Organic chemistry

1st stage
2nd course
Part 1

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Introduction

- According to chemical literature, there are more than 60 million known organic compounds.
- Each compound has its own physical properties, such as melting point for solids, and boiling point for liquid.
- Each compound has its own chemical reactivity.

introduction

- Organic compounds can be classified into **families** according to their **structural features**.
- The members of each family often **have similar chemical behavior**.
- The structural features that make it possible to classify compounds called **functional groups**.
- **Functional group** is an atom or a group of atoms with characteristic chemical and physical properties, it tend to be the reactive part of the molecule.

Hydrocarbon:

- **Hydrocarbons** are Certain compounds containing only two elements, hydrogen and carbon
- Hydrocarbons are divided into two main classes, **Aliphatic** and **Aromatic**.
- **Aliphatic hydrocarbons** are further divided in to families:
- Alkanes, alkenes, alkynes and their cyclic analogues (cycloalkanes, cycloalkenes and so on).

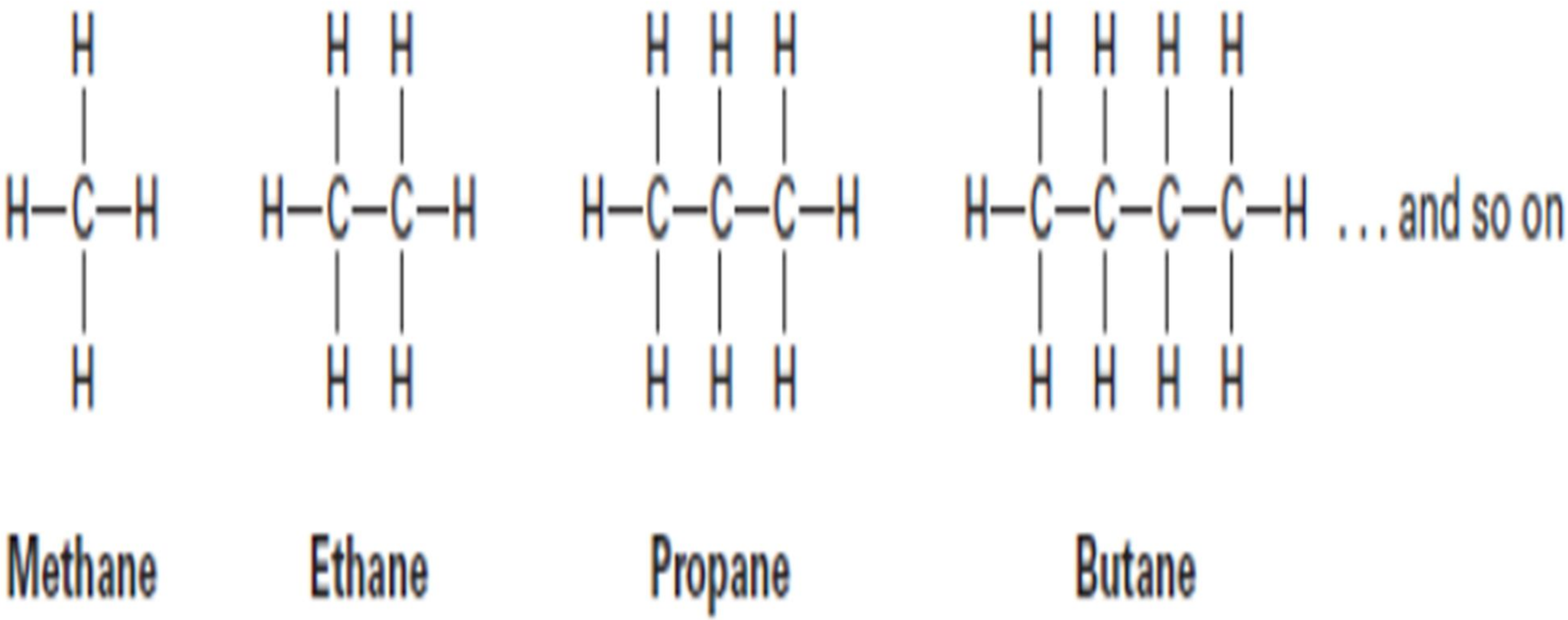
Hydrocarbons

- Aliphatic
  - **Alkanes**
  - **Alkenes**
  - **Alkynes**
  - **Cyclic Aliphatic**
- Aromatic

Alkanes

- **Alkanes** are the simplest family of molecules that contain the carbon– carbon single bond.
- Alkanes are often described as ***saturated hydrocarbons***.
- **hydrocarbons** because they contain only carbon and hydrogen,
- **saturated** because they have only C-C and C-H single bonds.
- They have the general formula $\mathbf{C_{\mathit{n}}H_{2\mathit{n}+2}}$, where ***n*** is an integer.
- Alkanes are also occasionally called **aliphatic** compounds.

Alkanes



Alkanes

- Think about the ways that carbon and hydrogen might combine to make alkanes. With one carbon and four hydrogen, only one structure is possible: methane, CH_4.
- Similarly, there is only one combination of two carbons with six hydrogens (ethane, CH_3CH_3).
- and only one combination of three carbons with eight hydrogens (propane, $CH_3CH_2CH_3$).
- However, When larger numbers of carbons and hydrogens combine more than one structure is possible.
- For example, there are ***two*** substances with the formula C_4H_{10} the four carbons can all be in a Straight row (butane), or they can be as a branch (isobutane).
- Similarly, there are three C_5H_{12} molecules, and so on for larger alkanes.

CH_4

Methane, CH_4

CH_3CH_3

Ethane, C_2H_6

$CH_3CH_2CH_3$

Propane, C_3H_8

$CH_3CH_2CH_2CH_3$

Butane, C_4H_{10}

$$\begin{array}{c} \quad CH_3 \\ \quad | \\ CH_3CHCH_3 \end{array}$$

Isobutane, C_4H_{10} (2-methylpropane)

$CH_3CH_2CH_2CH_2CH_3$

Pentane, C_5H_{12}

$$\begin{array}{c} \qquad CH_3 \\ \qquad | \\ CH_3CH_2CHCH_3 \end{array}$$

2-Methylbutane, C_5H_{12}

$$\begin{array}{c} CH_3 \\ | \\ CH_3CCH_3 \\ | \\ CH_3 \end{array}$$

2,2-Dimethylpropane, C_5H_{12}

- Compounds like butane and pentane, whose carbons are all connected in a row, are called **straight-chain alkanes**, or *normal alkanes.*
- Compounds like 2-methylpropane (isobutane), 2-methylbutane, and 2,2-dimethylpropane, whose carbon chains branch, are called **branched-chain alkanes**.
- Compounds like the two C_4H_{10} molecules and the three C_5H_{12} molecules, which have the same formula but different structures, are called *isomers.*
- **Isomers** are compounds that have the **same numbers** and **kinds** of atoms **but differ in the way the atoms are arranged**.
- Compounds like butane and isobutane, whose atoms are connected differently, are called **constitutional isomers**.

TABLE 3-2 Number of Alkane Isomers

Formula	Number of isomers
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4347
$C_{20}H_{42}$	366,319
$C_{30}H_{62}$	4,111,846,763

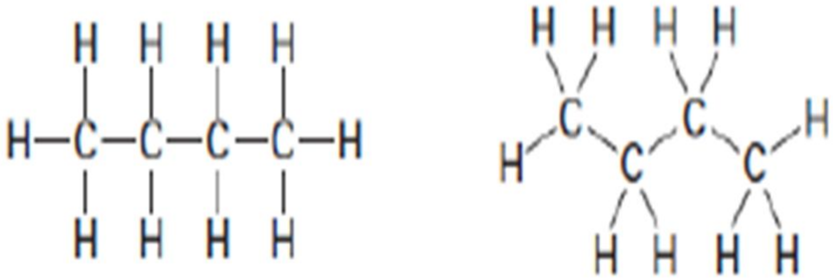
Alkanes

- **Constitutional isomers** are compounds that have the same molecular formula and different connectivity.
- Constitutional isomerism is not limited to alkanes it occurs widely throughout organic chemistry.
- Constitutional isomers may have different carbon skeletons (as in isobutane and butane), different functional groups (as in ethanol and dimethyl ether), or different locations of a functional group along the chain (as in isopropylamine and propylamine).
- constitutional isomers are always different compounds with different properties but with the same formula.

Different carbon skeletons C_4H_{10}	$\begin{array}{c} CH_3 \\ \vert \\ CH_3CHCH_3 \end{array}$ **2-Methylpropane (isobutane)**	and	$CH_3CH_2CH_2CH_3$ **Butane**
Different functional groups C_2H_6O	CH_3CH_2OH **Ethanol**	and	CH_3OCH_3 **Dimethyl ether**
Different position of functional groups C_3H_9N	$\begin{array}{c} NH_2 \\ \vert \\ CH_3CHCH_3 \end{array}$ **Isopropylamine**	and	$CH_3CH_2CH_2NH_2$ **Propylamine**

Alkanes

- given alkane can be drawn in many ways. For example, the straight chain, four-carbon alkane called butane can be represented by any of the structures shown in **Figure 3-2**.
- These structures don't imply any particular three-dimensional geometry for butane; they indicate only the connections among atoms. In practice, chemists rarely draw all the bonds in a molecule and usually refer to butane by the condensed structure, $CH_3CH_2CH_2CH_3$ or $CH_3(CH_2)_2CH_3$. Still more simply, butane can be represented as n-C_4H_{10}, where *n* denotes *normal* (straight-chain) butane.



$CH_3{-}CH_2{-}CH_2{-}CH_3$ $CH_3CH_2CH_2CH_3$ $CH_3(CH_2)_2CH_3$

Figure 3-2 some representations of butane, C_4H_{10}. The molecule is the same regardless of how it's drawn. These structures imply only that butane has a continuous chain of four carbon atoms; they do not imply any specific geometry.

Alkanes

- Straight-chain alkanes are named according to the number of carbon atoms they contain, as shown in **Table 3-3**.
- With the exception of the first four compounds (methane, ethane, propane, and butane) whose names have historical roots, the alkanes are named based on **Greek numbers**.
- The suffix -***ane*** is added to the end of each name to indicate that the molecule identified is an alkane.
- Thus, pent*ane* is the five-carbon alkane; hex*ane* is the six carbon alkane, and so on.
- We'll soon see that these alkane names form the basis for naming all other organic compounds, so at least the first ten should be memorized.

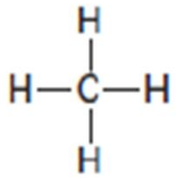
TABLE 3-3 Names of Straight-Chain Alkanes

Number of carbons (n)	Name	Formula (C_nH_{2n+2})	Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4	9	Nonane	C_9H_{20}
2	Ethane	C_2H_6	10	Decane	$C_{10}H_{22}$
3	Propane	C_3H_8	11	Undecane	$C_{11}H_{24}$
4	Butane	C_4H_{10}	12	Dodecane	$C_{12}H_{26}$
5	Pentane	C_5H_{12}	13	Tridecane	$C_{13}H_{28}$
6	Hexane	C_6H_{14}	20	Icosane	$C_{20}H_{42}$
7	Heptane	C_7H_{16}	30	Triacontane	$C_{30}H_{62}$
8	Octane	C_8H_{18}			

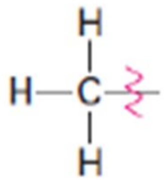
Alkyl Group

- If you imagine removing a hydrogen atom from an alkane, the partial structure that remains is called an **alkyl group**.
- Alkyl groups are not stable compounds themselves; they are simply parts of larger compounds.
- Alkyl groups are named by replacing the - *ane* ending of the parent alkane with an *-yl* ending.
- For example, removal of hydrogen from methane, CH_4, generates a *methyl* group, - CH3, and removal of hydrogen from ethane, CH_3CH_3, generates an *ethyl* group, - CH_2CH3. Similarly, removal of a hydrogen atom from the end carbon of any straight-chain alkane gives the series of straight-chain alkyl groups shown in **Table 3-4**.

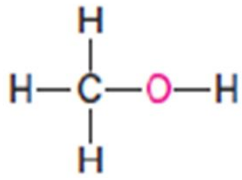
Combining an alkyl group with any of the functional groups listed earlier makes it possible to generate and name many thousands of compounds. For example:



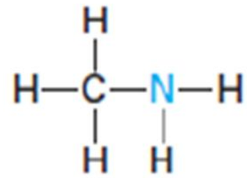
Methane



A methyl group



Methyl alcohol (methanol)



Methylamine

TABLE 3-4 Some Straight-Chain Alkyl Groups

Alkane	Name	Alkyl group	Name (abbreviation)
CH_4	Methane	$-CH_3$	Methyl (Me)
CH_3CH_3	Ethane	$-CH_2CH_3$	Ethyl (Et)
$CH_3CH_2CH_3$	Propane	$-CH_2CH_2CH_3$	Propyl (Pr)
$CH_3CH_2CH_2CH_3$	Butane	$-CH_2CH_2CH_2CH_3$	Butyl (Bu)
$CH_3CH_2CH_2CH_2CH_3$	Pentane	$-CH_2CH_2CH_2CH_2CH_3$	Pentyl, or amyl

Straight-Chain and Branched alkyl

- straight-chain alkyl groups are generated by removing hydrogen from an **end carbon**.
- branched alkyl groups are generated by removing a hydrogen atom from an **internal carbon.**
- Two alkyl groups can be generated from3 Carbon compound.
- four alkyl groups can be made from 4 carbon compounds as shown in **(Figure 3-3)**.

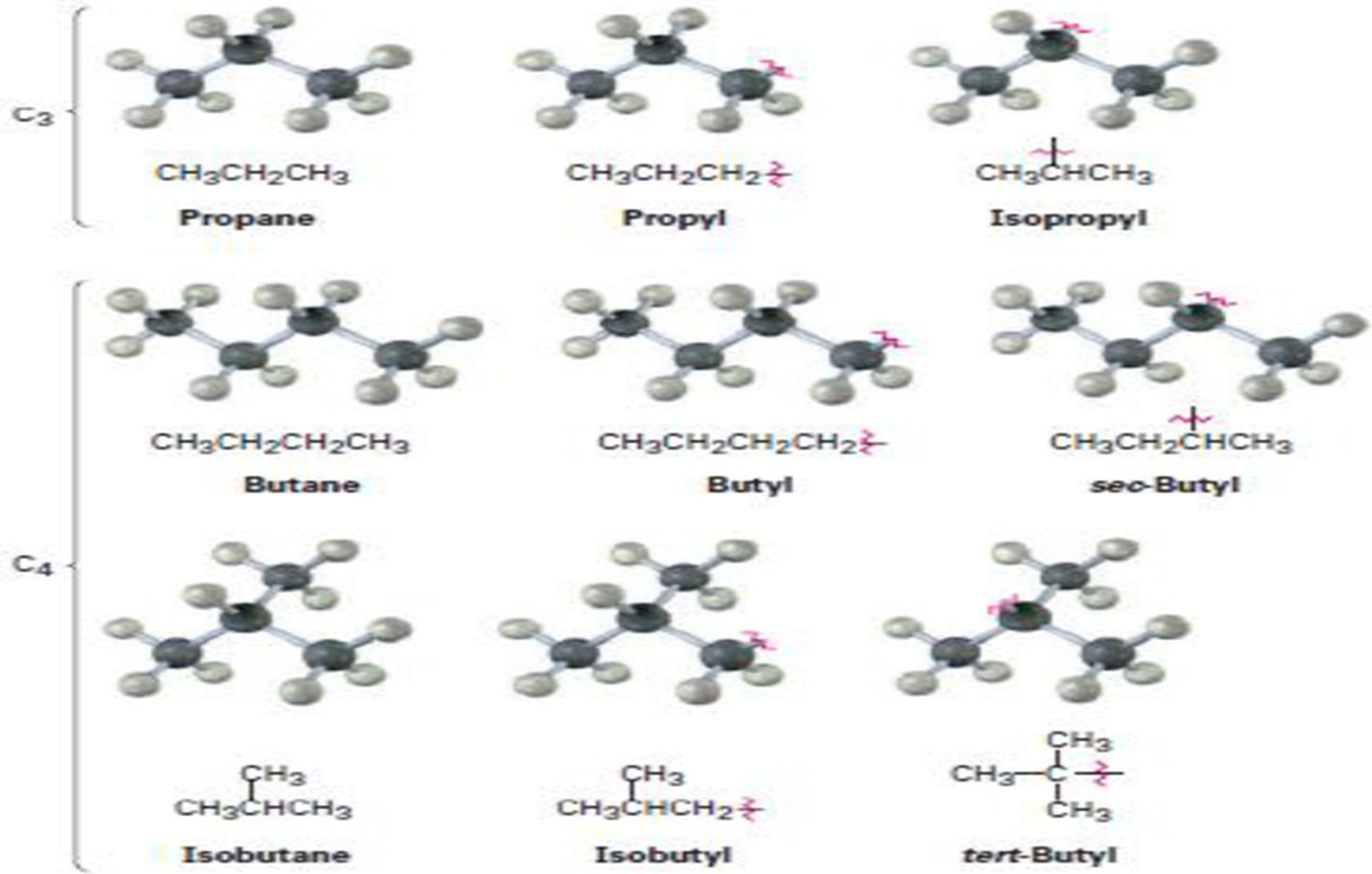
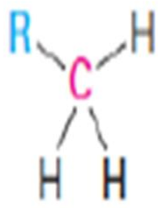


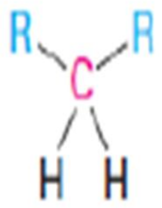
Figure 3-3 Alkyl groups generated from straight-chain alkanes.

Alkyl

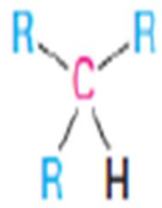
- One further comment about naming alkyl groups: the prefixes *sec*- (for secondary) and *tert*- (for tertiary) used for the C4 alkyl groups in Figure 3-3 refer to *the number of other carbon atoms attached to the branching carbon atom.*
- There are four possibilities: primary (1°), secondary (2°), tertiary (3°), and quaternary (4°).



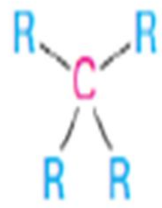
Primary carbon (1°)
is bonded to one
other carbon.



Secondary carbon (2°)
is bonded to two
other carbons.



Tertiary carbon (3°)
is bonded to three
other carbons.

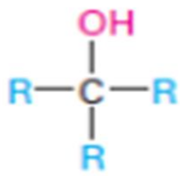


Quaternary carbon (4°)
is bonded to four
other carbons.

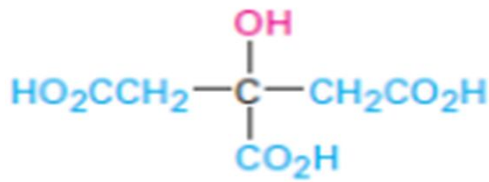
Alkyl

- The symbol **R** is used here and throughout organic chemistry to represent a *generalized* organic group.
- The R group can be methyl, ethyl, propyl, or any of a multitude of others.
- You might think of **R** as representing the **R**est of the molecule, which isn't specified.
- The terms *primary, secondary, tertiary,* and *quaternary* are routinely used in organic chemistry, and their meanings need to become second nature(Be familiar) . For example, if we were to say, ―Citric acid is a tertiary alcohol, we would mean that it has an alcohol functional group (-OH) bonded to a carbon atom that is itself bonded to three other carbons.

Alkyl

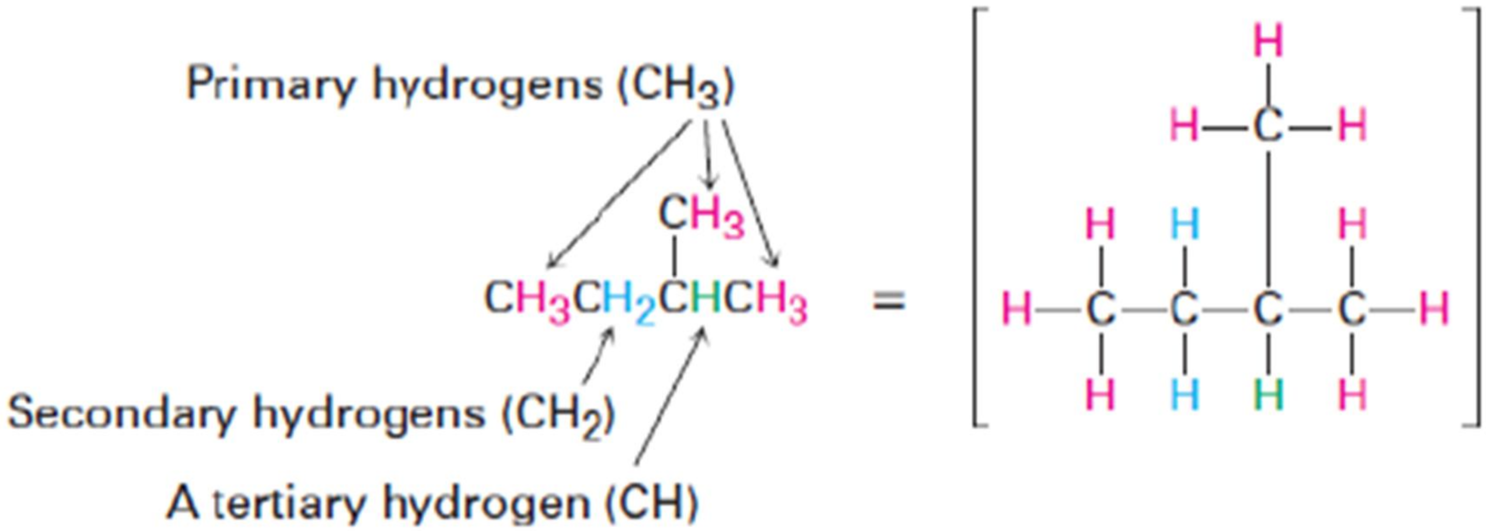


General class of tertiary alcohols, R_3COH



Citric acid—a specific tertiary alcohol

- In addition, we also speak of hydrogen atoms as being primary, secondary, or tertiary.
- Primary hydrogen atoms are attached to primary carbons (RCH3)
- secondary hydrogens are attached to secondary carbons (R2CH2)
- and tertiary hydrogens are attached to tertiary carbons (R3CH).
- There is, of course, no such thing as quaternary hydrogen.


Primary hydrogens (CH3)
CH3CH2CHCH3
CH3
Secondary hydrogens (CH2)
A tertiary hydrogen (CH)
=

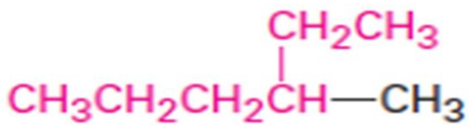
Naming of Alkanes(Nomenclature)

- A chemical name typically has four parts in the *IUPAC system of nomenclature*: prefix, parent, locant, and suffix.
- the prefix identifies the various **substituent** groups in the molecule
- the parent selects a main part of the molecule and tells how many carbon atoms are in that part
- the locants give the positions of the functional groups and substituents
- the suffix identifies the primary functional group.

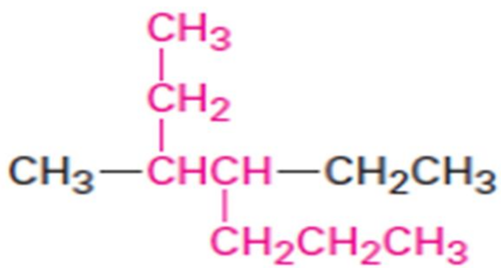
Naming of Alkanes(Nomenclature)

➢ **Step 1**

- **Find the parent hydrocarbon.**
- **(a)** Find the longest continuous chain of carbon atoms in the molecule, and use the name of that chain as the parent name. The longest chain may not always be apparent from the manner of writing; you may have to —turn corners.



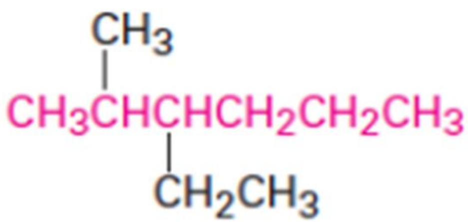
Named as a substituted hexane



Named as a substituted heptane

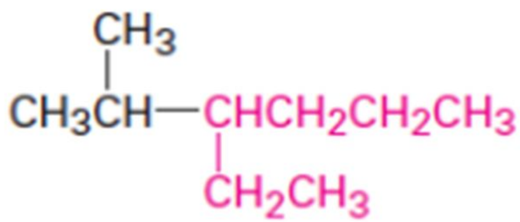
Naming Alkanes

- **(b)** If two different chains of equal length are present, choose the one with the larger number of branch points as the parent.



Named as a hexane with *two* substituents

NOT



as a hexane with *one* substituent

Naming Alkanes

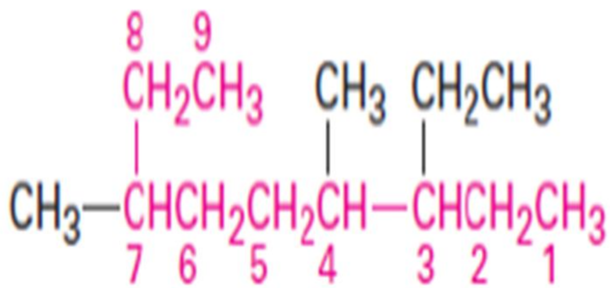
➢ **Step 2**

- **Number the atoms in the longest chain.**
- **(a)** Beginning at the end nearer the first branch point, number each carbon atom in the parent chain.

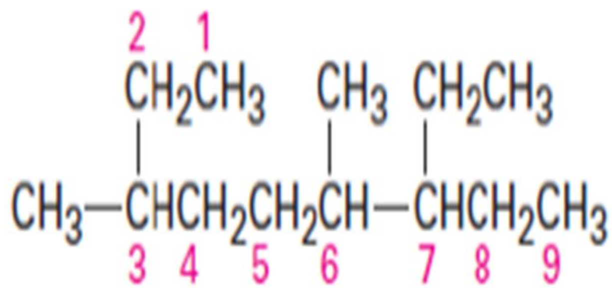
The first branch occurs at C3 in the proper system of numbering, not at C4.

Naming Alkanes

- **(b)** If there is branching an equal distance away from both ends of the parent chain, begin numbering at the end nearer the second branch point.



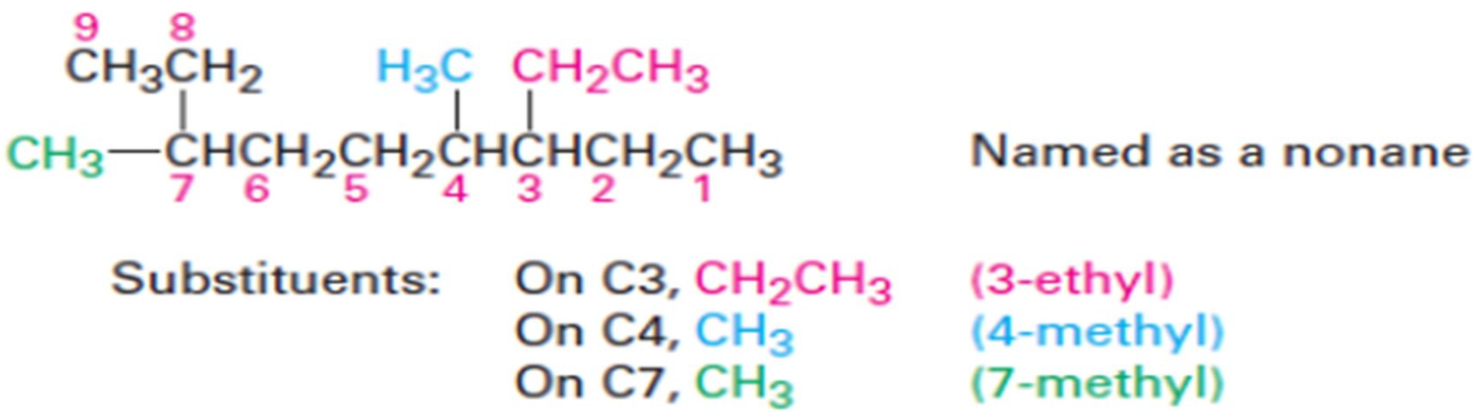
NOT



Naming Alkanes

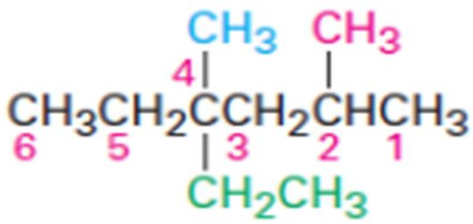
- **Step 3**

- **Identify and number the substituents.**
- **(a)** Assign a number, or *locant,* to each substituent to locate its point of attachment to the parent chain.



Naming Alkanes

- **(b)** If there are two substituents on the same carbon, give both the same number. There must be as many numbers in the name as there are substituents.



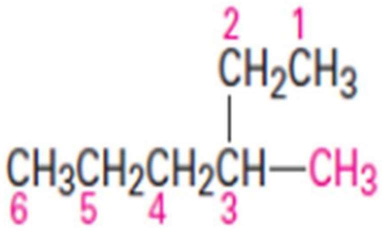
Named as a hexane

Substituents:	On C2, CH_3		(2-methyl)
	On C4, CH_3		(4-methyl)
	On C4, CH_2CH_3		(4-ethyl)

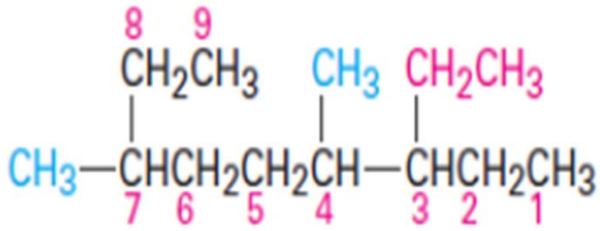
Naming Alkanes

➢ **Step 4**

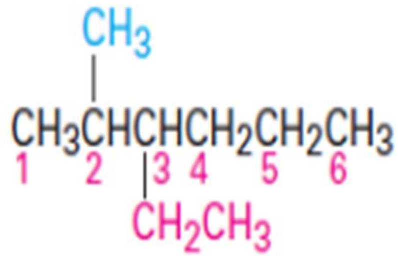
- **Write the name as a single word.**
- Use hyphens to separate the different prefixes, and use commas to separate numbers. If two or more different substituents are present, cite them in alphabetical order. If two or more identical substituents are present on the parent chain, use one of the multiplier prefixes *di*-, *tri*-, *tetra*-, and so forth, but don't use these prefixes for alphabetizing. Full names for some of the examples we have been using are as follows:



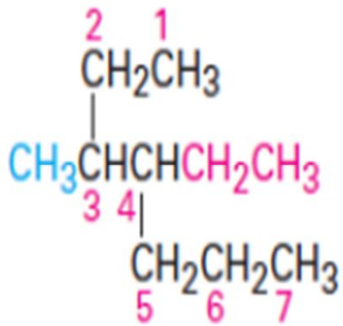
3-Methylhexane



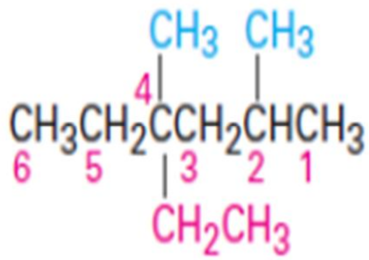
3-Ethyl-4,7-dimethylnonane



3-Ethyl-2-methylhexane



4-Ethyl-3-methylheptane

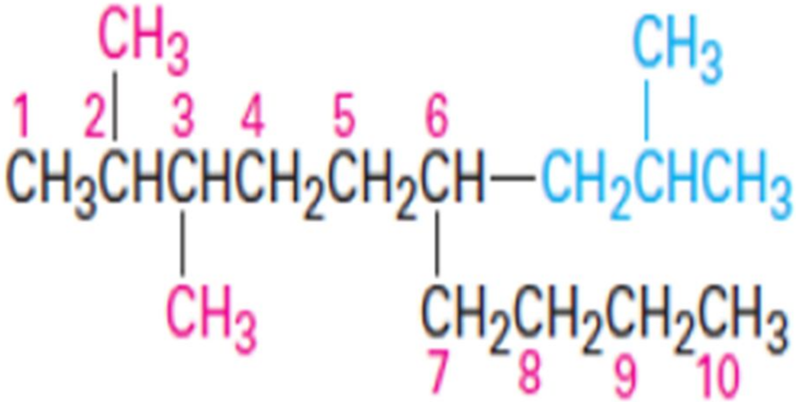


4-Ethyl-2,4-dimethylhexane

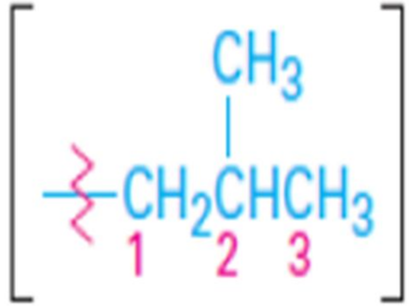
Naming Alkanes

- **Step 5**

- **Name a branched substituent as though it were itself a compound.**
- In some particularly complex cases, a fifth step is necessary. It occasionally happens that a substituent on the main chain is itself branched. In the following case, for instance, the substituent at C6 is a three-carbon chain with a methyl group. To name the compound fully, the branched substituent must first be named.



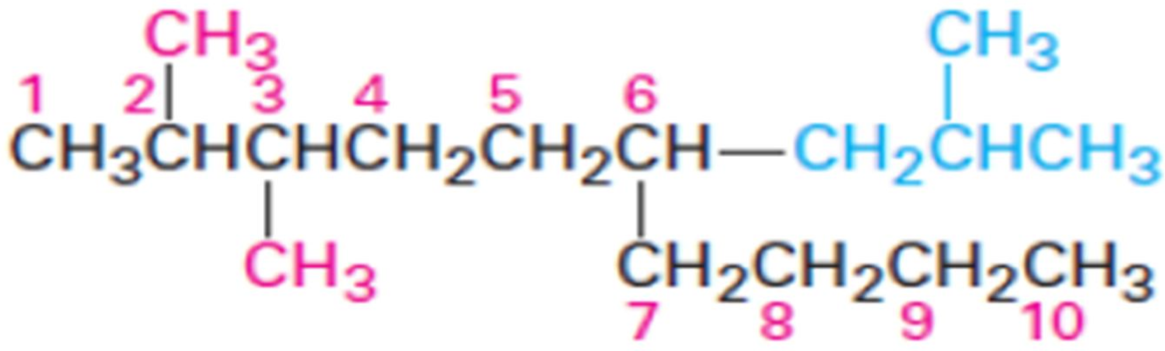
Named as a 2,3,6-
trisubstituted decane



A 2-methylpropyl
substituent

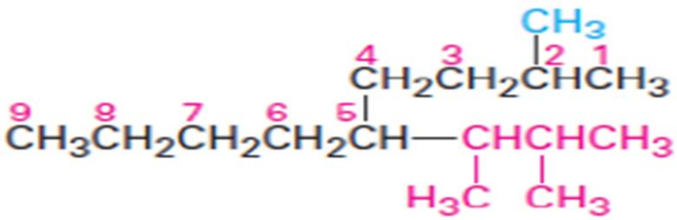
Naming Alkanes

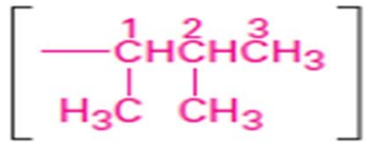
- Number the branched substituent beginning at the point of its attachment to the main chain, and identify it—in this case, a 2-methylpropyl group.
- The substituent is treated as a whole and is alphabetized according to the first letter of its complete name, including any numerical prefix. It is set off in parentheses when naming the entire molecule.



2,3-Dimethyl-6-(2-methylpropyl)decane

As a further example:

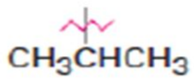




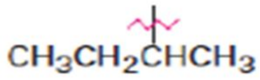
5-(1,2-Dimethylpropyl)-2-methylnonane

A 1,2-dimethylpropyl group

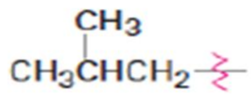
For historical reasons, some of the simpler branched-chain alkyl groups also have nonsystematic, common names, as noted earlier.



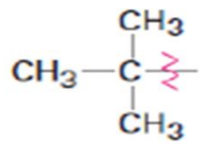
Isopropyl (*i*-Pr)



sec-Butyl (*sec*-Bu)



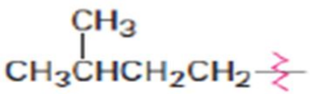
Isobutyl



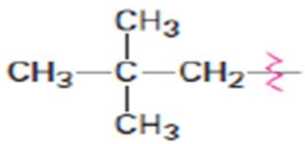
tert-Butyl (*t*-butyl or *t*-Bu)

3-Carbon alkyl group

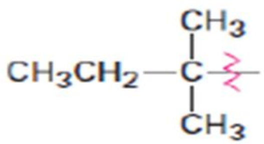
4-Carbon alkyl groups



Isopentyl, also called isoamyl (*i*-amyl)



Neopentyl

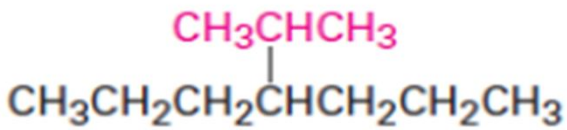


tert-Pentyl, also called *tert*-amyl (*t*-amyl)

5-Carbon alkyl groups

Naming Alkanes

- The common names of these simple alkyl groups are so well entrenched in the chemical literature that IUPAC rules make allowance for them. Thus, the following compound is properly named either 4-(1-methylethyl) heptane or 4-isopropylheptane. There's no choice but to memorize these common names; fortunately, there are only a few of them.



4-(1-Methylethyl)heptane or 4-Isopropylheptane

Naming Alkanes

- When writing an alkane name, the non-hyphenated prefix iso- is considered part of the alkyl-group name for alphabetizing purposes, but the hyphenated and italicized prefixes *sec*- and *tert*- are not. Thus, isopropyl and isobutyl are listed alphabetically under *i,* but *sec*-butyl and *tert*-butyl are listed under *b*