3.3: ALKANES

learning objectives

- name alkanes using IUPAC (systematic) and selected common name nomenclature
- draw the structure of alkanes from IUPAC (systematic) and selected common names

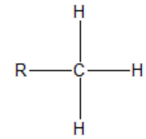
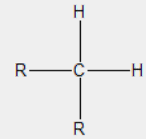
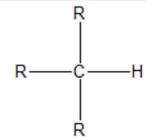
Alkanes are hydrocarbons that can be described by the general formula C_nH_{2n+2}. They consist only of carbon and hydrogen and contain only single bonds. Alkanes are also known as "saturated hydrocarbons."

The following table contains the systematic names for the first twenty straight chain alkanes. It will be important to familiarize yourself with these names because they will be the basis for naming many other organic molecules throughout your course of study.

Name	Molecular Formula	Condensed Structural Formula
Methane	CH_4	CH_4
Ethane	C_2H_6	CH_3CH_3
Propane	C_3H_8	$CH_3CH_2CH_3$
Butane	C_4H_{10}	$CH_3(CH_2)_2CH_3$
Pentane	C_5H_{12}	$CH_3(CH_2)_3CH_3$
Hexane	C_6H_{14}	$CH_3(CH_2)_4CH_3$
Heptane	C_7H_{16}	$CH_3(CH_2)_5CH_3$
Octane	C_8H_{18}	$CH_3(CH_2)_6CH_3$
Nonane	C_9H_{20}	$CH_3(CH_2)_7CH_3$
Decane	$C_{10}H_{22}$	$CH_3(CH_2)_8CH_3$
Undecane	$C_{11}H_{24}$	$CH_3(CH_2)_9CH_3$
Dodecane	$C_{12}H_{26}$	$CH_3(CH_2)_{10}CH_3$
Tridecane	$C_{13}H_{28}$	$CH_3(CH_2)_{11}CH_3$
Tetradecane	$C_{14}H_{30}$	$CH_3(CH_2)_{12}CH_3$
Pentadecane	$C_{15}H_{32}$	$CH_3(CH_2)_{13}CH_3$
Hexadecane	$C_{16}H_{34}$	$CH_3(CH_2)_{14}CH_3$
Heptadecane	$C_{17}H_{36}$	$CH_3(CH_2)_{15}CH_3$
Octadecane	$C_{18}H_{38}$	$CH_3(CH_2)_{16}CH_3$
Nonadecane	$C_{19}H_{40}$	$CH_3(CH_2)_{17}CH_3$
Eicosane	$C_{20}H_{42}$	$CH_3(CH_2)_{18}CH_3$

CARBON ATOM CLASSIFICATIONS

To assign the prefixes sec-, which stands for secondary, and tert-, for tertiary, it is important that we first learn how to classify carbon atoms. If a carbon is attached to only one other carbon, it is called a primary carbon. If a carbon is attached to two other carbons, it is called a seconday carbon. A tertiary carbon is attached to three other carbons and last, a quaternary carbon is attached to four other carbons. These terms are summarixed with an example in the table below.

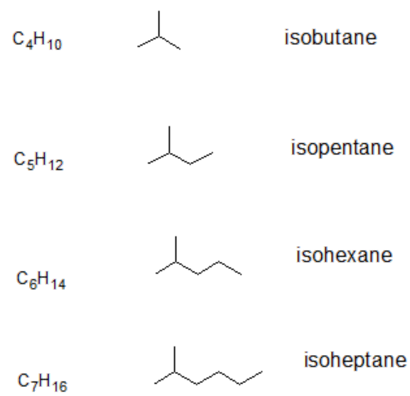
Classification	Example
methyl	CH_4
primary	
secondary	
tertiary	

USING COMMON NAMES WITH BRANCHED ALKANES

Certain branched alkanes have common names that are still widely used today. These common names make use of prefixes, such as ***iso***-, ***sec***-, ***tert***-, and ***neo***-.

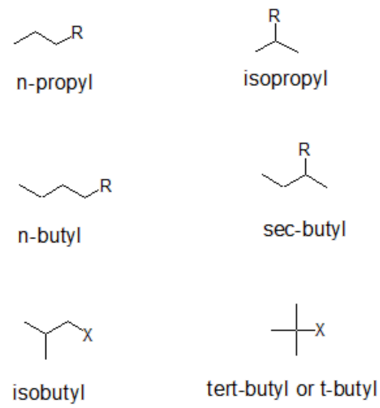
Isoalkanes

The prefix ***iso***-, which stands for isomer, is commonly given to 2-methyl alkanes. In other words, if there is methyl group located on the second carbon of a carbon chain, we can use the prefix ***iso***-. The prefix will be placed in front of the alkane name that indicates the *total* number of carbons as in isopentane which is the same as 2-methylbutane and isobutane which is the same as 2-methylpropane. The pattern is illustrated below



Sec- and Tert-alkanes

Secondary and tertiary alkanes can be further distinguished from their "iso-counter parts" by applying comparing the carbon classifications. The common names for three and four carbon branches are summarized below. Notice that the "iso" prefix is joined directly to the alkyl name. When alphabetizing branches, the "i" is considered. For "sec" and "tert", the prefix is separated from the alkyl name and is NOT considered when alphabetizing branches.



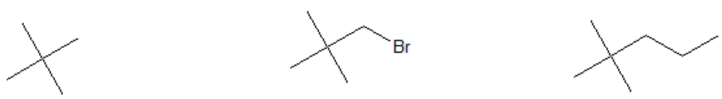
For some compounds, the common names bring a simple a simple elegance to the experience.

Common: 4-sec-butylheptane
IUPAC: 3-methyl-4-propylheptane

Common: 4-t-butyl-3-isopropylheptane
IUPAC: 4-*tert*-butyl-3-ethyl-2-methylheptane

Neo-alkanes

A five carbon alkane and the corresponding five carbon branch can form a structural pattern commonly known as neopentane and neopentyl respectively. The prefix neo- can also be applied to larger alkanes as shown below.



IUPAC:	2,2-dimethylpropane	1-bromo-2,2-dimethylpropane	2,2-dimethylpentane
Common:	neopentane	neopentylbromide	neoheptane

ALKYL GROUPS

An alkyl group is formed by removing one hydrogen from the alkane chain and is described by the formula C_nH_{2n+1}. The removal of this hydrogen results in a stem change from **-ane** to **-yl**. Take a look at the following examples.

$CH_4 \longrightarrow CH_3^-$
Methane → Methyl

$CH_3CH_2CH_3 \longrightarrow CH_3CH_2CH_2^-$
Propane → Propyl

The same approach can be used with any of the alkanes in the table above and with common names.

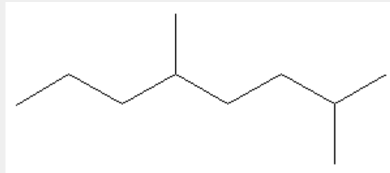
ALKYL GROUP COMMON NAMES THAT SOUND LIKE ALKENES

In long hydrocarbon chains there can be many $-CH_2-$ groups in a series. These internal $-(CH_2)_n-$ groups are names using the homologous series stem with the suffice "ene" even though there are NO carbon-carbon double bonds present. For example, the common name for dichloromethane, CH_2Cl_2, is methylene chloride; and the common names for the major ingredients in antifreeze are ethylene glycol ($CH_2(OH)CH_2OH$) and propylene glycol ($CH_2(OH)CH_2(OH)CH_3$), in spite of the fact that there are no carbon-carbon double bonds in any of these three compounds.

THREE BASIC PRINCIPLES OF NAMING

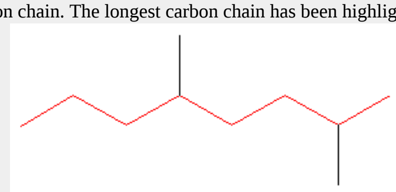
1. Choose the longest, most substituted carbon chain containing a functional group.
2. A carbon bonded to a functional group must have the lowest possible carbon number. If there are no functional groups, then any substitute present must have the lowest possible number.
3. Take the alphabetical order into consideration; that is, after applying the first two rules given above, make sure that your substitutes and/or functional groups are written in alphabetical order.

Example

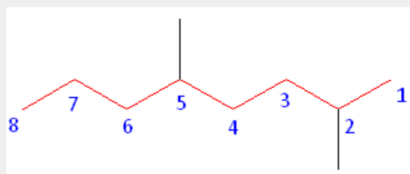


Solution

Rule #1 Choose the longest, most substituted carbon chain containing a functional group. This example does not contain any functional groups, so we only need to be concerned with choosing the longest, most substituted carbon chain. The longest carbon chain has been highlighted in red and consists of eight carbons.

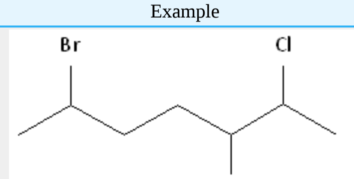


Rule #2 Carbons bonded to a functional group must have the lowest possible carbon number. If there are no functional groups, then any substitute present must have the lowest possible number. Because this example does not contain any functional groups, we only need to be concerned with the two substitutes present, that is, the two methyl groups. If we begin numbering the chain from the left, the methyls would be assigned the numbers 4 and 7, respectively. If we begin numbering the chain from the right, the methyls would be assigned the numbers 2 and 5. Therefore, to satisfy the second rule, numbering begins on the right side of the carbon chain as shown below. This gives the methyl groups the lowest possible numbering.



In this example, there is no need to utilize the third rule. Because the two substitutes are identical, neither takes alphabetical precedence with respect to numbering the carbons. This concept will become clearer in the next example.

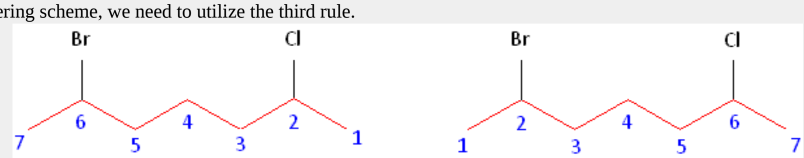
Example



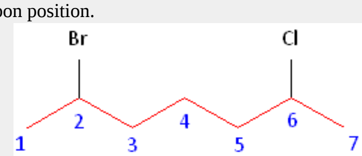
Solution

Rule #1 Choose the longest, most substituted carbon chain containing a functional group. This example contains two functional groups, bromine and chlorine. The longest carbon chain has been highlighted in red and consists of seven carbons.

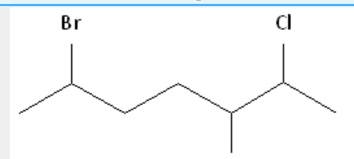
Rule #2 Carbons bonded to a functional group must have the lowest possible carbon number. If there are no functional groups, then any substitute present must have the lowest possible number. In this example, numbering the chain from the left or the right would satisfy this rule. If we number the chain from the left, bromine and chlorine would be assigned the second and sixth carbon positions, respectively. If we number the chain from the right, chlorine would be assigned the second position and bromine would be assigned the sixth position. In other words, whether we choose to number from the left or right, the functional groups occupy the second and sixth positions in the chain. To select the correct numbering scheme, we need to utilize the third rule.



Rule #3 After applying the first two rules, take the alphabetical order into consideration. Alphabetically, bromine comes before chlorine. Therefore, bromine is assigned the second carbon position, and chlorine is assigned the sixth carbon position.

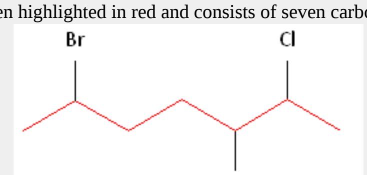


Example

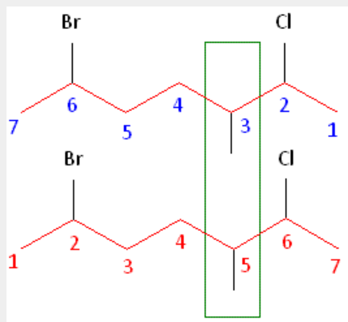


Solution

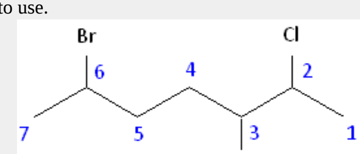
Rule #1 Choose the longest, most substituted carbon chain containing a functional group. This example contains two functional groups, bromine and chlorine, and one substitute, the methyl group. The longest carbon chain has been highlighted in red and consists of seven carbons.



Rule #2 Carbons bonded to a functional group must have the lowest possible carbon number. After taking functional groups into consideration, any substitutes present must have the lowest possible carbon number. This particular example illustrates the **point of difference principle**. If we number the chain from the left, bromine, the methyl group and chlorine would occupy the second, fifth and sixth positions, respectively. This concept is illustrated in the second drawing below. If we number the chain from the right, chlorine, the methyl group and bromine would occupy the second, third and sixth positions, respectively, which is illustrated in the first drawing below. The position of the methyl, therefore, becomes a **point of difference**. In the first drawing, the methyl occupies the third position. In the second drawing, the methyl occupies the fifth position. To satisfy the second rule, we want to choose the numbering scheme that provides the lowest possible numbering of this substitute. Therefore, the first of the two carbon chains shown below is correct.



Therefore, the first numbering scheme is the appropriate one to use.



Once you have determined the correct numbering of the carbons, it is often useful to make a list, including the functional groups, substitutes, and the name of the parent chain.

Parent chain: heptane 2-Chloro 3-Methyl 6-Bromo

6-bromo-2-chloro-3-methylheptane

EXERCISES

Write the IUPAC (systematic) name for each of the compounds below. The parent chains have numbered for the first two compounds to help you begin.

a)
b)
c)

SOLUTIONS

a) 9-chloro-7-ethyl-2,2,4-tromethyldecane

b) 3-chloro-5-ethyl-4,4-dimethylheptane

c) 2-bromo-6-ethyloctane