Tishk International University

Faculty of Dentistry

Department of Basic Science

Organic Chemistry

Hydrocarbons

2nd lecture

1st grade

Organic compounds:

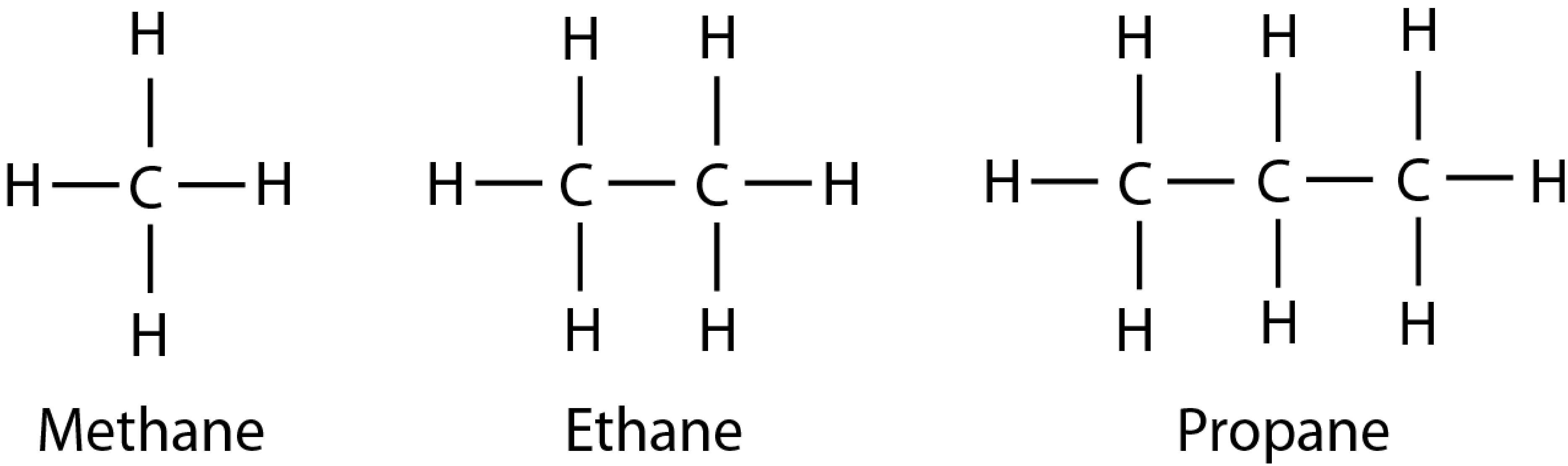
Organic chemistry is the study of carbon compounds. **Organic compounds** typically contain carbon (C) and hydrogen (H), and sometimes oxygen (O), sulfur (S), nitrogen (N), phosphorus (P), or a halogen (F, Cl, Br, and I). The formulas of organic compounds are written with carbon first, followed by hydrogen, and then any other elements.

Many organic compounds are ***nonpolar*** molecules, are ***not soluble*** in water, and are ***less dense*** than water.

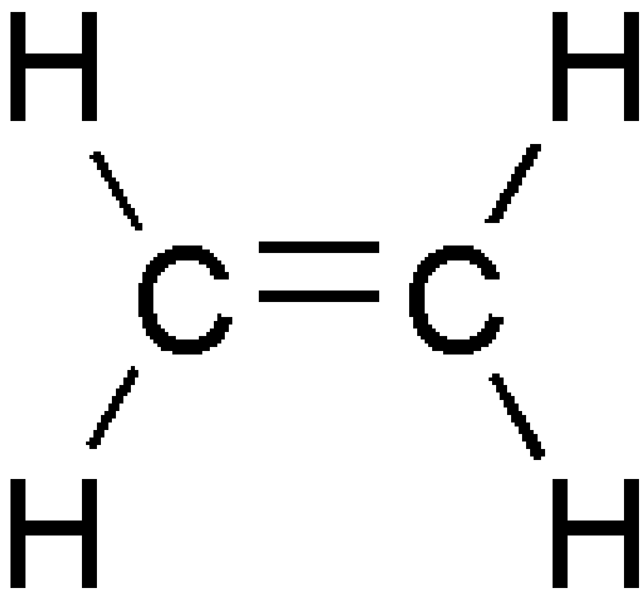
Hydrocarbons:

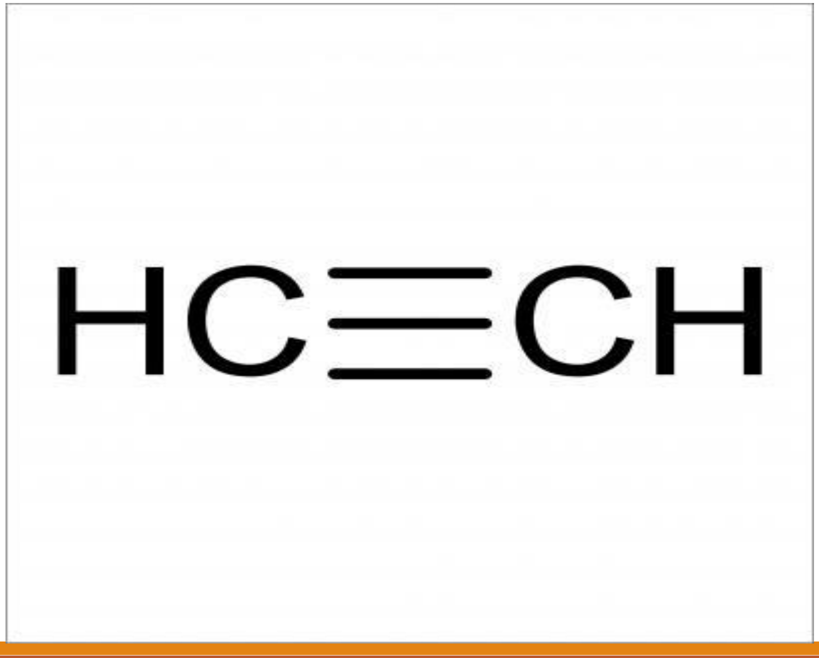
They are compounds that contain only carbon and hydrogen atoms**.**

Generally, compounds such as the *alkanes*, whose molecules contain only *single* bonds, are referred to as ***saturated*** compounds because these compounds contain the maximum number of hydrogen atoms that the carbon compound can possess.



Compounds with *multiple* bonds, such as *alkenes*, *alkynes*, and *aromatic* hydrocarbons, are called ***unsaturated*** compounds because they possess fewer hydrogen atoms, and they are capable of reacting with hydrogen under the proper conditions.

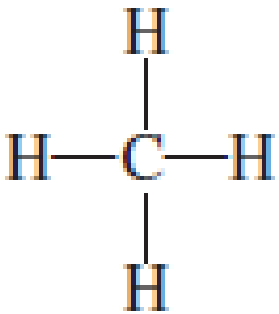




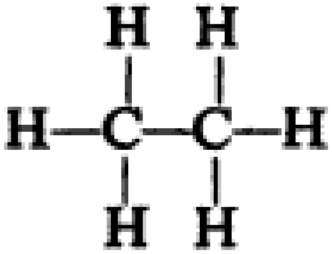
❖ Structural formulas for hydrocarbons:

➢ Expanded structural formula:

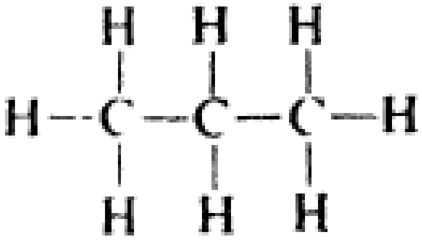
We can draw an **expanded structural formula** of a compound by *showing* all the *bonds between atoms*.



Methane



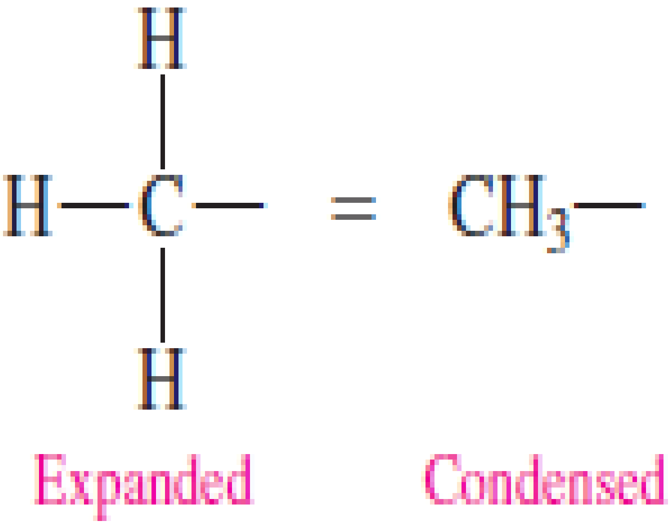
ethane

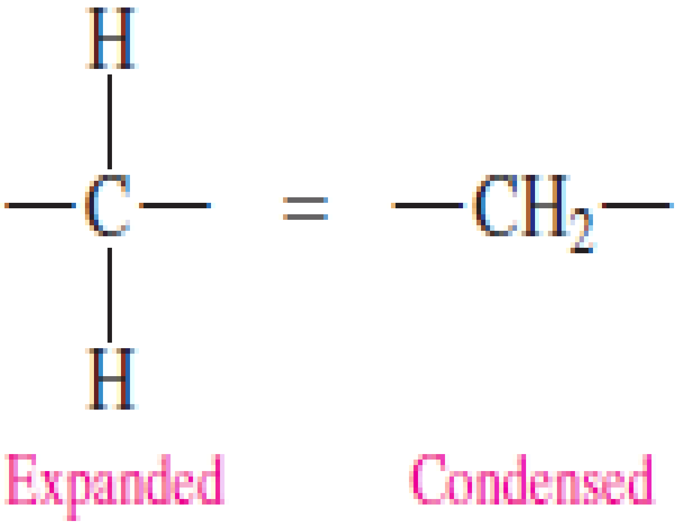


propane

➢ Condensed structural formulas:

In a **condensed structural formula**, each carbon atom and its attached hydrogen atoms are written as a ***group***. A ***subscript*** indicates the ***number of hydrogen*** atoms bonded to each carbon atom.



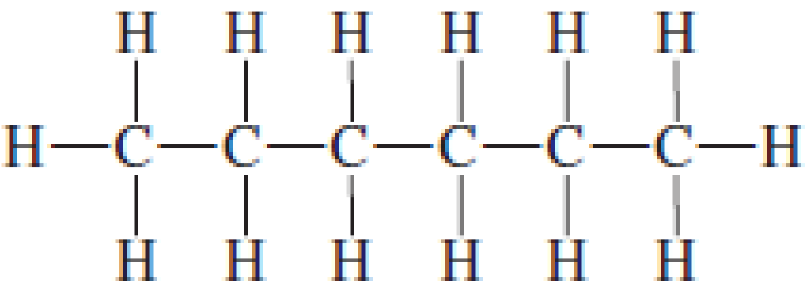


➢ Skeletal formula:

When an organic molecule consists of a chain of three or more carbon atoms, the carbon atoms do not lie in a ***straight*** line. Carbon bonds arrange in a ***zigzag pattern***. The structure called the ***line-bond*** or ***skeletal formula*** represents only the carbon skeleton, in which carbon atoms are represented as the ***ends*** of each line or as ***corners in a zigzag line***. The hydrogen atoms are not shown, *but each carbon is understood to have the proper number of atoms including hydrogen atoms to give four bonds.*

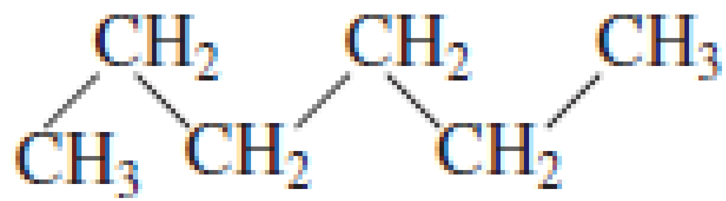
By contrast, the ***molecular formula*** gives the total number of each kind of atom but does not indicate their arrangement in the molecule.

Expanded Structural Formula

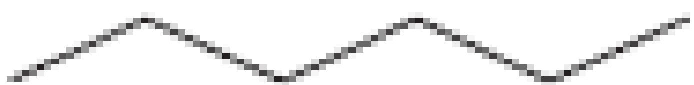


Condensed Structural Formulas

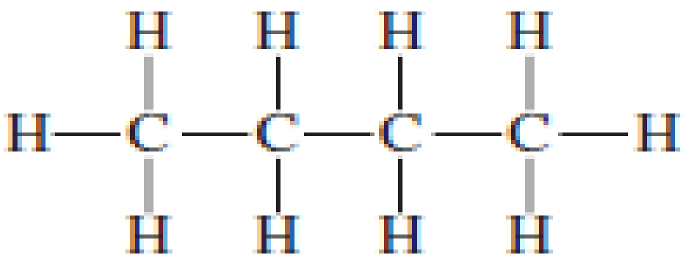
$$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$$



Skeletal Formula



Expanded Structural Formula



Condensed Structural Formulas

$$CH_3—CH_2—CH_2—CH_3$$

Skeletal Formulas

IUPAC nomenclature of alkanes

Today, chemists use a systematic nomenclature developed and updated by the International Union of Pure and Applied Chemistry (IUPAC).

The names for several of the **unbranched alkanes** are listed below. The ending for all of the names of alkanes is (-*ane)*. *The stems of the names of most of the alkanes* are of Greek and Latin origin. For example *(one*, *two*, *three*, *four*, *and five)* become *(meth*-, *eth*-, *prop*-, *but*-, *and pent*-*)*.

Number of Carbon Atoms	Prefix	Name	Molecular Formula
1	Meth	Methane	CH_4
2	Eth	Ethane	C_2H_6
3	Prop	Propane	C_3H_8
4	But	Butane	C_4H_{10}
5	Pent	Pentane	C_5H_{12}
6	Hex	Hexane	C_6H_{14}
7	Hept	Heptane	C_7H_{16}
8	Oct	Octane	C_8H_{18}
9	Non	Nonane	C_9H_{20}
10	Dec	Decane	$C_{10}H_{22}$

Name	Number of Carbon Atoms	Structure
Undecane	11	$CH_3(CH_2)_9CH_3$
Dodecane	12	$CH_3(CH_2)_{10}CH_3$
Tridecane	13	$CH_3(CH_2)_{11}CH_3$
Tetradecane	14	$CH_3(CH_2)_{12}CH_3$
Pentadecane	15	$CH_3(CH_2)_{13}CH_3$
Hexadecane	16	$CH_3(CH_2)_{14}CH_3$
Heptadecane	17	$CH_3(CH_2)_{15}CH_3$
Octadecane	18	$CH_3(CH_2)_{16}CH_3$
Nonadecane	19	$CH_3(CH_2)_{17}CH_3$
Eicosane	20	$CH_3(CH_2)_{18}CH_3$

Nomenclature of alkyl groups:

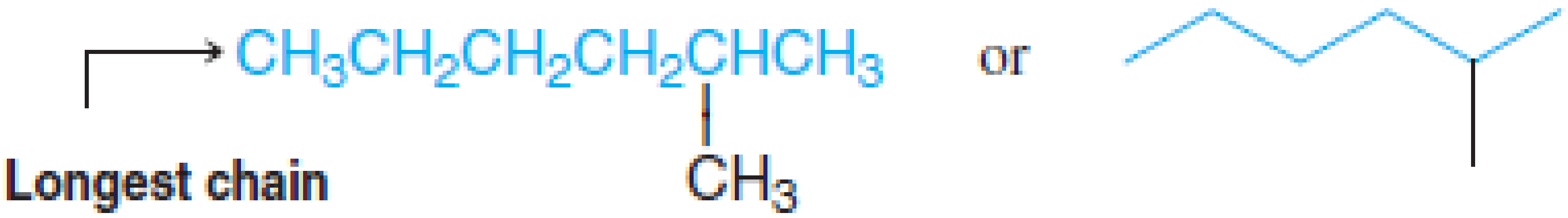
In the IUPAC names for alkanes, a carbon branch is named as an **alkyl group**, which is an alkane that is missing ***one hydrogen*** atom. The alkyl group is named by replacing the (-*ane)* ending of the corresponding alkane name with (-*yl).*

Substituent	Name
$CH_3—$	Methyl
$CH_3—CH_2—$	Ethyl
$CH_3—CH_2—CH_2—$	Propyl
$CH_3—\overset{\vert}{CH}—CH_3$	Isopropyl
F—, Cl—, Br—, I—	Fluoro, chloro, bromo, iodo

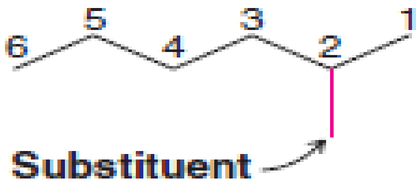
Nomenclature of branched-chain alkanes

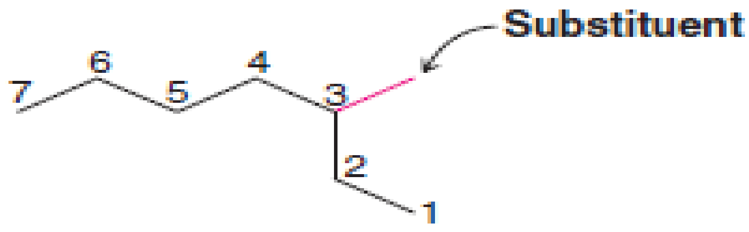
Branched-chain alkanes are named according to the following rules:

1. Locate the longest continuous chain of carbon atoms; this chain determines the parent name for the alkane.

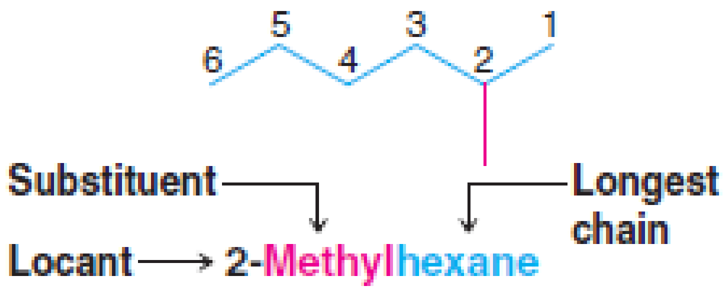


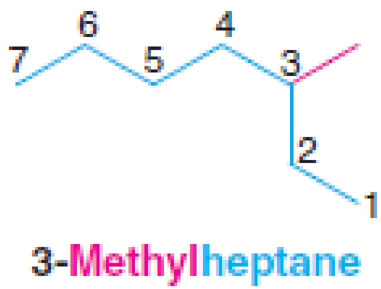
2. Number the longest chain beginning with the end of the chain nearer the substituent.



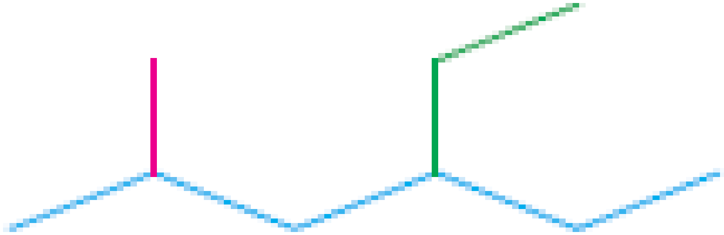


3. Use the numbers obtained by application of rule 2 to designate the location of the substituent group.



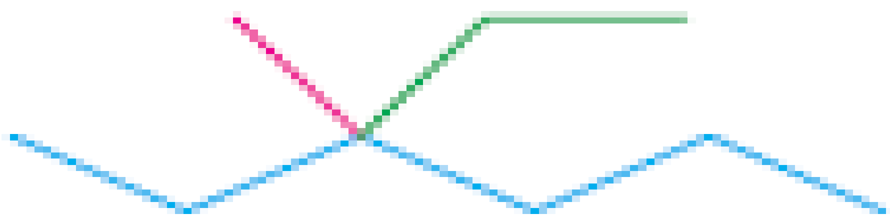


4. When two or more substituents are present, give each substituent a number corresponding to its location on the longest chain.



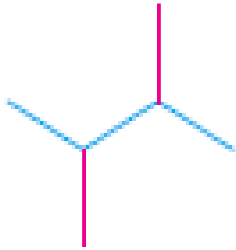
4-Ethyl-2-methylhexane

5. When two substituents are present on the same carbon atom, use that number twice:

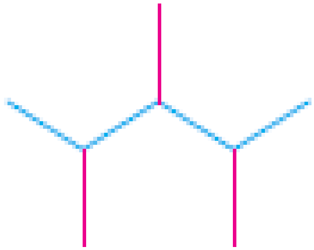


3-Ethyl-3-methylhexane

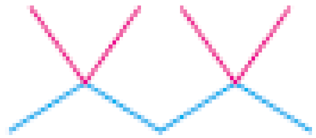
6. When two or more substituents are identical, indicate this by the use of the prefixes *di*-, *tri*-, *tetra*-, and so on.



2,3-Dimethylbutane

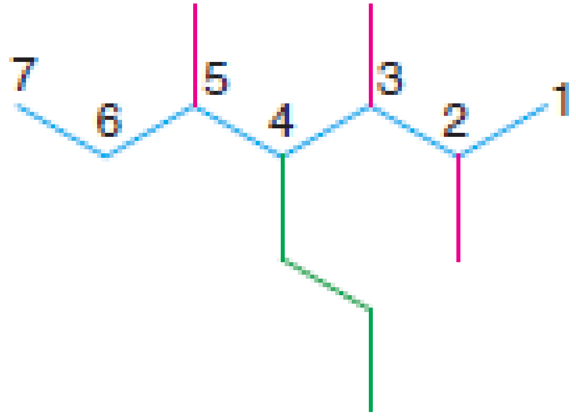


2,3,4-Trimethylpentane



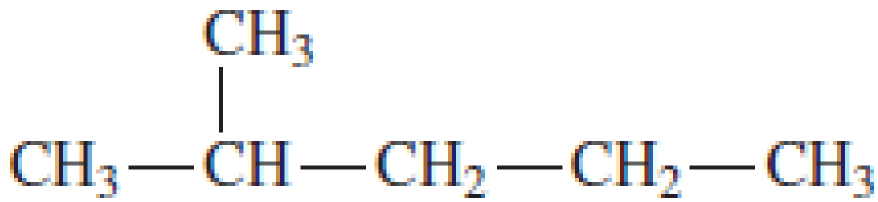
2,2,4,4-Tetramethylpentane

7. When two chains of equal length compete for selection as the parent chain, choose the chain with the greater number of substituents:



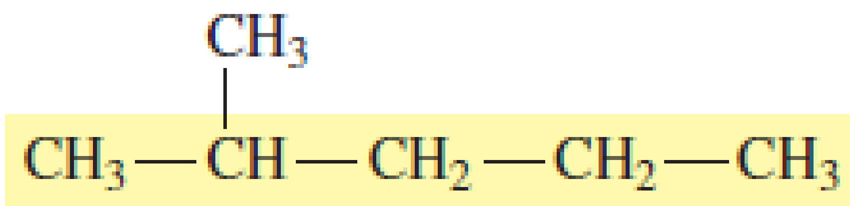
2,3,5-Trimethyl-4-propylheptane
(four substituents)

Example: **Give IUPAC naming for the following compound?**



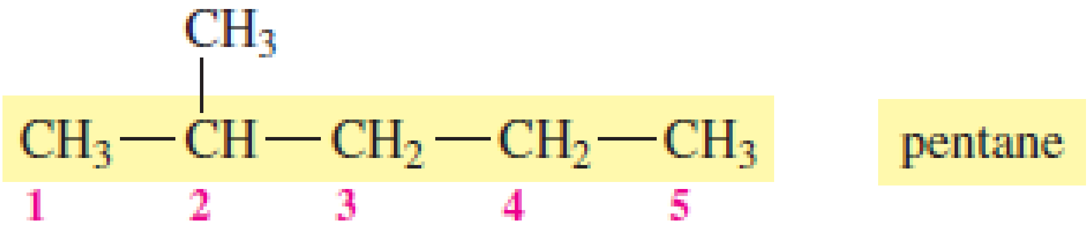
Solution:

Step 1: Write the alkane name of the longest chain of carbon atoms. In this alkane, the longest chain has five carbon atoms, which is *pentane*.

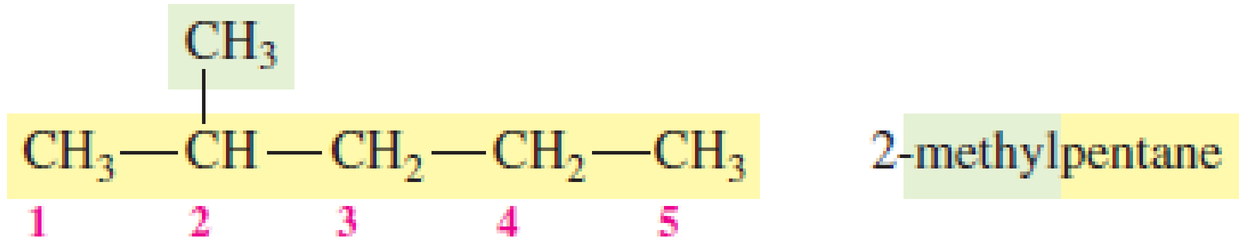


pentane

Step 2: Number the carbon atoms starting from the end nearer a substituent. Number the chain from 1 to 5 starting at the end nearer the branch of (CH_3). Once you start numbering, continue in that same direction.

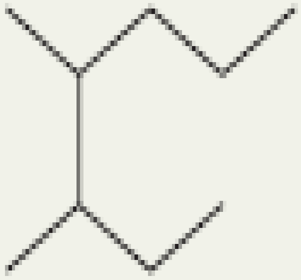


Step 3: Give the location and name of each substituent (alphabetical order) as a prefix to the name of the main chain. Place a hyphen between the number and the substituent name.



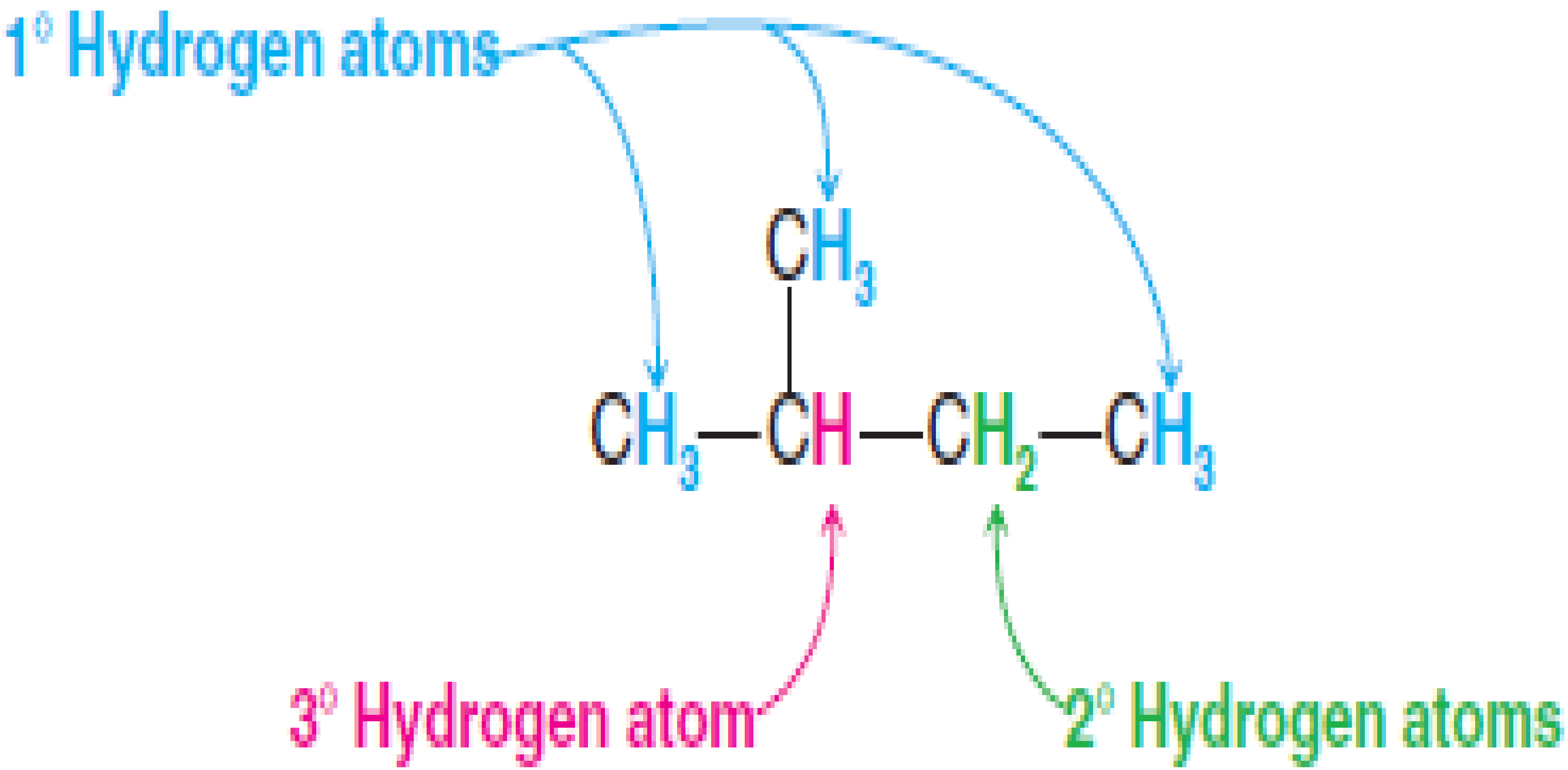
Example:

Provide an IUPAC name for the following alkane.

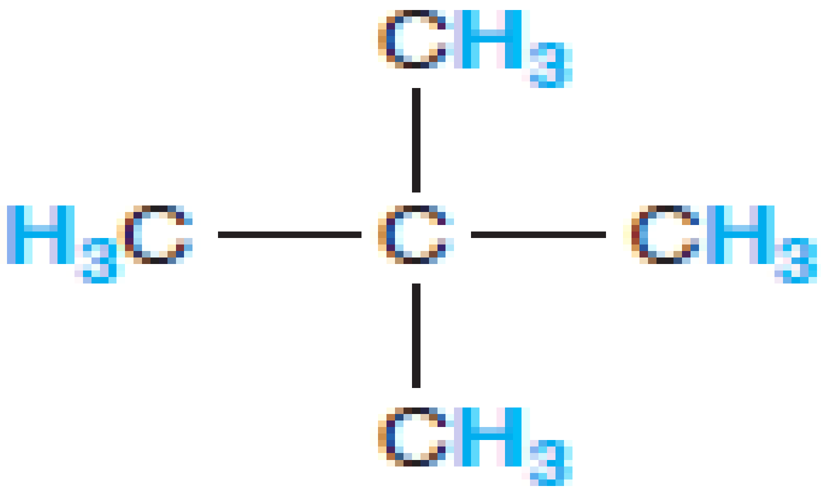


Classification of hydrogen atoms

The hydrogen atoms of an alkane are classified on the basis of the carbon atom to which they are attached. A hydrogen atom attached to a ***primary carbon*** atom is a primary (1°) hydrogen atom, and so forth. The following compound, 2-methylbutane, has primary, secondary (2°), and tertiary (3°) hydrogen atoms:


1° Hydrogen atoms
CH3
CH3—CH—CH2—CH3
3° Hydrogen atom
2° Hydrogen atoms

On the other hand, ***2,2-dimethylpropane***, a compound has only primary hydrogen atoms:



Physical properties of alkanes

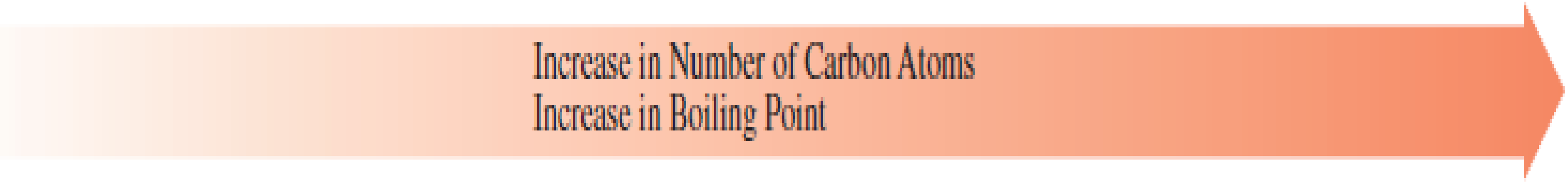
If we examine the ***unbranched*** alkanes, we notice that each alkane differs from the preceding alkane by ***one*** — $\boldsymbol{CH_2}$ — group. Butane, for example, is $CH_3(CH_2)_2CH_3$ and pentane is $CH_3(CH_2)_3CH_3$. A series of compounds like this, where each member differs from the next member by a constant unit, is called a ***homologous series***. Members of a homologous series are called ***homologues***.

Name	Number of Carbon Atoms	Structure
Methane	1	CH_4
Ethane	2	CH_3CH_3
Propane	3	$CH_3CH_2CH_3$
Butane	4	$CH_3(CH_2)_2CH_3$
Pentane	5	$CH_3(CH_2)_3CH_3$
Hexane	6	$CH_3(CH_2)_4CH_3$
Heptane	7	$CH_3(CH_2)_5CH_3$
Octane	8	$CH_3(CH_2)_6CH_3$
Nonane	9	$CH_3(CH_2)_7CH_3$
Decane	10	$CH_3(CH_2)_8CH_3$

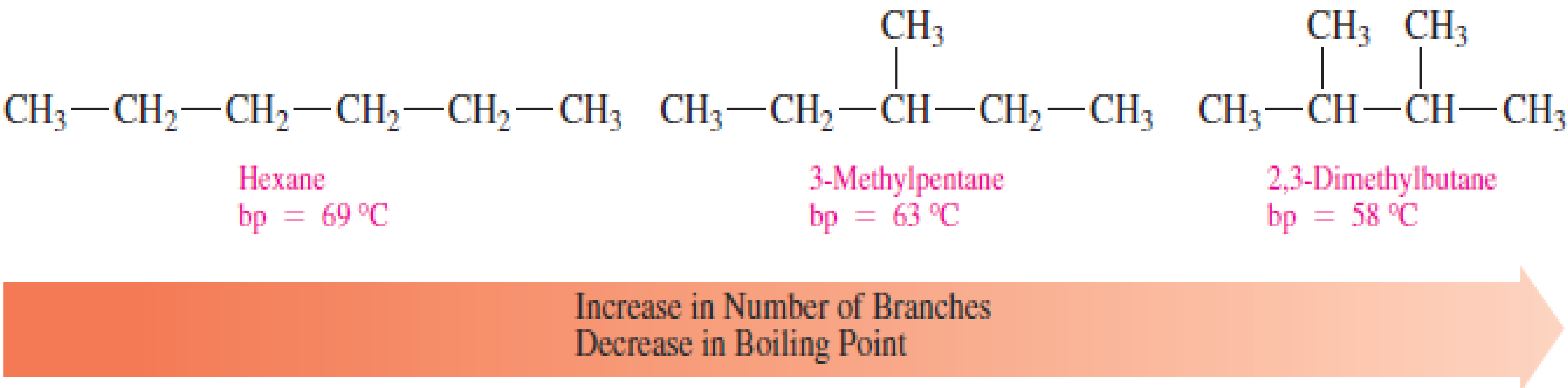
- At room temperature (25°C) and 1 atm pressure the first four members of the homologous series of unbranched alkanes ***(1 to 4) carbon atoms*** (methane, ethane, propane, and butane) are ***gases***.
- The $\boldsymbol{C_5}$—$\boldsymbol{C_{17}}$ unbranched alkanes (pentane to heptadecane) are ***liquids***; alkanes having (5 to 8) carbon atoms (pentane, hexane, heptane, and octane) are highly volatile liquids.
- The unbranched alkanes with ***18 and more*** carbon atoms are ***solids.***

1. **Boiling points:** The boiling points of the unbranched alkanes show a regular ***increase*** with increasing molecular weight in the homologous series of straight-chain alkanes. Branching of the alkane chain, ***lowers*** the boiling point.

CH_4	CH_3-CH_3	$CH_3-CH_2-CH_3$	$CH_3-CH_2-CH_2-CH_3$	$CH_3-CH_2-CH_2-CH_2-CH_3$
Methane	Ethane	Propane	Butane	Pentane
bp = −164 °C	bp = −89 °C	bp = −42 °C	bp = 0.5 °C	bp = 36 °C



The boiling points of branched alkanes are generally lower than the straight-chain isomers. The branched-chain alkanes tend to be more compact, which reduces the points of contact between the molecules.



Cycloalkanes have higher boiling points than the straight-chain alkanes with the same number of carbon atoms. Because rotation of carbon bonds is restricted, cycloalkanes maintain a rigid structure. Cycloalkanes with their rigid structures can be stacked closely together, which gives them many points of contact and therefore many attractions to each other.

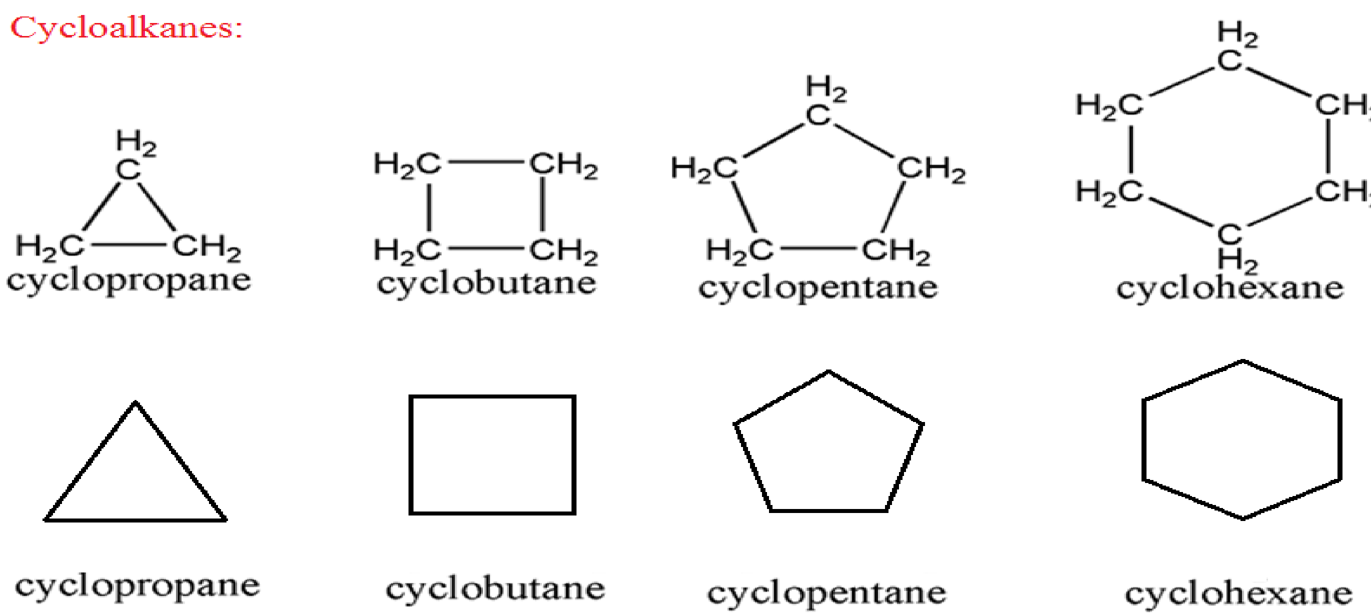
2. Melting point: melting points of unbranched alkanes show a regular increase with increasing molecular weight in the homologous series of straight-chain alkanes. branched alkanes have fewer attractions, they have lower melting and boiling points.

3. Density: Alkanes are the ***least*** dense of all groups of organic compounds; having densities considerably less than 1.00 g mL^{-1}. As a result, petroleum (a mixture of hydrocarbons rich in alkanes) floats on water.

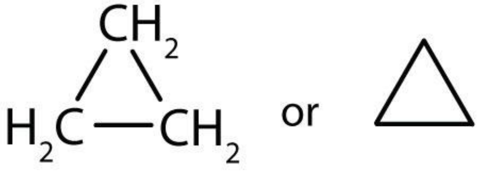
4. Solubility: Alkanes are almost totally ***insoluble*** in water because of their very low polarity and their inability to form hydrogen bonds. Liquid alkanes are soluble in one another, and they generally dissolve in solvents of low polarity. Good solvents for them are benzene, carbon tetrachloride, chloroform, and other hydrocarbons.

Cycloalkanes

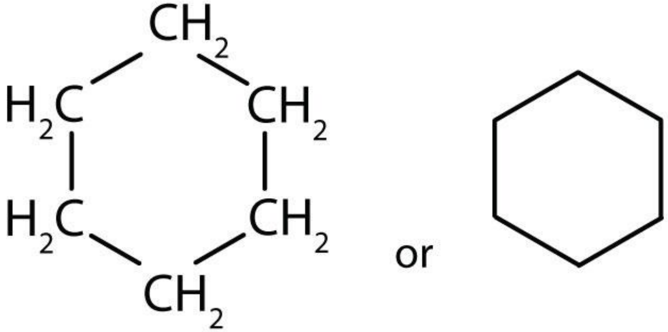
Cycloalkanes are alkanes in which all or some of the carbon atoms are arranged in a ring. Alkanes have the general formula **(C_nH_{2n+2})**; cycloalkanes containing a single ring have two fewer hydrogen atoms and thus have the general formula **(C_nH_{2n})**.



The simplest cycloalkane, cyclopropane, C_3H_6, has a ring of ***three*** carbon atoms bonded to ***six*** hydrogen atoms. Most often, a cycloalkane is drawn using its skeletal formula, which appears as a simple geometric figure. As seen for alkanes, each corner of the skeletal formula for a cycloalkane represents a carbon atom. A cycloalkane is named by adding the prefix ***cyclo*** to the name of the alkane with the same number of carbon atoms.

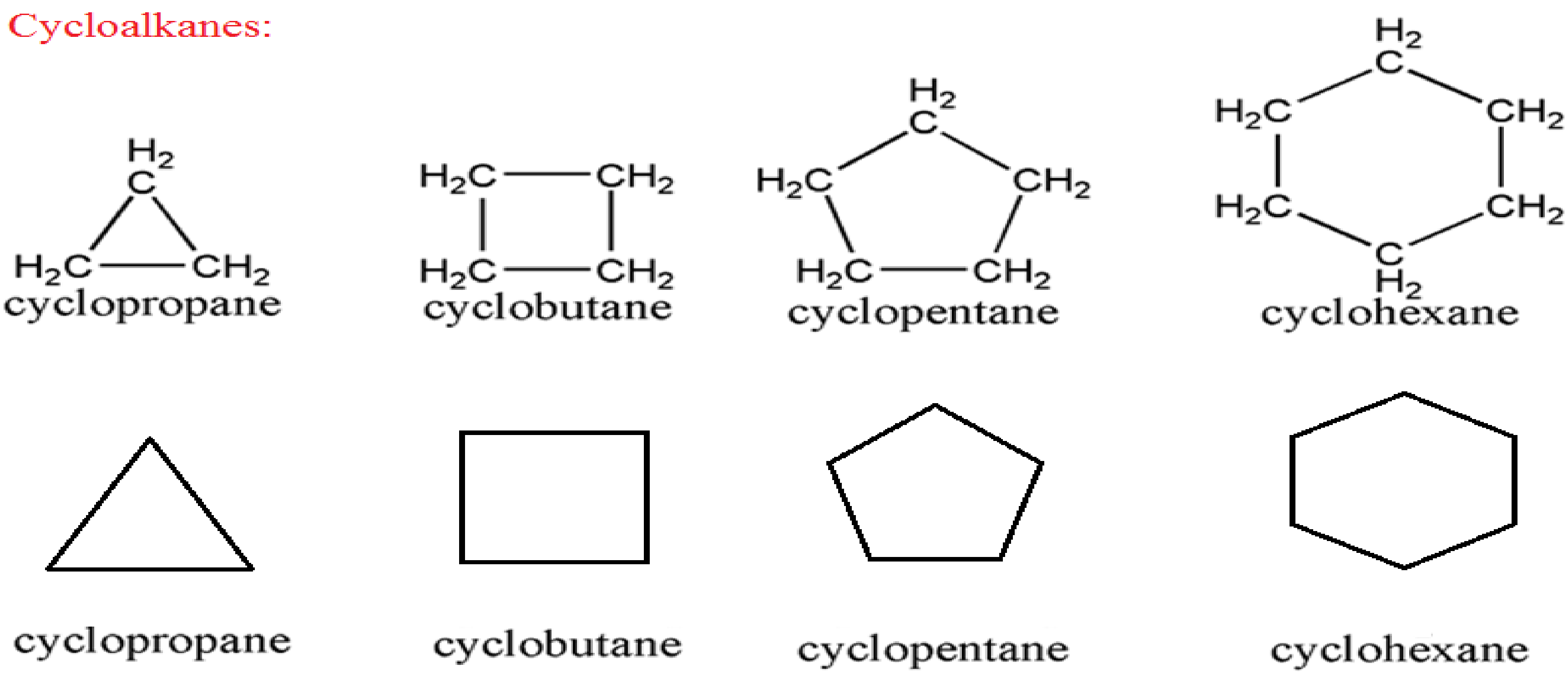


cyclopropane



cyclohexane

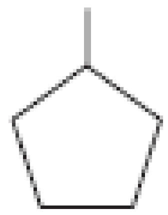
Alkanes and cycloalkanes are so similar that many of their properties can be considered side by side. Some differences remain. However, certain structural features arise from the rings of cycloalkanes.



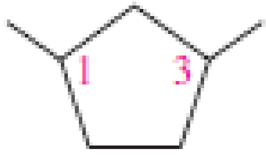
Monocyclic alkane compounds (substituted):

- Naming substituted cycloalkanes is as follow:

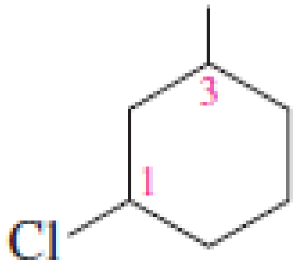
We name them as ***alkyl-cycloalkanes*** *and* ***halo-cycloalkanes***, and so on. If only one substituent is present, it is not necessary to *designate its position*. When two substituents are present, we number the ring beginning with the substituent first in the *alphabet and number in the direction that gives the next substituent the* ***lower*** *number possible.*



Methylcyclopentane

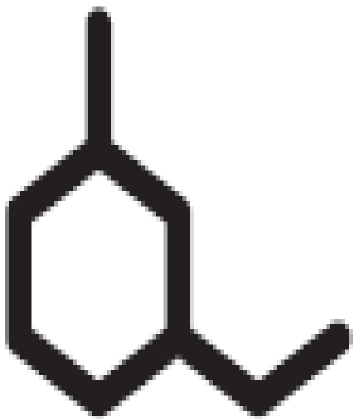


1,3-Dimethylcyclopentane

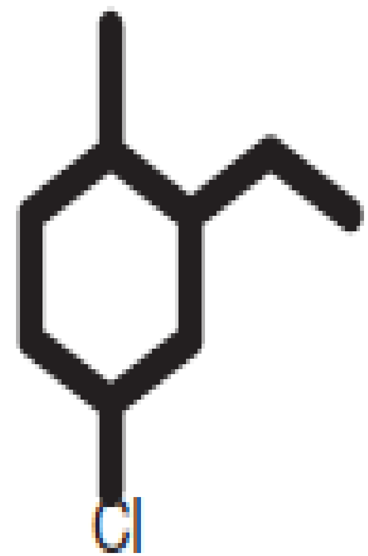


1-Chloro-3-methylcyclohexane

When three or more substituents are present, we begin at the substituent that leads to the ***lowest set of locants***:



1-Ethyl-3-methylcyclohexane
(*not* 1-ethyl-5-methylcyclohexane)

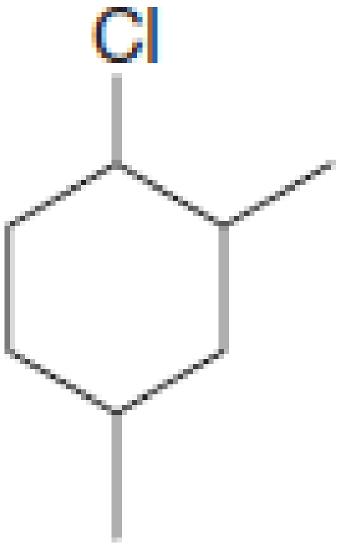


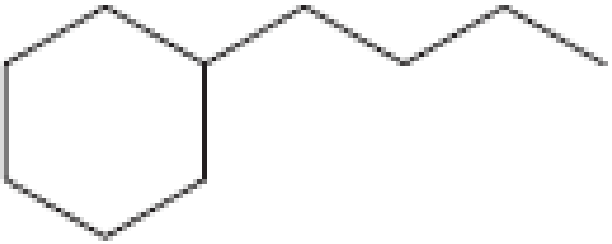
4-Chloro-2-ethyl-1-methylcyclohexane
(*not* 1-chloro-3-ethyl-4-methylcyclohexane)

When a single ring system is attached to a single chain with a ***greater number*** of carbon atoms, or when more than one ring system is attached to a single chain, then it is appropriate to name the compounds as ***cycloalkylalkanes***. For example,

1-Cyclobutylpentane

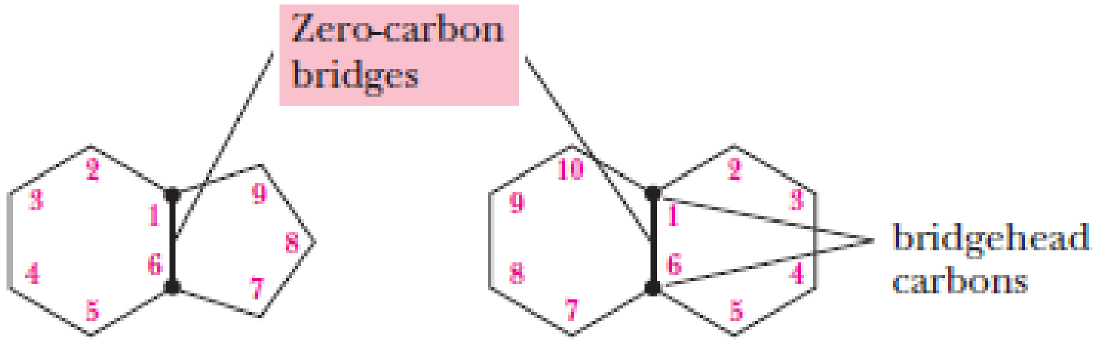
Q: Give names for the following substituted alkanes:





Bicycloalkanes:

An alkane that contains two rings that share two carbon atoms is classified as a **bicycloalkane**. The shared carbon atoms are called **bridgehead carbons**, and the carbon chain connecting them is called a **bridge.**



Bicyclo[4.3.0]nonane (Hydrindane)   Bicyclo[4.4.0]decane (Decalin)

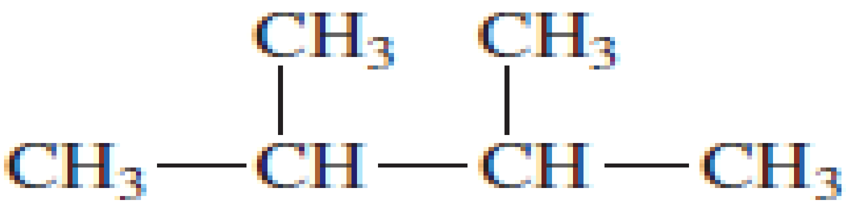
Homework:

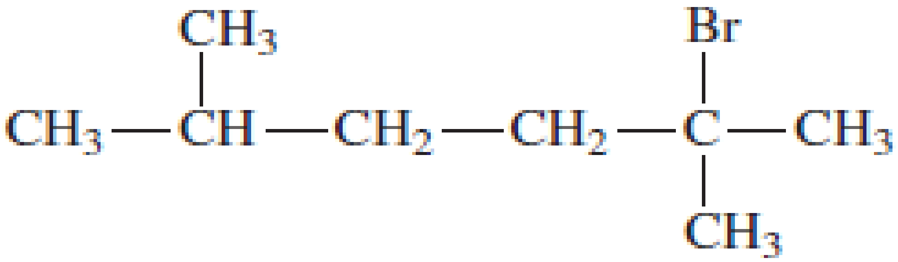
1- Draw the condensed structural formula and give the name for the following skeletal formula:

2- Identify primary, secondary and tertiary hydrogen atoms in the following structures of alkanes:

$CH_3CH_2CH_2CH_3$ $CH_3CH_2CH_3$

3- Give IUPAC naming for the following compound?





References:

1. Organic chemistry by morrison and boyd.
2. Organic chemistry by solomon and fryhl, 10th Edition, 2011.