IUPAC nomenclature

STRUCTURAL REPRESENTATION OF ORGANIC COMPOUNDS

Complete, condensed and bond line structural formulas

- Organic compounds structures are represented in several ways.

1. The *Lewis structure or dot structure, dash structure,* condensed structure and bond line structural formulas are some of the specific types.
2. The Lewis structures, however, can be simplified by representing the two-electron covalent bond by a dash (–).

These structures can also be represented by the following ways

$CH_3\ CH_3$ H_2C $H_2C\ HC\ HC$

Ethane Ethene

organic chemists use another way of representing the structures, in which only lines are used. In this bond-line structural representation of organic compounds, carbon and hydrogen atoms are not shown and the lines representing carbon-carbon bonds are drawn in a zig-zag fashion.

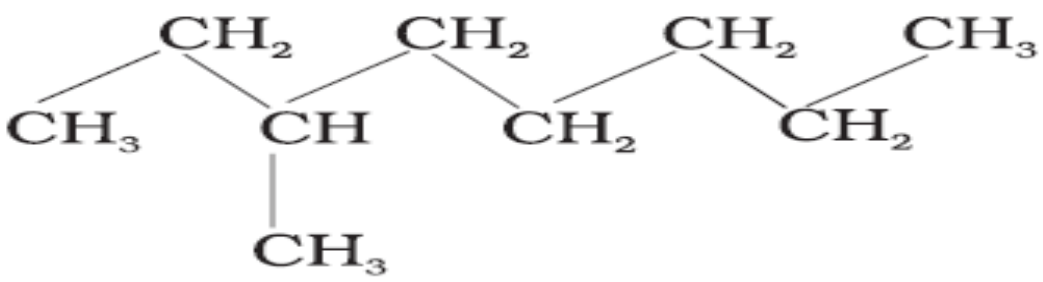
For example

3-Methyloctane can be represented in various forms as:

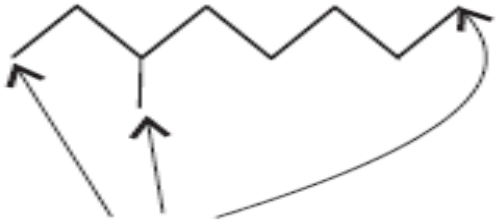
i) $CH_3CH_2CHCH_2CH_2CH_2CH_2CH_3$

CH_3

(b)

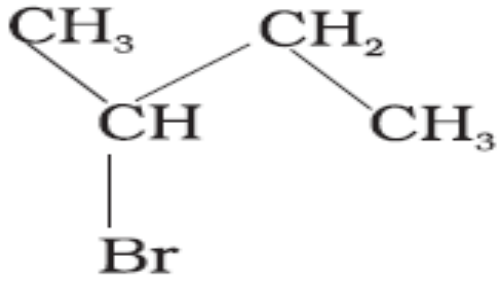


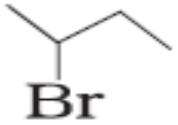
(c)



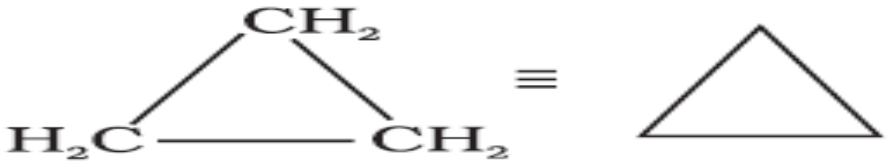
Terminals represent methyl group

(ii) Various ways of representing 2-bromo butane are:

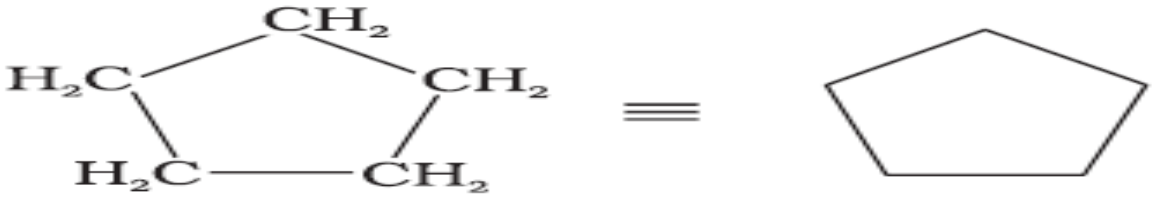
(a) $CH_3CHBrCH_2CH_3$ (b) 

(c) 

In cyclic compounds, the bond-line formulas may be given as follows:



Cyclopropane



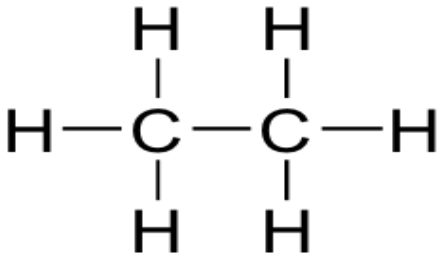
Cyclopentane

chlorocyclohexane

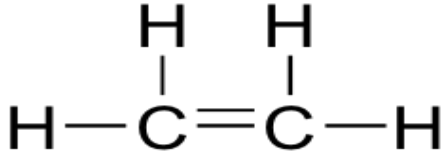
Thus, ethane (C_2H_6), ethene (C_2H_4), ethyne (C_2H_2)

Such structural representations are called

complete structural formula



eth**ane**
(an alk**ane**)



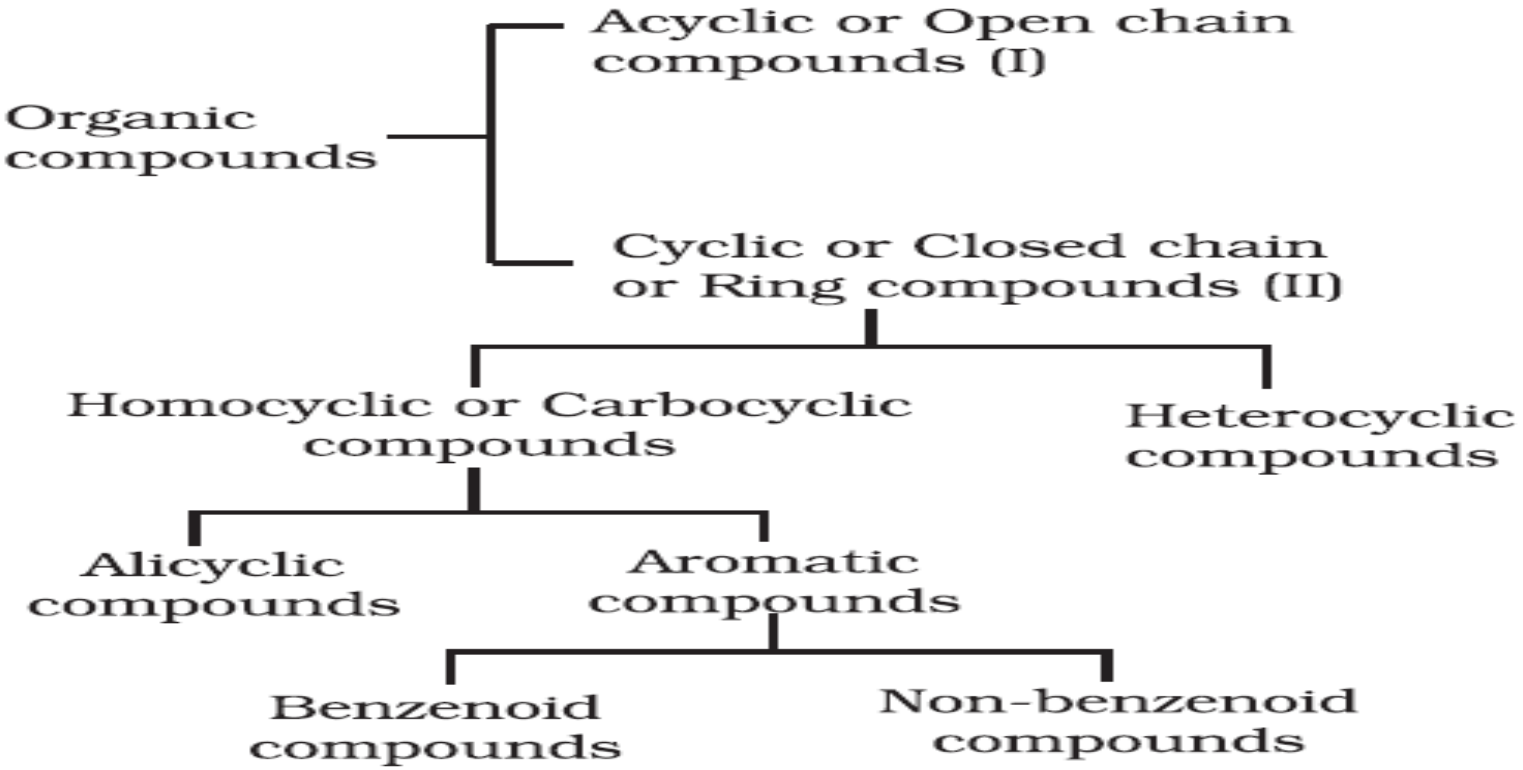
eth**ene**
(an alk**ene**)

eth**yne**
(an alk**yne**)

Common or Trivial Names of Some Organic Compounds

Compound	Common name
CH_4	Methane
$H_3CCH_2CH_2CH_3$	*n*-Butane
$(H_3C)_2CHCH_3$	Isobutane
$(H_3C)_4C$	Neopentane
$H_3CCH_2CH_2OH$	*n*-Propyl alcohol
$HCHO$	Formaldehyde
$(H_3C)_2CO$	Acetone
$CHCl_3$	Chloroform
CH_3COOH	Acetic acid
C_6H_6	Benzene
$C_6H_5OCH_3$	Anisole
$C_6H_5NH_2$	Aniline
$C_6H_5COCH_3$	Acetophenone
$CH_3OCH_2CH_3$	Ethyl methyl ether

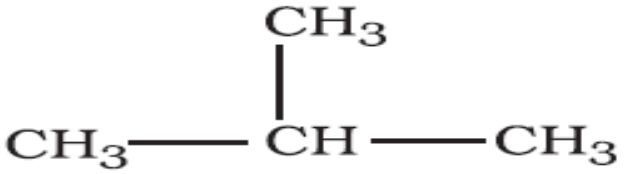
CLASSIFICATION OF ORGANIC COMPOUNDS



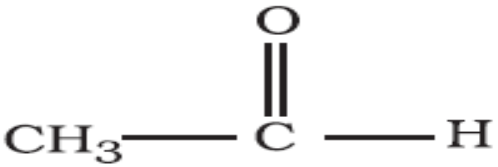
Acyclic or open chain compounds

These compounds are also called as **aliphatic** compounds and consist of straight or branched chain compounds, for example:

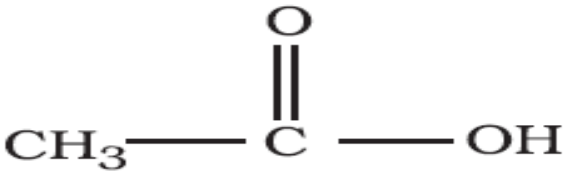
Ethane



Isobutane



Acetaldehyde

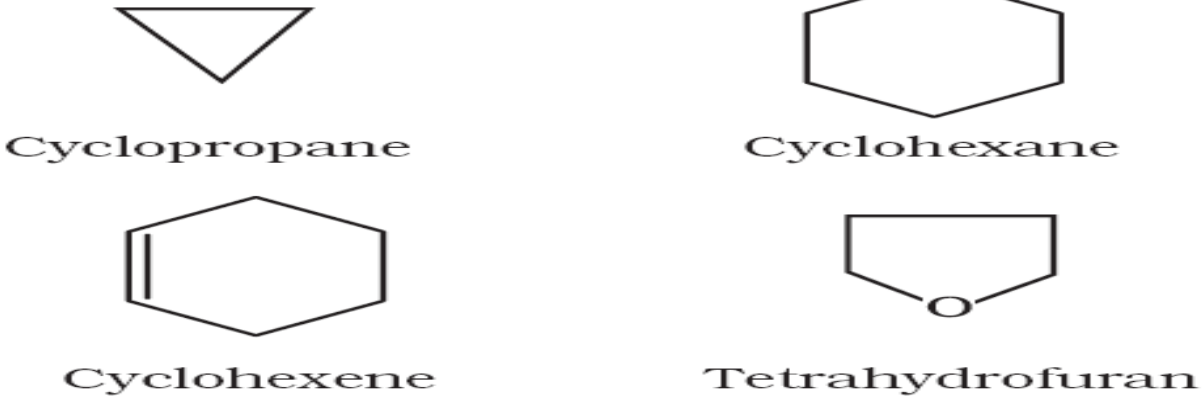


Acetic acid

Alicyclic or closed chain or ring compounds

Alicyclic (aliphatic cyclic) compounds contain carbon atoms joined in the form of a ring (homocyclic). Sometimes atoms other than carbon are also present in the ring (heterocylic).

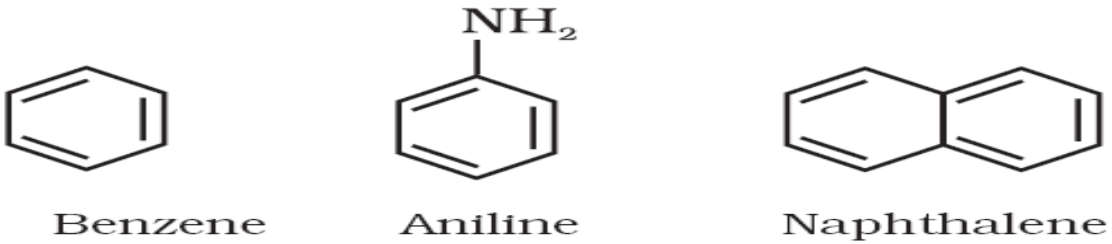
Some examples are



Aromatic compounds

Aromatic compounds are special types of compounds. These include benzene and other related ring compounds (benzenoid).

Benzenoid aromatic compounds

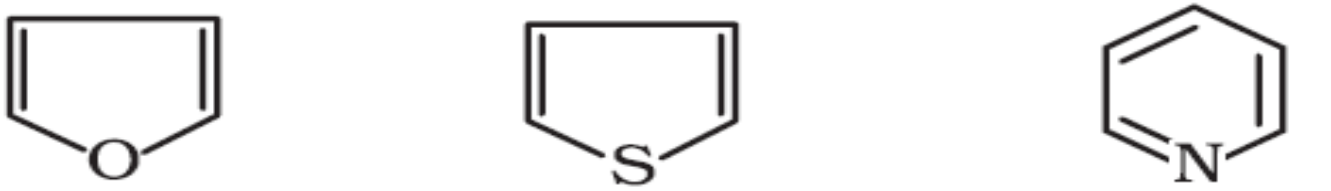


Benzene Aniline Naphthalene

Non-benzenoid compound

Tropolone

Heterocyclic aromatic compounds



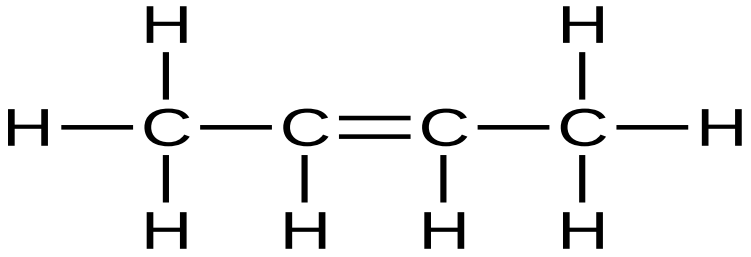
Furan Thiophene Pyridine

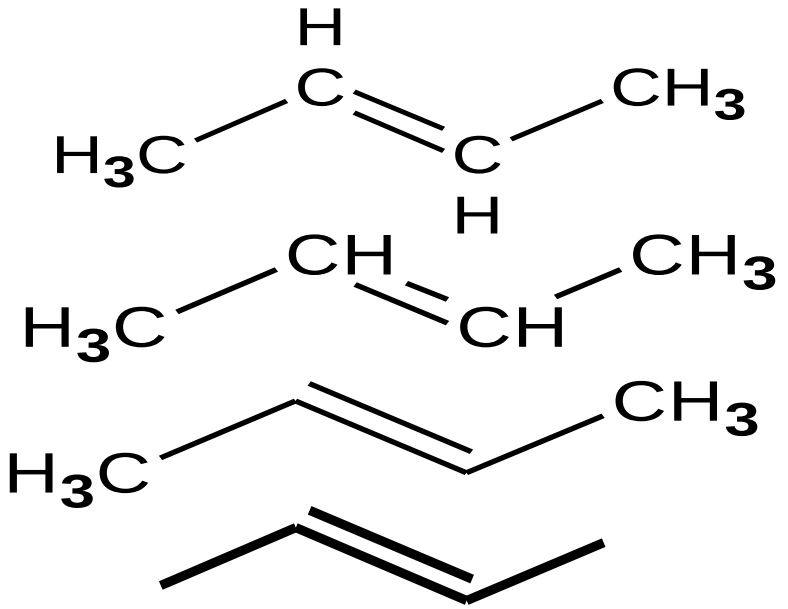
NOMENCLATURE OF ORGANIC COMPOUNDS

In order to clearly identify compound, a systematic method of naming has been developed and is known as the **IUPAC (International Union of Pure and Applied Chemistry) system of nomenclature.**

Drawing bondline Structures:

2-butene





$H_3C-CH=CH-CH_3$

Draw the condensed structure for the above !”

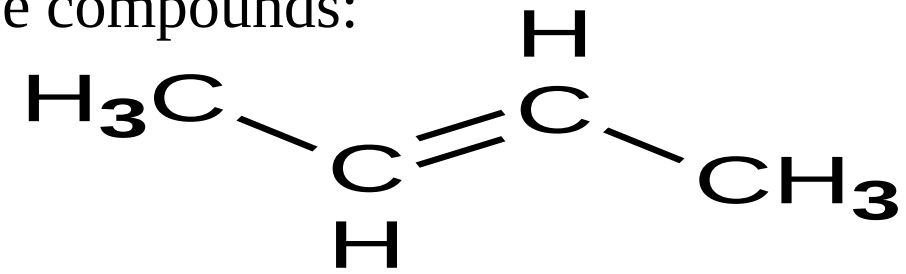
On a test, choose a method that shows all H’s

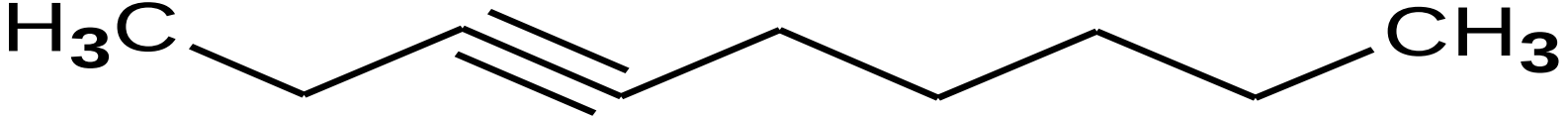
Using brackets can also shorten some formulas:

$CH_3CH_2CH_2CH_2CH_2CH_3$ vs. $CH_3(CH_2)_4CH_3$

TRY THESE

1. What are the 3 classes of hydrocarbons, based on number of carbon-carbon bonds?
2. Give the 10 organic homologous prefixes, in order, from 1-10.
3. Name these compounds:

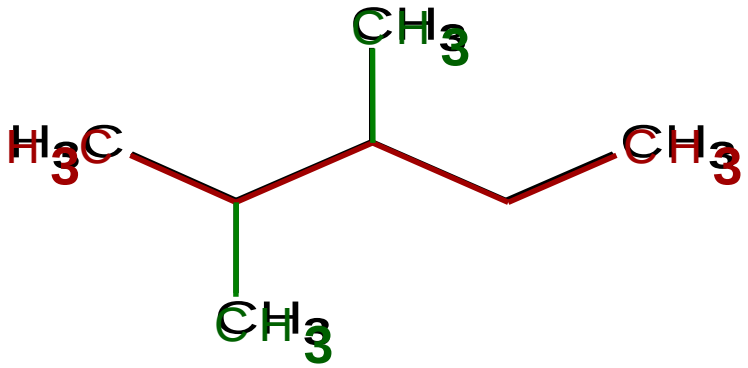




Naming Side Chains

- The names of molecules with branches are based on: side chains, root

  2,3-dimethylpentane



- The “root” or “parent chain” is usually the longest possible hydrocarbon chain.
- The root must include multiple bonds if they are present. If a cyclic structure is present it will be the root even if it is not the longest chain.
- Side chains are also called “side branches” or “alkyl groups”. Their names end in -yl.

<u>Common side chains</u> :

-CH_3 methyl, -CH_2CH_3 ethyl, -$CH_2CH_2CH_3$ propyl

IUPAC Rules for Naming Hydrocarbons

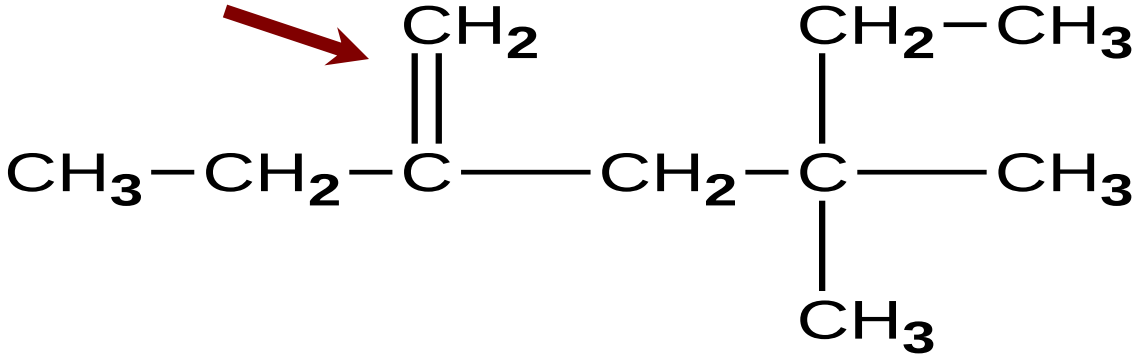
1. Choose the correct ending: -ane, -ene, or -yne
2. Determine the longest carbon chain. Where a double or triple bond is present, choose the longest chain that includes this bond. If there is a cyclic structure present, the longest chain starts and stops within the cyclic structure.
3. Assign numbers to each C of the parent chain. For alkenes and alkynes the first carbon of the multiple bond should have the smallest number. For alkanes the first branch (or first point of difference) should have the lowest #. Carbons in a multiple bond must be numbered consecutively.
4. Attach a prefix that corresponds to the number of carbons in the parent chain. Add cyclo- to the prefix if it is a cyclic structure.

IUPAC Rules for Naming Hydrocarbons

5. Determine the correct name for each branch (“alkyl” groups include methyl, ethyl, propyl, etc.)
6. Attach the name of the branches alphabetically, along with their carbon position, to the front of the parent chain name. Separate numbers from letters with hyphens (e.g. 4-ethyl-2-methyldecane)
7. When two or more branches are identical, use prefixes (di-, tri-, etc.) (e.g. 2,4-dimethylhexane). Numbers are separated with commas. Prefixes are ignored when determining alphabetical order. (e.g. 2,3,5-trimethyl-4-propylheptane)
8. When identical groups are on the same carbon, repeat the number of this carbon in the name. (e.g. 2,2-dimethylhexane)

Naming Side Chains

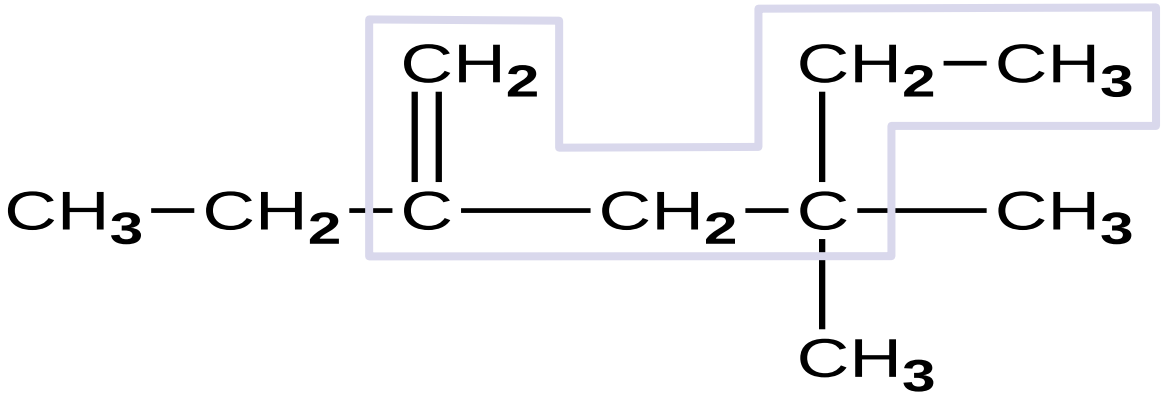
Example: use the rules on this handout to name the following structure



Rule 1: choose the correct ending

ene

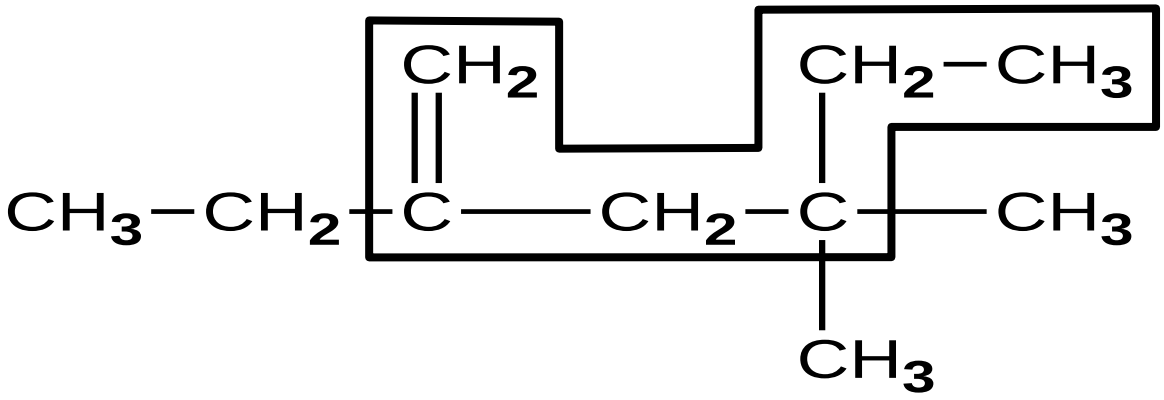
Naming Side Chains



Rule 2: determine the longest carbon chain

ene

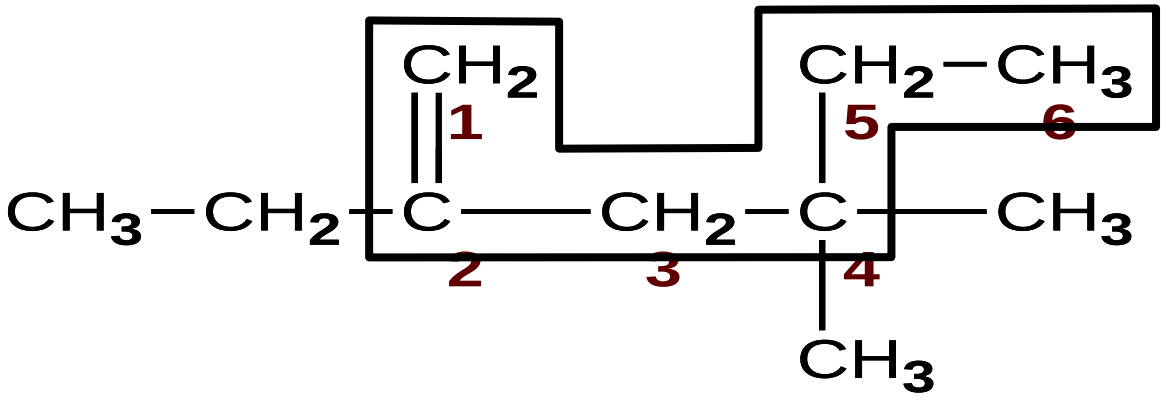
Naming Side Chains



Rule 3: Assign numbers to each carbon

ene

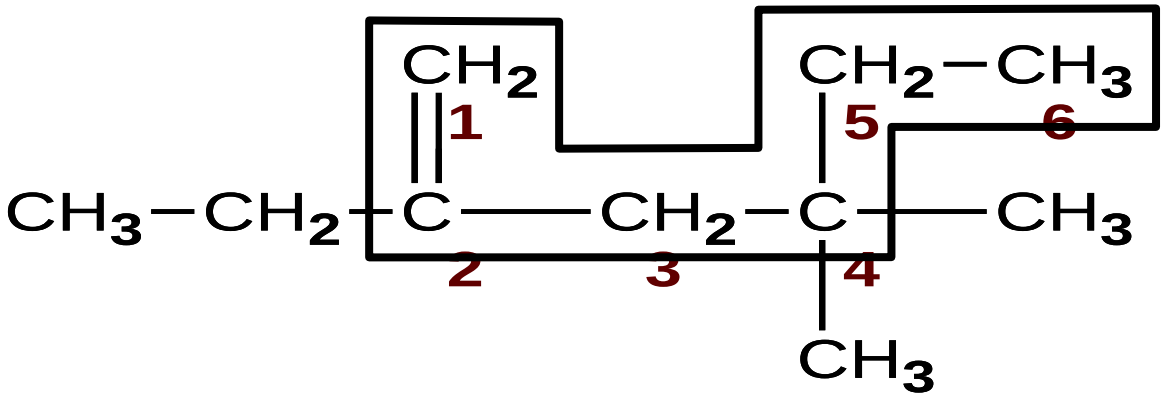
Naming Side Chains



Rule 3: Assign numbers to each carbon

ene

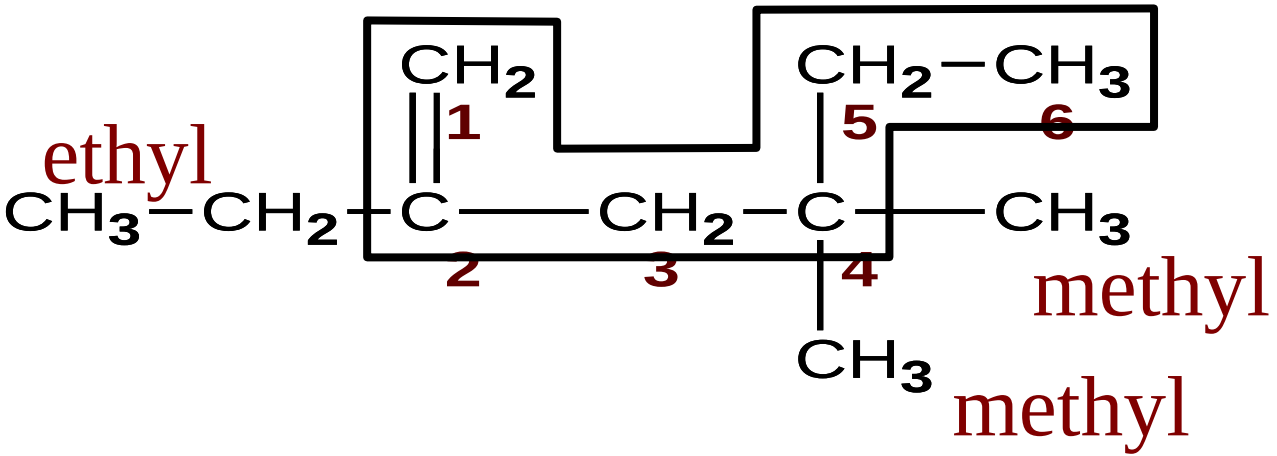
Naming Side Chains



Rule 4: attach prefix (according to # of Cs)

1-hexene

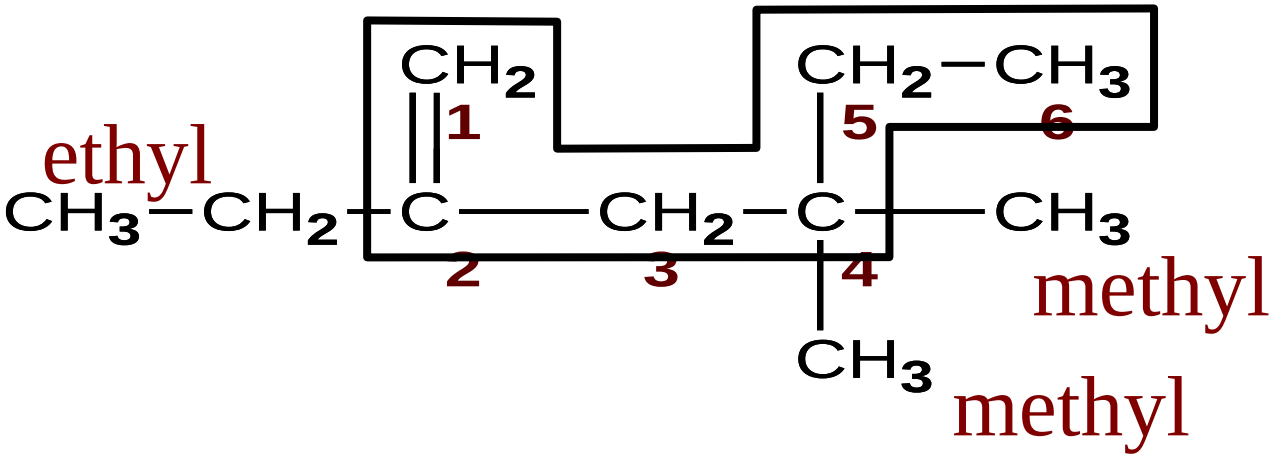
Naming Side Chains



Rule 6: attach name of branches alphabetically

2-ethyl-4-methyl-4-methyl-1-hexene

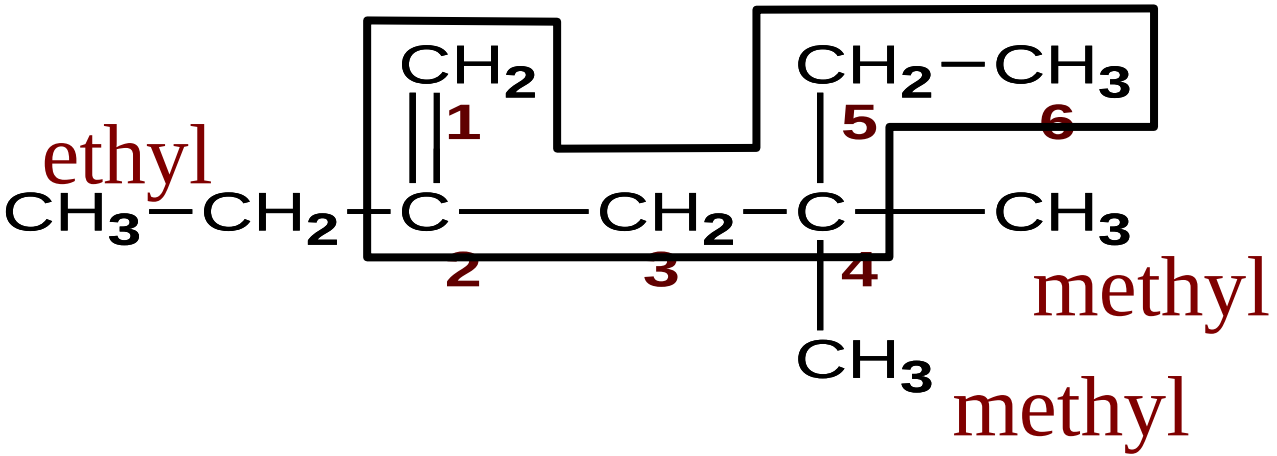
Naming Side Chains



Rule 7,8: group similar branches

2-ethyl-4-methyl-4-methyl-1-hexene

Naming Side Chains



Rule 7,8: group similar branches

2-ethyl-4,4-dimethyl-1-hexene

Rules for naming IUPAC compounds

- I. for branched chain alkanes:-

a) Identify the longest carbon chain

b) *When there are two or more parent chains of identical length, choose the parent chain with the greater number of substituents.*

c) Identify and name the substituent(s).

- **for One substituent** start numbering from the end that gives the substituent the lower number.

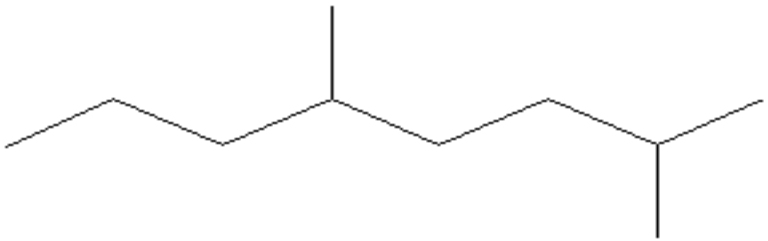
- **Two or more identical substituents**: number from the end that gives the lower number to the substituent encountered first.
- *The number of times the substituent occurs is indicated by a prefix di-, tri-, tetra-, penta-, hexa-, and so on.*
- *A comma is used to separate position numbers.*

- **Two or more different substituents**: list the substituents in alphabetical order and number from the end that gives the lower number to the substituent encountered first. If there are different substituents in equivalent positions at opposite ends of the parent chain, give the substituent of lower alphabetical order the lower number.
- *Prefixes such as di-, tri-, tetra-, penta-, hexa-, and so on are not included in alphabetizing.*

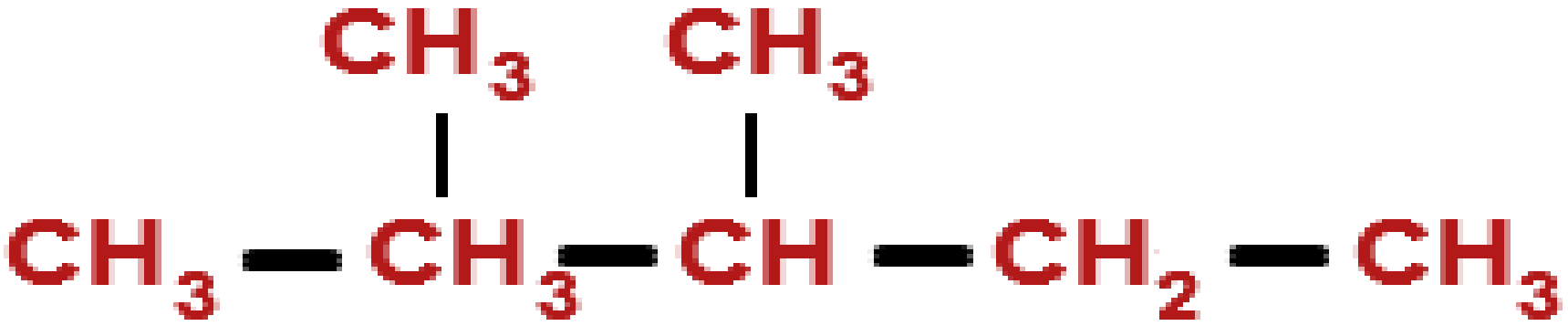
Draw the structures of the following compounds

- 1) hexanethioyl chloride
- 2) 3-methyl pent-i-oic acid
- Propane 1,2,3 tricarboxylic acid.
- Propane 1,2,3 trial

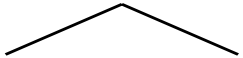
Name the following compounds

- 1) $CH_2=CH-CH=CH_2$
- 2) $HOCH_2(CH_2)_3CH_2COCH_3$
- 3) $CH_3CH(CH_3)CH_2CHCH_2$
- 4)$COOHCH_2CH_2CHCH_2CH_2COOH$
- 5) 

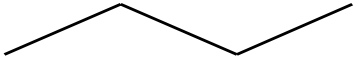
Name the following compound…..



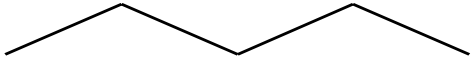
Alkane Nomenclature



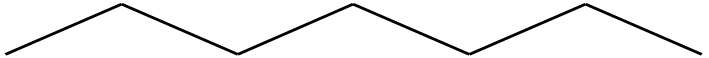
Propane



Butane



Pentane



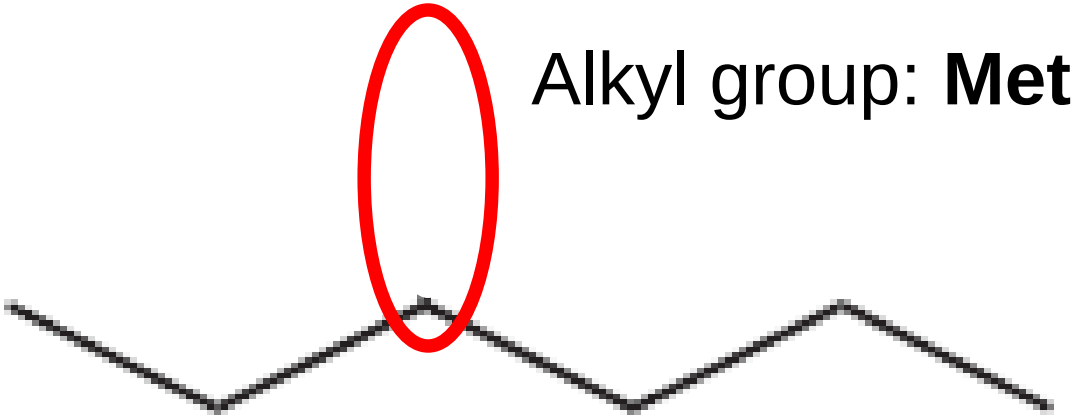
Heptane

- Condensed Structural Formula
- Actually Zig-Zag Structures
- All Carbons sp^3 Hybridized

Alkane Nomenclature

Name the smaller rows that branch off of the larger rows as if they were little independent alkanes of their own, better known as ***alkyl groups***.

Alkane Nomenclature



Alkyl group: **Methyl**

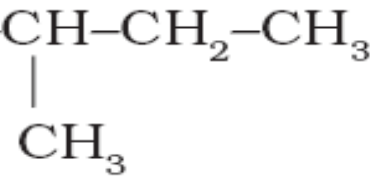
Hexane or n-hexane

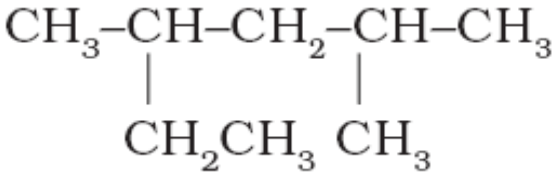
Alkyl Group Nomenclature

Unbranched Alkyl Groups

# C	Name	#C	Name
1	Methyl	11	Undecyl
2	Ethyl	12	Dodecyl
3	Propyl	13	Tridecyl
4	Butyl	14	Tetradecyl
5	Pentyl	15	Pentadecyl
6	Hexyl	16	Hexadecyl
7	Heptyl	17	Heptadecyl
8	Octyl	18	Octadecyl
9	Nonyl	19	Nonadecyl
10	Decyl	20	Eicosyl

Branched chain hydrocarbons: In a branched chain compound small chains of carbon atoms are attached at one or more carbon atoms of the parent chain. The small carbon chains (branches) are called alkyl groups.

(a) 

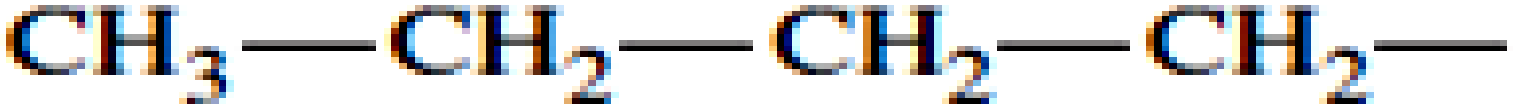
(b) 

In order to name such compounds, the names of alkyl groups are prefixed to the name of parent alkane. An alkyl group is derived from a saturated hydrocarbon by removing a
hydrogen atom from carbon. Thus, CH_4 becomes $-CH_3$ and is called *methyl group.*

Alkane Nomenclature

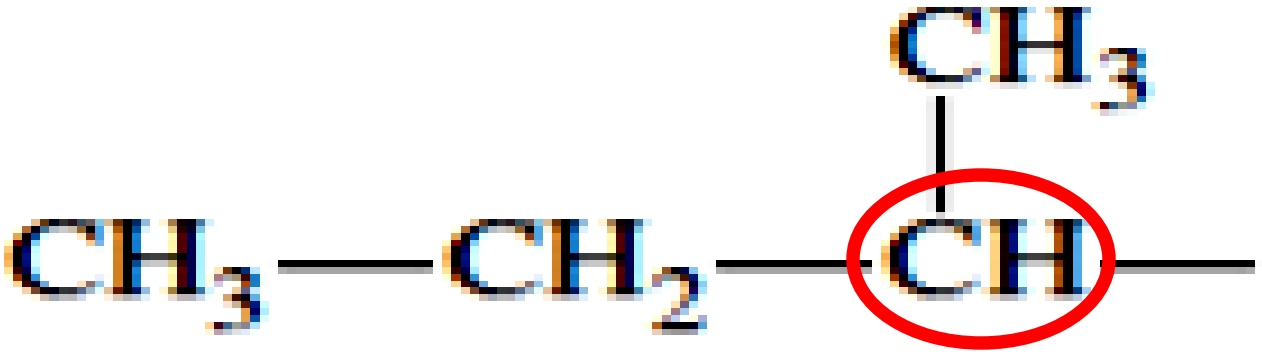
The carbons in an alkane are sometimes classified by how many ***other carbon atoms*** are stuck to them.

Alkane Nomenclature



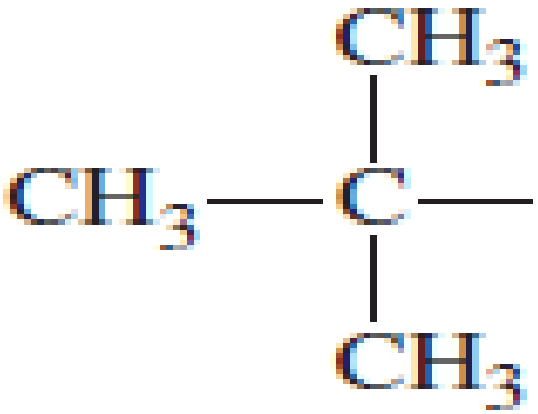
butyl group or *n*-butyl

Alkane Nomenclature



sec-butyl group

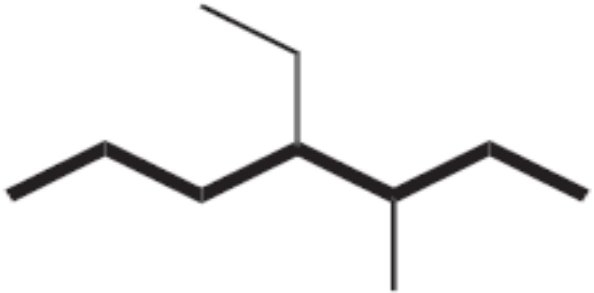
Alkane Nomenclature



tert-butyl group

Alkane Nomenclature: Rule 1

- The root name for an alkane is based on the longest unbroken chain of carbon atoms (called the “parent chain”).

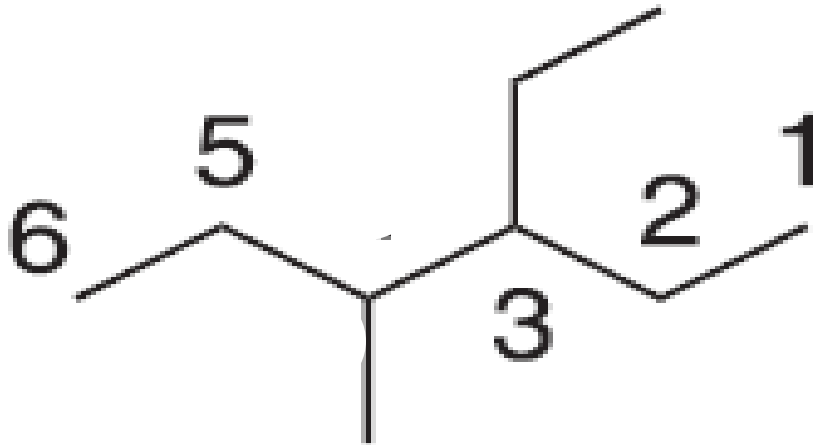


Derivative of **heptane**

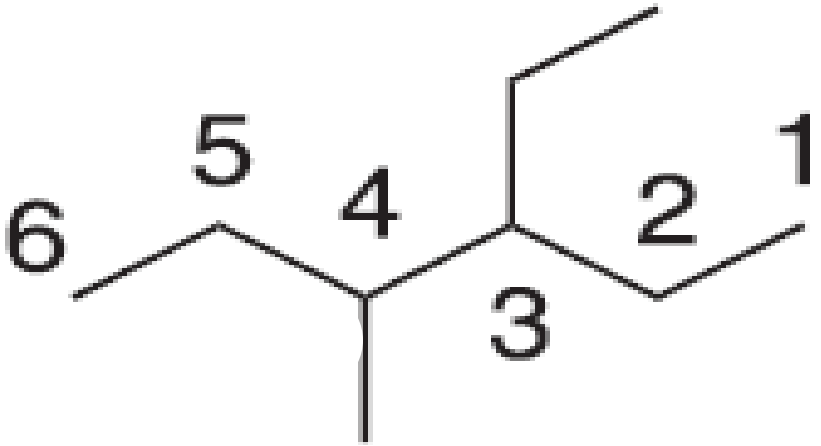
Alkane Nomenclature: Rule 1

When there are two longest chains of equal length, use the ***chain with the greater number of substituents*** as the main chain.

- Problem 3: Write the name of the compound.



answer

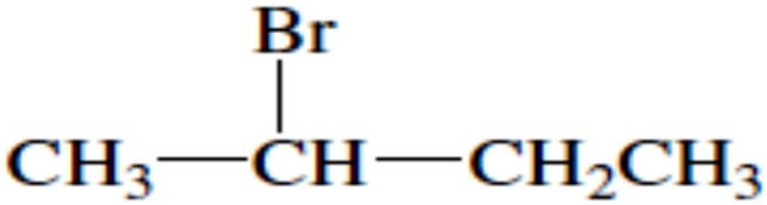


3-ethyl-4-methylhexane

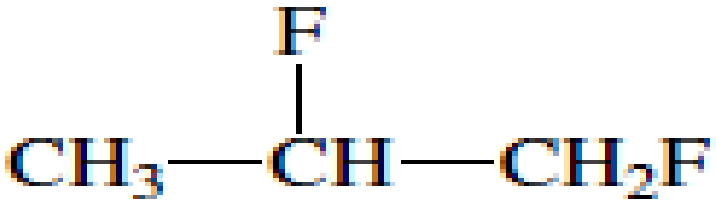
Haloalkanes

- Haloalkanes can be named just like alkanes, with the halogen atom treated as a substituent. Halogen substituents are named ***fluoro-, chloro-, bromo-,*** and ***iodo-.***
- When more than one halogen is present in the parent chain, they must be named ***alphabetically.***

Haloalkanes



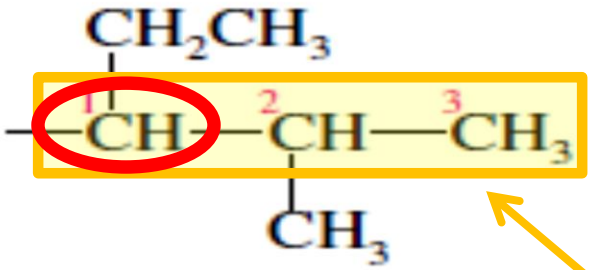
2-bromobutane



1,2-difluoropropane

Complex Substituents

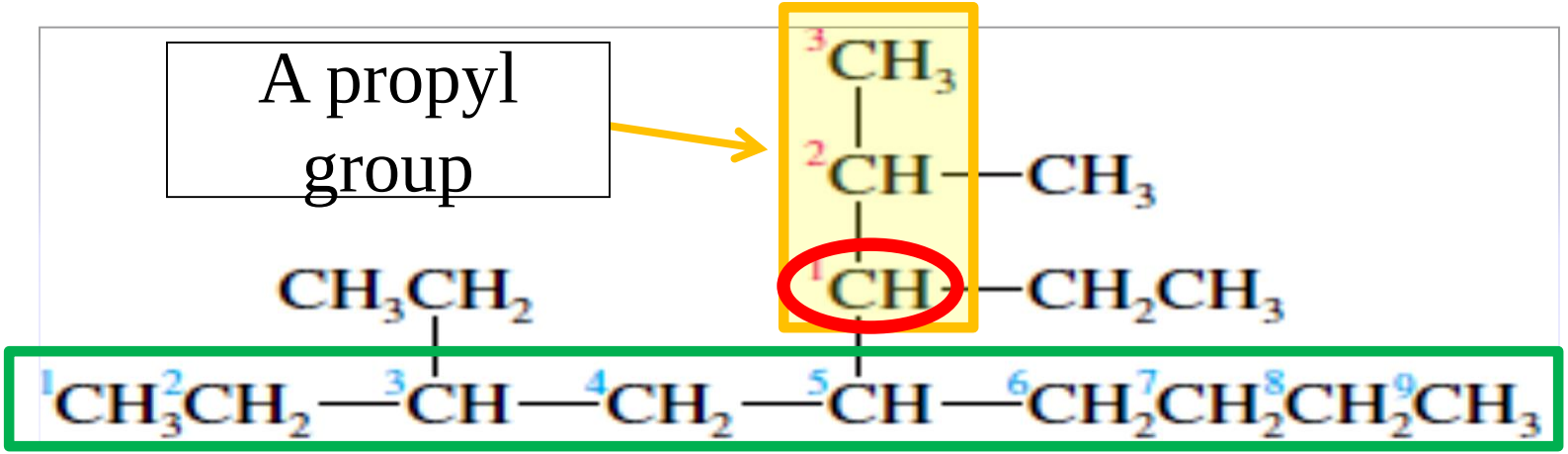
The substituents on the base alkyl group are listed with appropriate numbers, and ***parentheses*** are used to set off the name of the complex alkyl group.



A (1-ethyl-2-methylpropyl) group

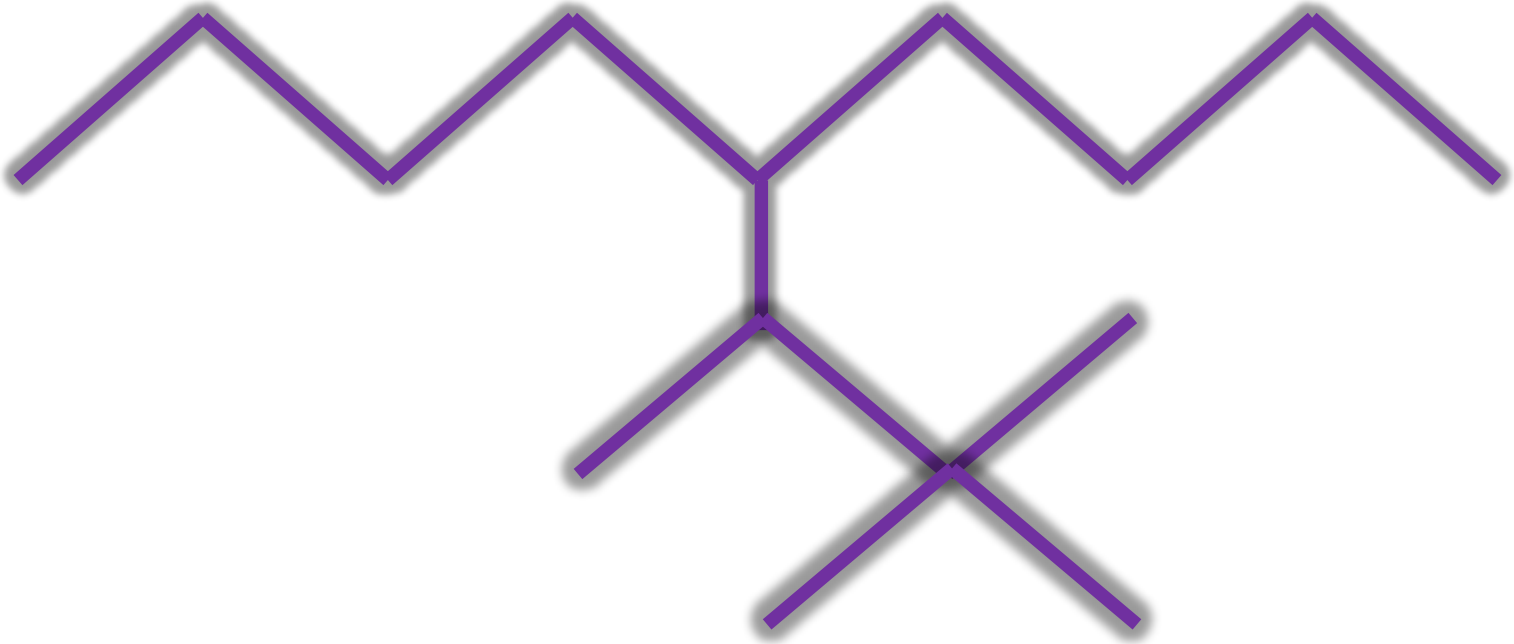
A propyl group

Complex Substituents

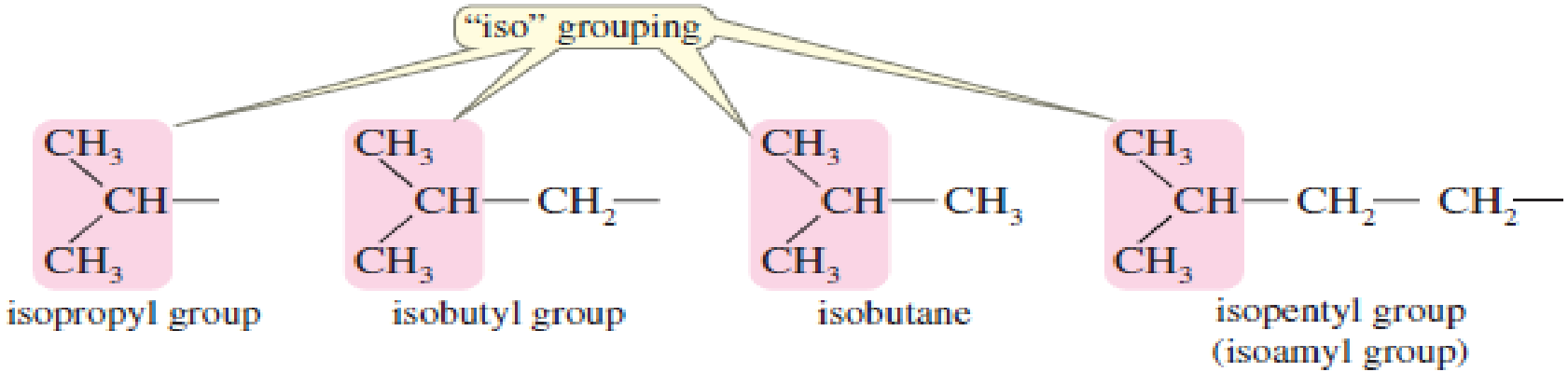


3-ethyl-5-(1-ethyl-2-methylpropyl)nonane

5-(1,2,2-trimethylpropyl)nonane



Alkane Nomenclature



Compounds containing polyfunctional groups

- Here a principle and a suboordinate functional group is taken.
- The choice of functional group is made out of the order of preference

The order of decreasing priority for some functional groups is: -COOH, $-SO_3H$, -COOR (R=alkyl group), COCl, $-CONH_2$, -CN,-HC=O, >C=O, -OH, -NH2, >C=C<, -C≡C- .

- Alkyl group , phenyl group halogens alkoxy group are always the prefixed substituents.

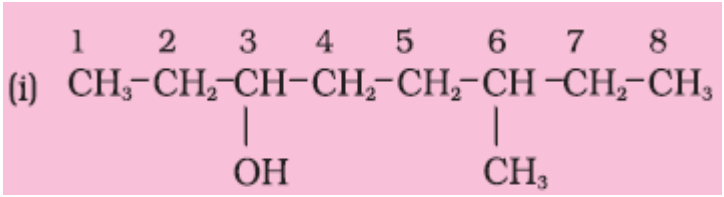
- Two or more identical groups are indicated by di, tri, tetra, etc.
- We represent an IUPAC name in the following way

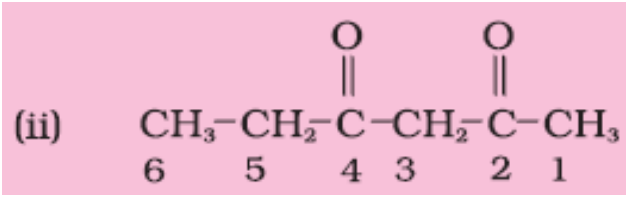
  prefix/ word root/ suffix
- “a” is added to the word root if the primary suffix is not added with a vowel.
- If “ene” if followed by y then the final “e” is cancelled

- If an unbranched carbon chain is directly linked to more than 2 like functional group , the organic compound is named as a derivative of the parent alkane which does not include the carbon atom of the functional group.

- Example pent-1,3,5 tricarboxylic acid.

Write the IUPAC names of the compounds from their given structures.

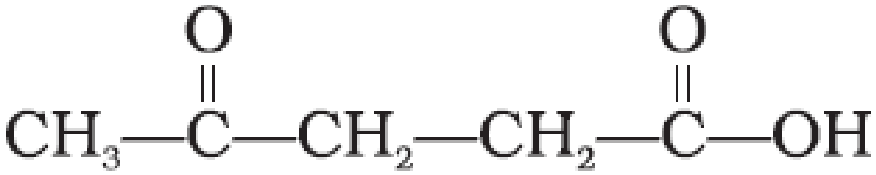
(i) 

(ii) 

6-Methyloctan-3-ol

Hexane- 2,4-dione

HW: Name the compound according to IUPAC system

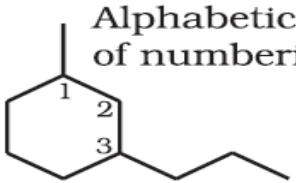


Cyclic compounds naming nomenclature

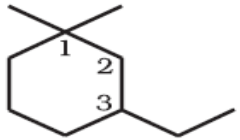
Cyclic Compounds: A saturated monocyclic :

Compound is named by prefixing '*cyclo' to the* corresponding straight chain alkane. If side chains are present, then the rules given above are applied. Names of some cyclic compounds
are given below.

Cyclopentane



1-Methyl-3-propylcyclohexane

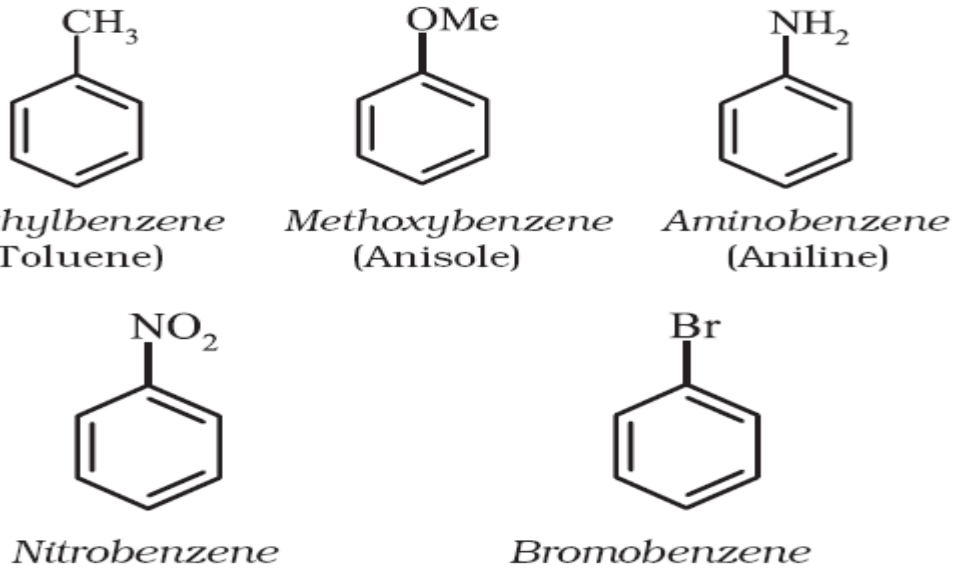


More branched carbon gets lower number

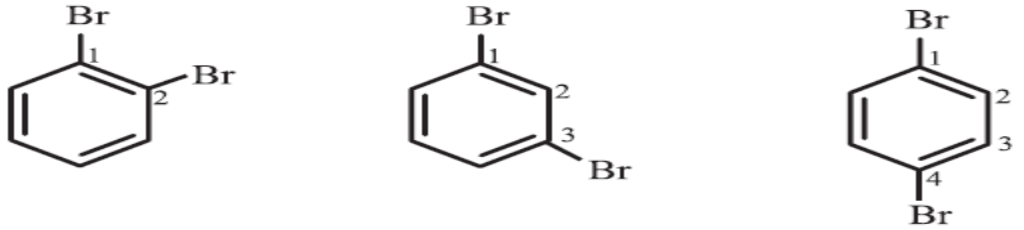
3-Ethyl-1,1-dimethylcyclohexane
(not 1-ethyl-3,3-dimethylcyclohexane)

Nomenclature of Substituted Benzene Compounds

For IUPAC nomenclature of substituted benzene compounds, the substituent is placed as prefix to the word *benzene as* shown in the following examples.



If benzene ring is disubstituted, the position of substituents is defined by numbering the carbon atoms of the ring such that the substituents are located at the lowest numbers possible.



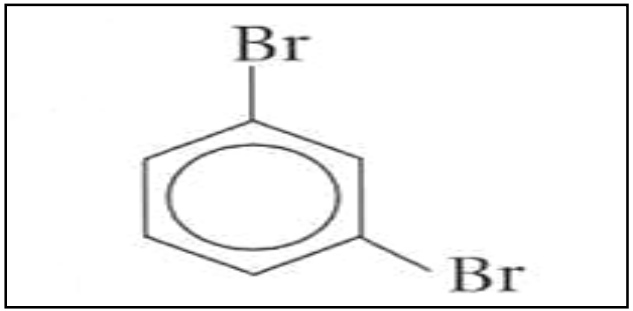
(a) 1,2-Dibromo-benzene

(b) 1,3-Dibromo-benzene

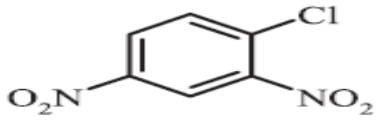
(c) 1,4-Dibromo-benzene

In the trivial system of nomenclature the terms *ortho (o), meta (m) and para (p) are used* as prefixes to indicate the relative positions 1,2- ;1,3- and 1,4- respectively.

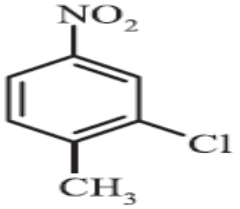
- *Draw the structural formula for 1,3-dibromobenzene.*



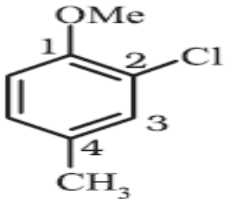
- Substituent of the base compound is assigned number1 and then the direction of numbering is chosen such that the next substituent gets the lowest number. The substituents appear in the name in alphabetical order.

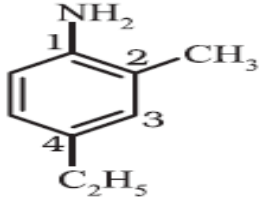


1-Chloro-2,4-dinitrobenzene
(not 4-chloro,1,3-dinitrobenzene)

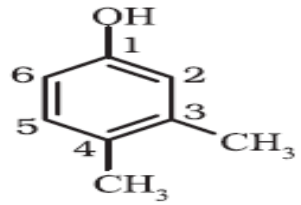


2-Chloro-1-methyl-4-nitrobenzene
(not 4-methyl-5-chloro-nitrobenzene)





2-Chloro-4-methylanisole *4-Ethyl-2-methylaniline*



3,4-Dimethylphenol