classify the following molecules as alcohol or ether.



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

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

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

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

Examples of aldehydes and ketones are:

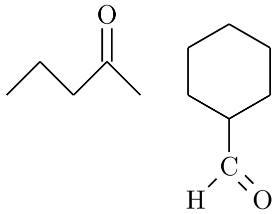
$$CH_3CH_2-\overset{\overset{\displaystyle O}{||}}{C}-H \qquad \text{or} \qquad CH_3-\overset{\overset{\displaystyle O}{||}}{C}-CH_3$$

Aldehyde Ether

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

Sample Problem 13

Classify the following molecules as an aldehyde or ketone



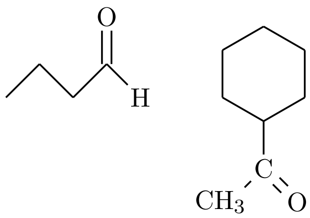
SOLUTION

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 an hydrocarbon and also an alcohol group:

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

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

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

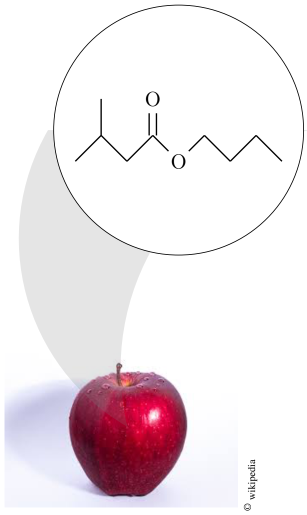
Examples of carboxylic acids and esters are:

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

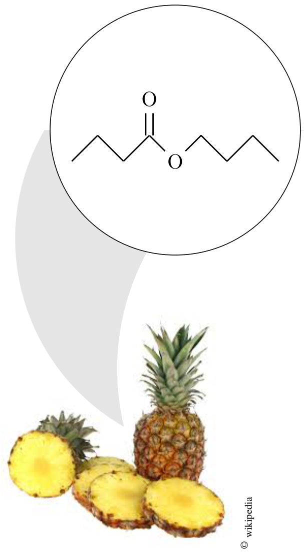
Carboxylic acid Esters

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

▼Ethyl isovalerate is an ester that flavors apples.

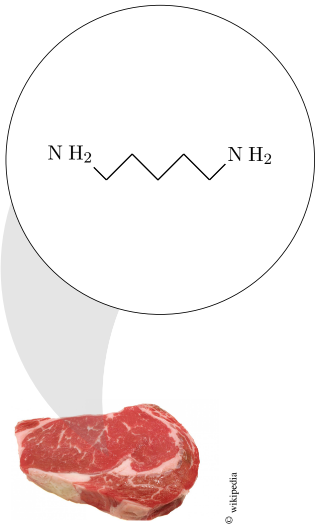


▼Butyl butyrate is an ester that flavors pineapple.

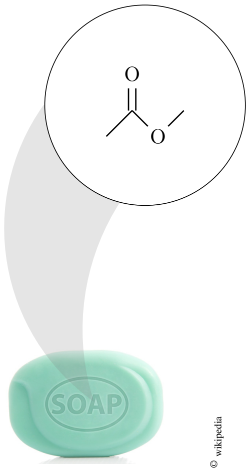


▼Diethyl ether was formerly used as a general anesthetic, until non-flammable drugs were developed.

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



▼Esters are found in soaps



▼Vinegar contains acetic acid, the smallest carboxylic acid.

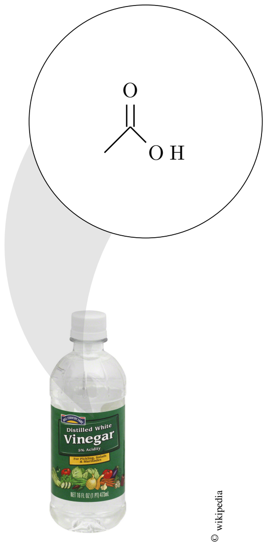
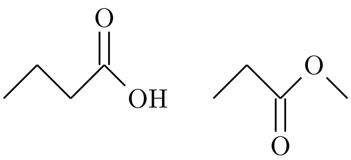


Figure 1.1 Some examples of functional groups with applications to real life.

Sample Problem 14

Classify the following molecules as an carboxylic acid or ester:

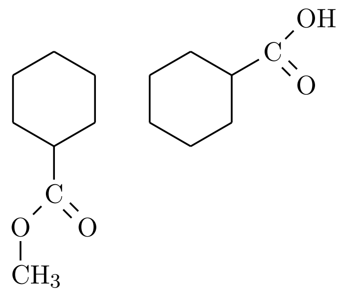


SOLUTION

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:



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

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

All these molecules are amines:

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

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

$$NH_2-\left(CH_2\right)_3-NH_2 \qquad\qquad NH_2-\left(CH_2\right)_5-NH_2$$

putrescine

cadaverine

Amides, on the other hand, contain a carbonyl group (C=O) connected to an amine group ($-\overset{|}{N}-$)

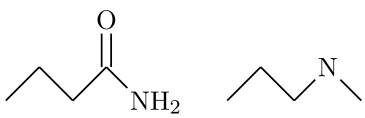
$$R-\overset{\displaystyle O}{\overset{||}{C}}-\overset{\displaystyle R''}{\overset{|}{N}}-R' \qquad \text{Amide}$$

Examples of amides are:

$$CH_3-\overset{\displaystyle O}{\overset{||}{C}}-NH_2 \qquad \text{or} \qquad CH_3-CH_2-\overset{\displaystyle O}{\overset{||}{C}}-\overset{\displaystyle H}{\overset{|}{N}}-CH_3$$

Sample Problem 15

Classify the following molecules as an amide or amine:



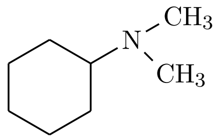
SOLUTION

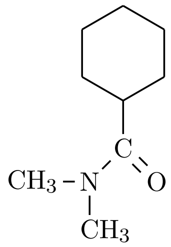
The molecule in the left is a amide as the carbonyl group (C=O) is connected to a nitrogen atom. Differently, the molecule in the right is an amine as the nitrogen group is not connected to any carbonyl group.

▶Answer: (left) amide; (right) amine.

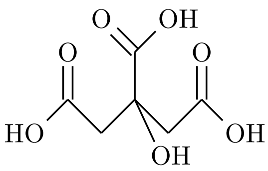
STUDY CHECK

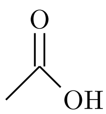
Classify the following molecules as an amide or amine:





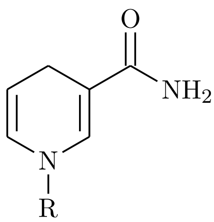
Identifying organic acids and bases Acid organic molecules, in general, contain one or more carboxylic acid groups. An example would be vinegar or citric acid, the acid found in citrus.



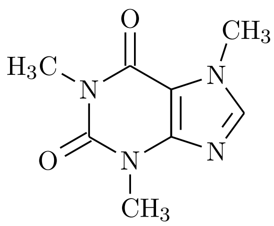


Citric acid Acetic Acid

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.



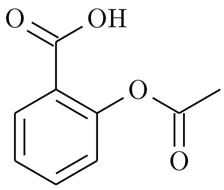
NADH



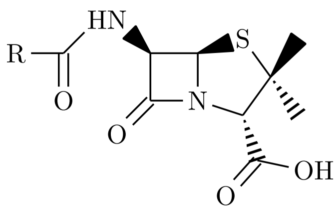
Caffeine

Sample Problem 16

Classify the following molecules as an acid or base:



Aspirin



Penicillin

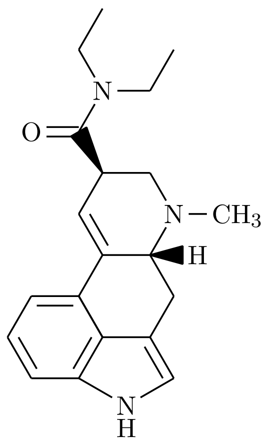
SOLUTION

Aspirin contains an acid group and hence it will be acidic. Penicillin contains both acidic and amine groups and hence will be both acidic and basic.

▶Answer: (left) acid; (right) both.

STUDY CHECK

Classify the following molecules as an carboxylic acid or base:



LDS

CHAPTER 1

ALKANES

1.1 Classify the following chemicals in two different categories. Give a rationale for your classification. For the group with more chemicals, further classify those chemicals in two categories. (a) KCl (b) C_2H_2 (c) C_4H_{10} (d) $FeO_{(s)}$ (e) C_6H_{12} (f) PH_3 (g) H_2O

1.2 Working in groups, select an everyday-life object (e.g a spoon) and guess whether the materials that made this object are mostly organic or inorganic (e.g mostly inorganic). Without revealing your answer, present the material you selected to another team member and ask him or her to give you his or her point or view regarding whether the materials that made this object are mostly organic or inorganic.

1.3 Indicate the molecular formula of the following organic compounds: (a) ethane (b) butane

1.4 Indicate the molecular formula of the following organic compounds: (a) methane (b) decane

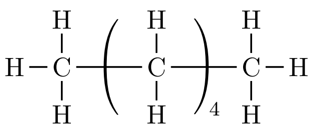
1.5 Name the following alkanes: (a) C_3H_8 (b) C_8H_{18}

1.6 Name the following alkanes: (a) C_5H_{12} (b) C_9H_{20}

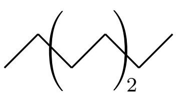
1.7 Write down the condensed formula of the following alkanes: (a) hexane (b) propane

1.8 Write down the expanded formula of the following alkanes: (a) pentane (b) decane

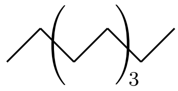
1.9 Write down the molecular formula for the chemical below:



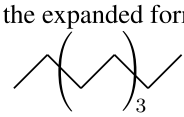
1.10 Write down the molecular formula for the chemical below:



1.11 Write down the molecular formula for the chemical below:



1.12 Write down the expanded formula for hexane.

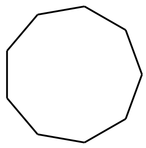


CYCLOALKANES

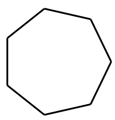
1.13 Indicate the molecular formula of the following cycloalkanes: (a) cyclobutane (b) cyclopentane

1.14 Indicate the molecular formula of the following cycloalkanes: (a) cyclopropane (b) cyclohexane

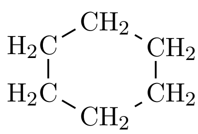
1.15 Name the following cycloalkane:



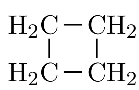
1.16 Name the following cycloalkane:



1.17 Name the following compound:



1.18 Name the following compound:



ALKANES WITH SUBSTITUENTS

1.19 Name the following compound:

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

1.20 Name the following compound:

$$\begin{array}{ccccccccccc} & & CH_3 & & & & & & & & \\ & & | & & & & & & & & \\ CH_3 & - & C & - & CH_2 & - & CH_2 & - & CH_2 & - & CH_3 \\ & & | & & & & & & & & \\ & & CH_3 & & & & & & & & \end{array}$$

1.21 Name the following compound:

$$\begin{array}{ccccccccccc} & & & & CH_3 & & & & & & \\ & & & & | & & & & & & \\ CH_3 & - & CH_2 & - & C & - & CH_2 & - & CH_2 & - & CH_3 \\ & & & & | & & & & & & \\ & & & & CH_3 & & & & & & \end{array}$$

1.22 Give the name for the following compound:

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

1.23 Give the name for the following compound:

$$\begin{array}{ccccccccc} & & C_2H_6 & & & & & & \\ & & | & & & & & & \\ CH_3 & - & CH & - & CH_2 & - & CH_2 & - & CH_3 \end{array}$$

1.24 Give the name for the following compound:

$$\begin{array}{ccccccccccc} & & Br & & NO_2 & & & & & & \\ & & | & & | & & & & & & \\ CH_3 & - & CH & - & CH & - & CH_2 & - & CH_2 & - & CH_3 \end{array}$$

1.25 Give the name for the following compound:

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

1.26 Give the name for the following compound:

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

1.27 Give the name for the following compound:

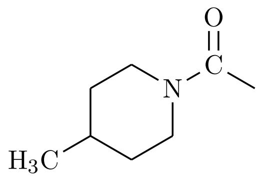
$$\begin{array}{ccccc} & & CH_3 & & \\ & & | & & \\ CH_3 & - & C & - & CH_3 \\ & & | & & \\ & & CH_2 - CH_3 & & \end{array}$$

1.28 Give the name for the following compound:

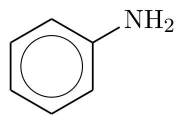
$$\begin{array}{ccccccccccc} & & & & CH_2 - CH_3 & & & & & & \\ & & & & | & & & & & & \\ CH_3 & - & CH_2 & - & CH & - & CH_2 & - & CH_2 & - & CH_3 \end{array}$$

FUNCTIONAL GROUPS

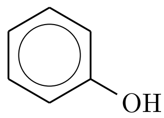
1.29 Identify the functional groups in the following molecule:



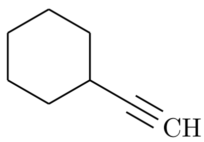
1.30 Identify the functional groups in the following molecule:



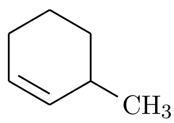
1.31 Identify the functional groups in the following molecule:



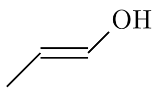
1.32 Identify the functional groups in the following molecule:



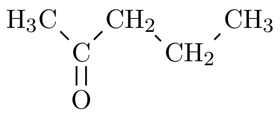
1.33 Identify the functional groups in the following molecule:



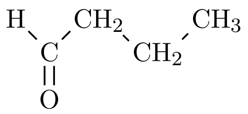
1.34 Identify the functional groups in the following molecule:



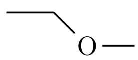
1.35 Identify the functional groups in the following molecule:



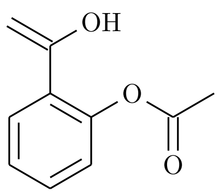
1.36 Identify the functional groups in the following molecule:



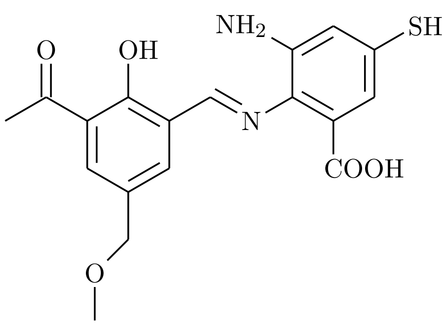
1.37 Identify the functional groups in the following molecule:



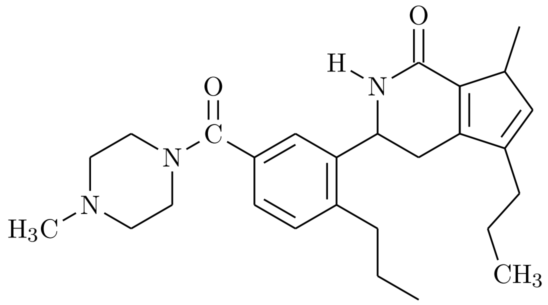
1.38 Identify the functional groups in the following molecule:

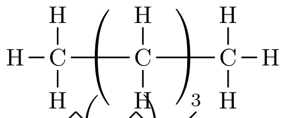
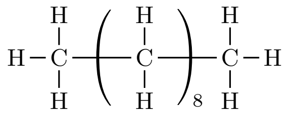
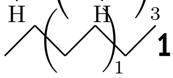


1.39 Identify the functional groups in the following molecule:



1.40 Identify the functional groups in the following molecule:



Answers **1.1** (a) KCl (ionic, inorganic) (b) C_2H_2 (covalent, organic) (c) C_4H_{10} (covalent, organic) (d) $FeO_{(s)}$ (ionic, inorganic) (e) C_6H_{12} (covalent, organic) (f) PH_3 (covalent, inorganic) (g) H_2O (covalent, inorganic) **1.2** Not given **1.3** (a) ethane (C_2H_6) (b) butane (C_4H_{10}) **1.4** (a) methane (CH_4) (b) decane ($C_{10}H_{22}$) **1.5** (a) C_3H_8 (Propane) (b) C_8H_{18} (Octane) **1.6** (a) C_5H_{12} (Pentane) (b) C_9H_{20} (nonane) **1.7** (a) $CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$ (b) $CH_3-CH_2-CH_3$ **1.8** (a)  (b)  **1.9** C_6H_{14},hexane**1.10** C_8H_{18}, octane**1.11** $C_{10}H_{22}$, decane**1.12**  **1.13** (a) cyclobutane C_4H_8 (b) cyclopentane C_5H_{10} **1.14** (a) C_4H_8 (b) C_6H_{12}

1.15 Cyclononane**1.16** Cycloheptane **1.17** Cyclohexane **1.18** Cyclopropane**1.19** 2-methylpentane**1.20** 2,2-dimethylhexane**1.21** 3,3-dimethylhexane**1.22** 2,3-dimethylhexane**1.23** 2-ethylpentane**1.24** 2-bromo-3-nitrohexane**1.25** 3-ethylhexane**1.26** 3-methylpentane**1.27** 2,3-dimethylbutane**1.28** 3-ethylhexane**1.29** amide**1.30** amine and aromatic**1.31** alcohol and aromatic**1.32** alkyne**1.33** alkene**1.34** alkene and alcohol**1.35** ketone**1.36** aldehyde**1.37** ether**1.38** alchol, atomatic, alkene, ester**1.39** (top left) ketone; (bottom) ether; (top left) alcohol; (top right) amino and thiol; (bottom left) acid; there are also two aromatic rings**1.40** there are an amine, two amides, an aromatic ring and two alkanes