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www.aepstudycircle.com

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2ND FLOOR, SATKOUDI COMPLEX, THANA CHOWK, RAMGARH - 829122-JH

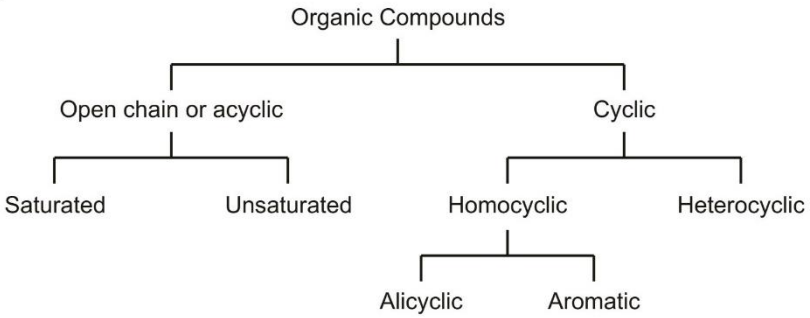
ORGANIC CHEMISTRY
VOLUME 02

CHAPTER 6

Classification of Organic Compounds

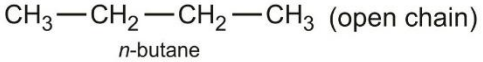
CLASSIFICATION

The Organic compounds are classified as

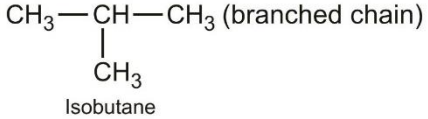


OPEN CHAINS

1. These compounds contain straight or branched chain of carbon atoms and are called as open chain or acyclic compounds.



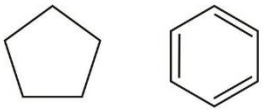
n-butane



Isobutane

2. **Cyclic :** The compounds in which terminal carbon atoms join with each other to form ring like structures are called as cyclic or closed chain or ring compounds. These are of two types

(i) **Homocyclic compounds** where the atoms are all of similar type *e.g.*,

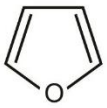


(ii) **Heterocyclic compounds** a wide variety of important organic compounds are derived from benzene, by replacing one of the hydrogens with a different functional group. They can have both common & systematic names.

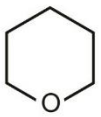
- Halogen-containing
- Hydrocarbon Derivatives
- Oxygen-containing
- Nitrogen-containing
- Sulfur-containing
- Polyaromatics

Ethylene Oxide
Oxirane
C_2H_4O

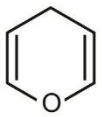
Tetrahydrofuran
Oxolane
C_4H_8O



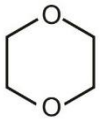
Furan
Oxole
C_2H_4O



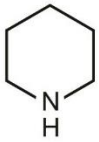
Tetrahydropyran
Oxane
$C_5H_{10}O$



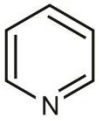
4H-Pyran
4H-oxine
C_5H_6O



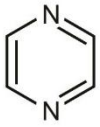
Ethylene Oxide
Oxirane
C_2H_4O



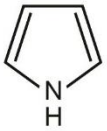
Piperidine
Azinane
$C_5H_{11}N$



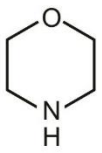
Pyridine
Azine
C_5H_5N



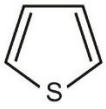
Pyrazine
1,4-diazine
$C_4H_4N_2$



Pyrrole
Azole
C_4H_5N



Morpholine



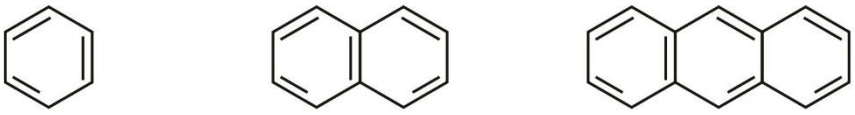
Thiophene
Thiole
C_4H_4S

The cyclic compounds are further divided into two types :

(i) **Alicyclic compounds :** The cyclic compounds which resembles with open chains i.e. aliphatic compounds are called alicyclic compounds *e.g.*,

Cyclopropane Cyclobutane Cyclopentane Cyclohexane

(ii) **Aromatic compounds :** In earlier days the compounds with pleasant smell were called aromatic compounds.



Benzene
(6π electrons)

Naphthalene
(10π electrons)

Anthralene
(14π electrons)

These are all aromatic compounds.

CHAPTER 7

Nomenclature of Alkanes

International Union of Pure and Applied Chemistry

I U P A C

Abbreviation	IUPAC
Motto	Advancing Chemistry Worldwide
Formation	1919
Type	International chemistry standards organization
Headquarters	Zurich, Switzerland
Region served	Worldwide
Official language	English
President	Mark Cesa
Website	www.iupac.org

The International Union of Pure and Applied Chemistry (IUPAC), is an international federation of National Adhering Organizations that represents chemists in individual countries. It is a member of the International Council for Science (ICSU). The international headquarters of IUPAC is in Zurich, Switzerland. The administrative office, known as the "IUPAC Secretariat". Is in Research Triangle Park, North Carolina, United States. This administrative office is headed by the IUPAC executive director, currently Lynn Soby.

Creation and history

The need for an international standard for chemistry was first addressed in 1860 by a committee headed by German scientist Friedrich August Kekule von Stradonitz. This committee was the first internatioinal conference to create an international conference to create an international naming system for organic compounds. The ideas that were formulated in that conference evolved into the official IUPAC nomenclature of organic chemistry. The IUPAC stands as a legacy of this meeting, making it one of the most important historical international collaborations of chemistry societies. Since this time, IUPAC has been the official organization held with the responsibility of updating and maintaining official organic nomenclature. IUPAC as such was established in 1919. One notable country excluded from this early IUPAC was Germany. Germany's exclusion was a result of prejudice towards Germans by the allied powers after World War I. Germany was finally admitted into IUPAC during World War II.


Friedrich August Kekule von Stradonitz

During World war II, IUPAC was affiliated with the Allied powers, but had little involvement during the war effort itself. After the war, West Germany was allowed back into IUPAC. Since World War II, IUPAC has been focused on standardizing nomenclature and methods in science without interruption.

ALKANES

In organic chemistry, an **alkane**, or **paraffin** (a historical name that also has other meanings), is a saturated hydrocarbon. Alkanes consist only of hydrogen and carbon atoms and all bonds are single bonds. Alkanes (technically, always acyclic or open-chain compounds) have the general chemical formula C_nH_{2n+2}. For example, Methane is CH_4, in which $n = 1$ (n being the number of carbon atoms).

☑ SPECIAL TOPIC

WHY ARE ALKANES CALLED PARRAFINS?

Paraffins is a latin word meaning (parum = little + affinis = reactivity). Alkanes are called paraffins because they have a little affinity towards a general reagent. In other words, alkanes are inert substances. They undergo reactions under drastic conditions.

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, and the suffix identifies the primary functional group.

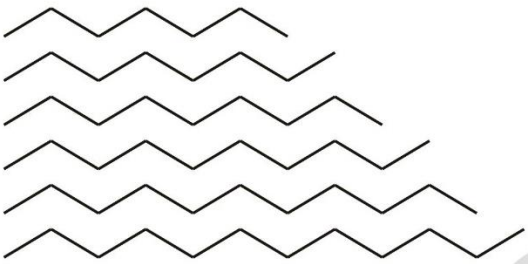
Locant — Prefix — Parent — Suffix

- Locant: Where are the substituents and functional groups?
- Prefix: What are the substituents?
- Parent: How many carbons?
- Suffix: What is the primary functional group?

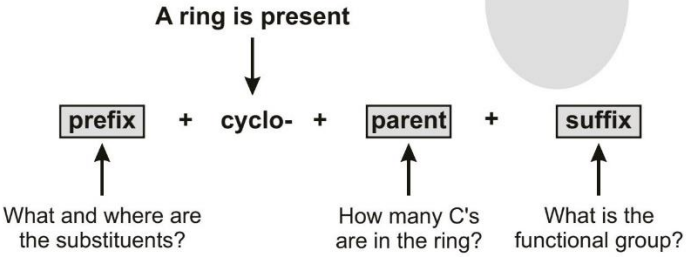
ACYCLIC HYDROCARBON

Methane	CH_4
Ethane	$H_3C — CH_3$
Propane	
Butane	
Pentane	
Hexane	

Heptane
Octane
Nonane
Decane
Undecane
Dodecane



NAMING CYCLOALKANES



CYCLIC HYDROCARBON

Cyclopropane

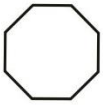
Cyclobutane

Cyclopentane

Cyclohexane

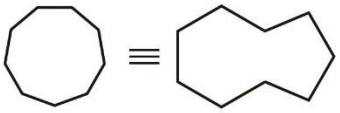
Cycloheptane

Cyclooctane

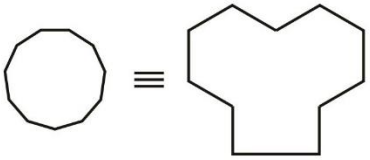


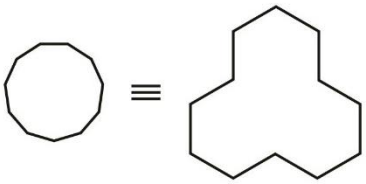
Cyclononane

Cyclodecane



Cycloundecane



Cyclododecane 

IUPAC SYSTEM OF NAMING COMPOUNDS

The IUPAC name of any organic compound essentially consists of three parts:

1. Word root **2.** Suffix **3.** Prefix

WORD ROOT

Word root is the basic unit of the name denoting the number of C atoms present in the principal chain (longest possible continuous chain of C atoms including the functional group and multiple bonds).

For C_1 to C_4, the normal common root based on names like meth, -eth-, and prop- are used. For C_5 or more carbon atoms chain, an extra letter (a) is used only if the primary suffix to be added to word root begins with a consonant.

Straight-chain alkanes take the suffix "-ane" and are prefixed depending on the number of carbon atoms in the chain, following standard rules. The first few are :

Number of carbons	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	20	30	40	50
Prefix	meth	eth	Prop	But	Pent	Hex	Hept	Oct	Non	Dec	Undec	Dodec	Tridec	Tetradec	Pentadec	Eicos	Triacont	Tetracont	Pentacont

SUFFIX

Suffix are of two types.

(i) Primary Suffix : is always added to word root to indicate whether the carbon chain is saturated or unsaturated. For saturated the primary suffix is 'ane'. For unsaturated (one double bond) it is -'ene' and for unsaturated (one triple bond) it is - 'yne'. If the number of double bonds is two or three, then the primary suffix is 'diene' or 'triene'. If there are two triple bonds then it is 'diyne'.

Example:

$HC \equiv CH$ ethyne; $CH_3 - CH = CH_2$ propene ; $CH_2 = CH - CH = CH_2$ Butadiene

('a' has been added to word root since primary suffix starts with a consonant 'd'.)

$HC \equiv C - C \equiv CH$ Butadiyne

(ii) Secondary Suffix: is added to primary suffix to indicate the nature of the functional group present in an organic compound.

For alcohol (— OH), -ol is added; for aldehydes (— CHO), -al is added.

For ketones (>C = O), -one is added; for acids (— COOH) -oic acid is added.

While adding the secondary suffix (to represent the functional group), the terminal 'e' of primary suffix is dropped. For example, CH_3CH_2OH is ethanol (e-dropped) and CH_2 = CHCHO is prop-2-en-1-al (e-dropped). However, it is not always dropped. For example, CH_3CH_2CN is propanenitrile (e-not dropped)

It should also be noted that locants are to be placed immediately before the part of the name to which they relate. For example, $\overset{3}{H}C \equiv \overset{2}{C} - \overset{1}{C}OOH$ is prop-2-yn-1-oic acid (working name 2-propynoic acid)

IUPAC Name

$ClC\overset{2}{H}_2\overset{1}{C}H_2OH$ is 2-chloroethan-1-ol (working name 2-chloroethanol)

PREFIX

These are also of two types.

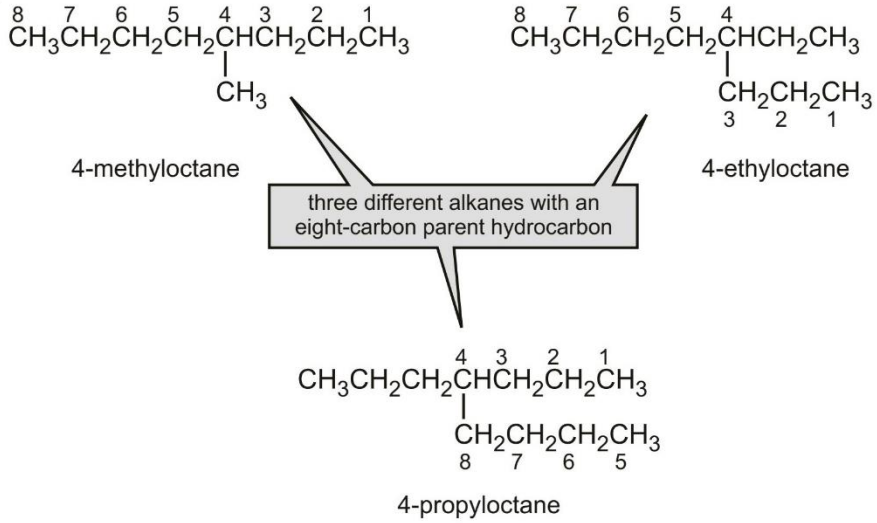
(i) **Primary Prefix:** It distinguishes between a cyclic and an acyclic compound. In a cyclic compound, the word 'cyclo' is used before the word root, for example,  is cyclopropane. If the prefix is not used, one can take the compound to be of open chain.

(ii) **Secondary Prefix:** Sometimes, certain groups are not considered functional groups. These are treated as substituents and added before the word root in an alphabetical order. For example, $C_2H_5 — O — C_2H_5$ is ethoxy ethane. In this, the secondary prefix is 'ethoxy', the word root is 'eth', and the primary suffix is 'ane'.

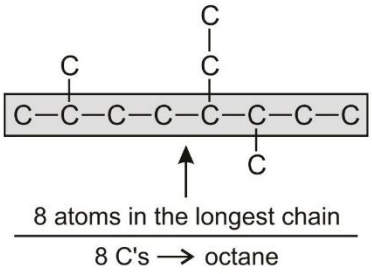
THE NOMENCLATURE OF ALKANES

The systematic name of an alkane is obtained using the following rules:

Determine the number of carbons in the longest continuous carbon chain. This chain is called the parent hydrocarbon . The longest continuous chain is not always in a straight line; sometimes you have to "turn a corner" to obtain the longest continuous chain.

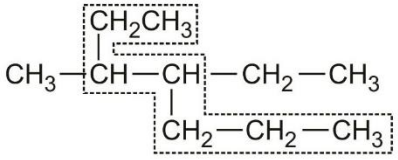


Find the parent carbon chain and add the suffix.



Rule 1 :

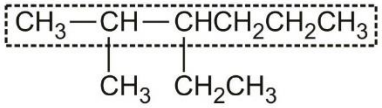
Longest chain rule : Select the longest continuous chain of carbon atoms. This is called the parent chain while all other carbon atoms which are not included in the parent chain are called branch chains or side chains or substituents.



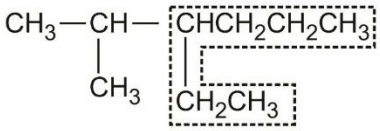
Longest chain contains seven carbon atoms and hence is named as a derivative of heptane

Rule 2 :

Rule for larger number of side chains : If two chains of equal lengths are possible, select the one with the larger number of side chains. For example,

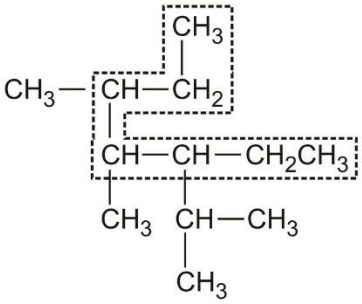


Named as hexane with **two** alkyl substituents (Correct)

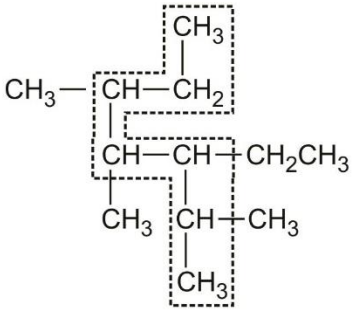


Named as hexane with **one** alkyl substituent (Wrong)

The series are called homologs. For example, butane is a homolog of propane, and both of these are homologs of hexane and decane.



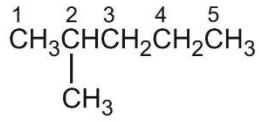
wrong
seven-carbon chain, but only three substituents



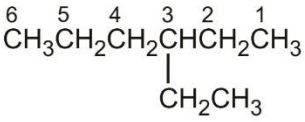
right
seven-carbon chain, four substituents

Rule 3 :

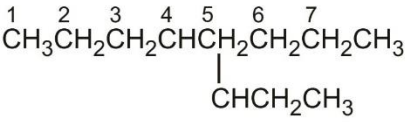
The name of any alkyl substituent that hangs off the parent hydrocarbon is placed in front of the name of the parent hydrocarbon, together with a number to designate the carbon to which the alkyl substituent is attached. The carbons in the parent chain are numbered in the direction that gives the substituent as low a number as possible. The substituents name and the name of the parent hydrocarbon are joined into one word. preceded by a hyphen that connects the substituent's number with its name.



2-methylpentane
not
4-methylpentane

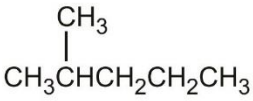


3-ethylhexane
not
4-ethylhexane



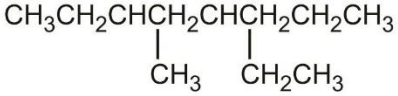
4-propyloctane
not
5-propyloctane

Only systematic names have numbers; common names never contain numbers



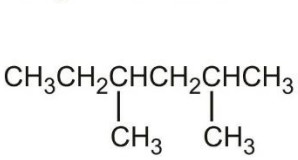
common name : isohexane
systematic names : 2-methypentane

If more than one substituent is attached to the parent hydrocarbon, the chain is numbered in the direction that will produce a name containing the lowest of the possible numbers.

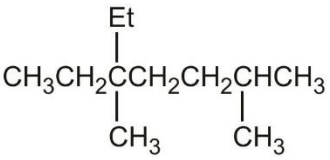


3-ethyl-5-methyloctane
not
4-ethyl-6-methyloctane
because 3 < 4

If two or more substituents are the same, the prefixes "di," "tri," and "tetra" are used to indicate how many identical substituents the compound has. The numbers indicating the locations of the identical substituents are listed together, separated by commas. There are no spaces on either side of a comma. There must be as many numbers in a name as there are substituents. The prefixes "di," "tri," "tetra," " sec ," and " tert " are ignored in alphabetizing substituents.

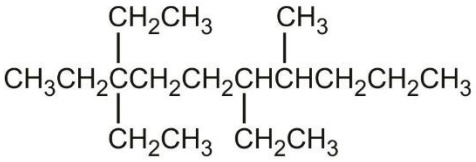


2,4-dimethylhexane

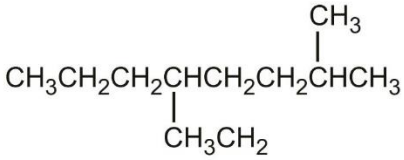


5-ethyl-2, 5-dimethylheptane

numbers are separated by a comma;
a number and a word are separated by a hyphen



3,3,6-triethyl-7-methyl decane



5-ethyl-2-methyloctane

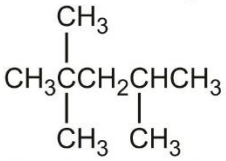
MISTAKES TO AVOID

Adding of punctuation:

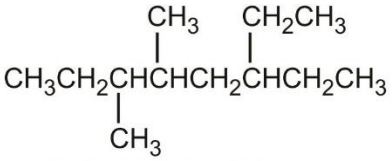
1. Commas are put between numbers (2, 5, 5 becomes 255)
2. Hyphens are put between a number and a letter (2,5,5 trimethylheptane becomes 2,5,5-trimethylheptane).
3. Successive words are merged into one word (trimethyl heptane becomes trimethylheptane)
   ❑ **NOTE :** IUPAC uses one-word names throughout. This is why all parts are connected.
4. When assigning the numbers (*i.e.*, the locants) while naming an organic compound there is NO rule based on summing the numbers.

Rule 4 :

1. When numbering in either direction leads to the same lowest number for one of the substituents, the chain is numbered in the direction that gives the lowest possible number to one of the remaining substituents.

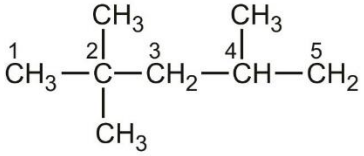


2,2,4-trimethylpentane
not
2,4,4-trimethylpentane
because 2 < 4

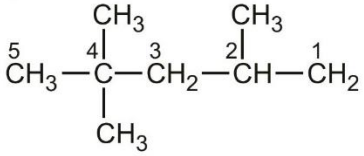


6-ethyl-3,4-dimethyloctane
not
3-ethyl-5,6-dimethyloctane
because 4 < 5

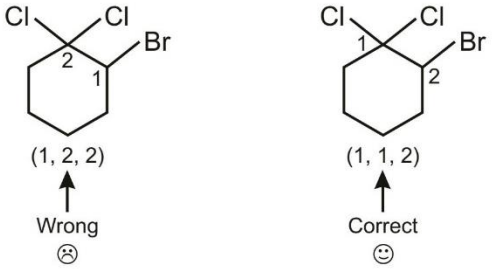
2. **Lowest set of locants rule :** *When two or more substituents are present, the lowest set of locants rule is applied*. According to this rule when two or more different sets of locants containing the same number of terms is possible, then that set of locants is the lowest which when compared term by term with other sets, each in order of increasing magnitude, has the lowest term at the first point of difference.
   That is why this rule is also sometimes called as first point of difference rule.



Set of locants = 2, 2, 4 (correct)

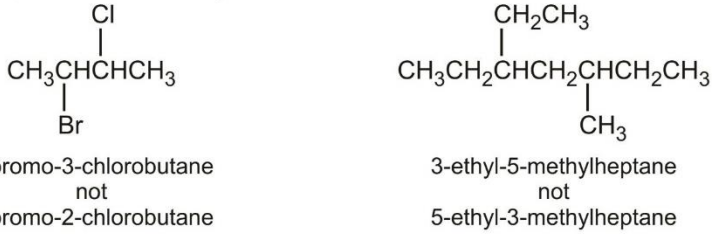


Set of locants = 2, 4, 4 (wrong)



Rule 5 :

If the same substituent numbers are obtained in both directions, the first group listed receives the lower number (according to alphabetical order).



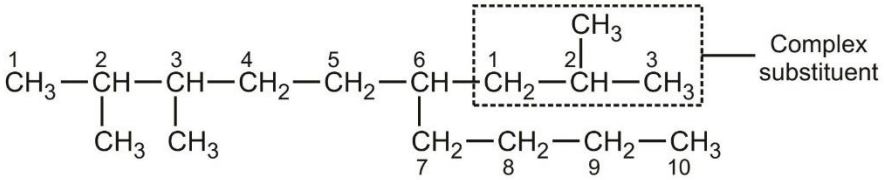
Rule 6 :

NAMING OF COMPLEX SUBSTITUENT

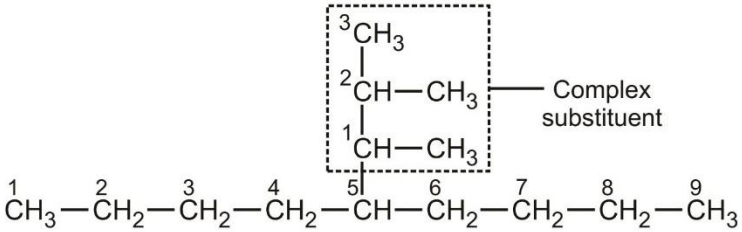
Alkyl group, R-	**Common name**	**Complex name** (if different)
CH_3-	methyl-	
CH_3CH_2-	ethyl-	
$CH_3CH_2CH_2$-	propyl-	
$(CH_3)_2CH$-	isopropyl-	(1-methylethyl)-
$CH_3CH_2CH_2CH_2$-	butyl-	
$CH_3-CH_2-\underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}}-$	sec-butyl- or s-butyl	(1-methylpropyl)-
$(CH_3)_2CHCH_2$-	isobutyl	(2-methylpropyl)-
$(CH_3)_3C$-	tert-butyl or t-butyl	(1,1-dimethylethyl)-

NUMBERING THE COMPLEX SUBSTITUENT

(a) In case the substituent on the parent chain is complex (*i.e.*, it has branched chain), it is named as a substituted alkyl group by numbering the carbon atom of this group attached to the parent chain as 1. The name of such a substituent is always enclosed in brackets to avoid confusion with the numbers of the parent chain. For example,



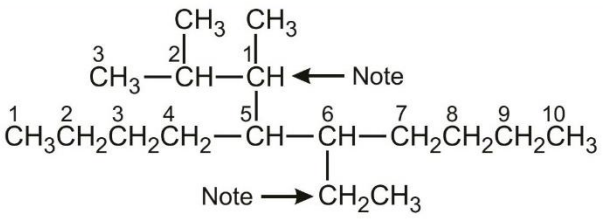
2, 3-Dimethyl-6-(2-methylpropyl)decane



5-(1, 2-Dimethylpropyl) nonane

(b) While deciding the alphabetical order of the various substituents, the name of the complex substituent is considered to begin with the first letter of the complete name, eventhough di, tri, iso, neo.

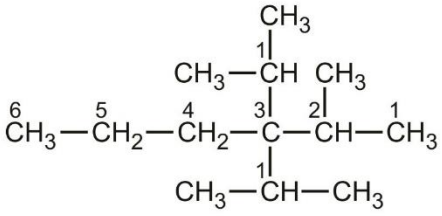
Solved Example



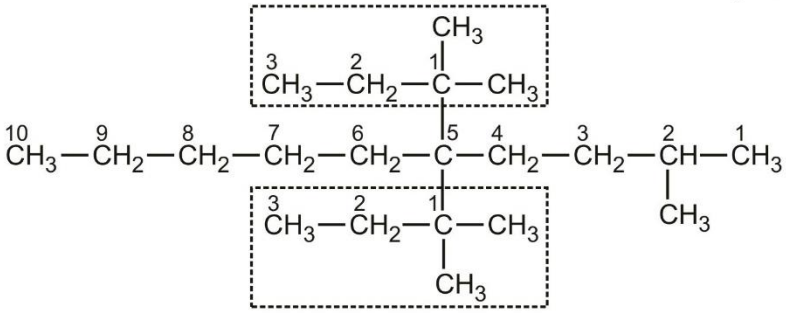
5-(1, 2-Dimethylpropyl)-6-ethyldecane

It may be noted here that the complete name of the complex substituent is dimethylbutyl. Since d of dimethylbutyl group comes first than e of the ethyl group in the alphabetical order, therefore, locant 5 is given to the complex substituent and 6 to the ethyl group.

(c) If the same complex substituent occurs more than once on the parent chain, prefixes bis (for two), tris (for three), tetrakis (for four), pentakis (for five) etc. are used before the name of the complex substituent. For example,



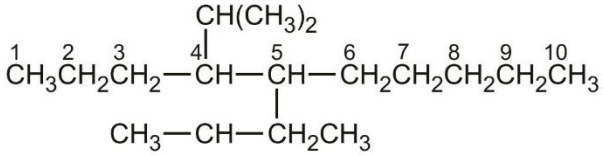
2-Methyl-3, 3-bis(1-methylethyl)hexane



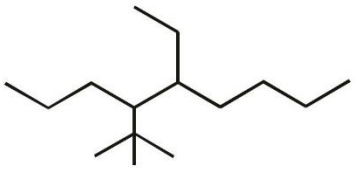
5, 5-Bis (1, 1-dimethylpropyl)-2-methyldecane

☞ Note that while deciding the alphabetical order of the various alkyl groups, **prefixes iso and neo are considered to be part of the fundamental name of the alkyl group while the prefixes sec, tert, di, tri are not.**

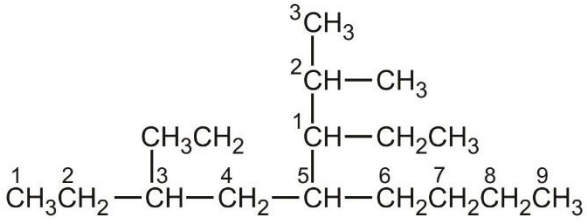
Solved Example



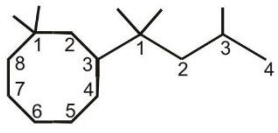
4-(Methylethyl)-5-(Methylpropyl)decane



4-(1,1-dimethylethyl)-5-ethylnonane
not 5-ethyl-4-(1,1-dimethylethyl) nonane



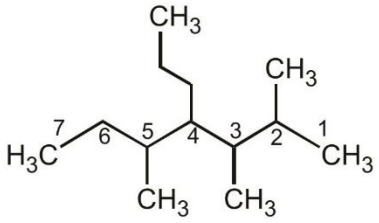
3-ethyl-5-(1-ethyl-2-methylpropyl)nonane



1,1 dimethyl-3-(1, 1,3-trimethylbutyl)cycloctane

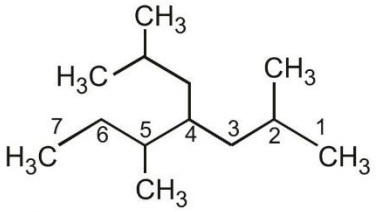
☞ If Chains of equal length are competing for selection as main chain in a saturated branched acyclic hydrocarbon, then the choice goes in series to :

(a) The chain which has the greatest number of side chains.



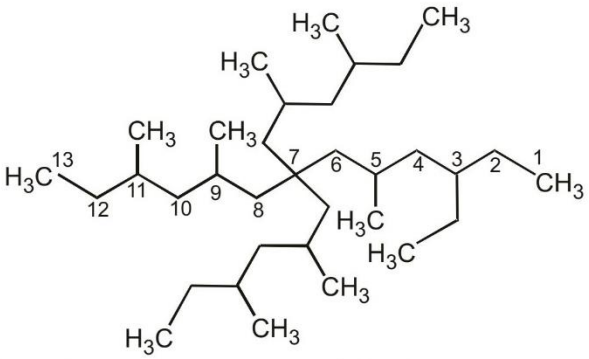
2,3,5-Trimethyl-4-propylheptane

(b) The chain whose side chains have the lowest-numbered locants.



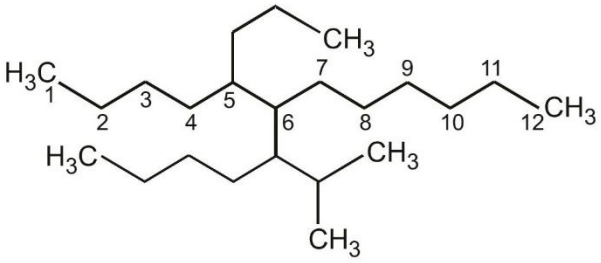
4-Isobutyl-2,5-dimethyl heptane

(c) The chain having the greatest number of carbon atoms in the smaller side chains.

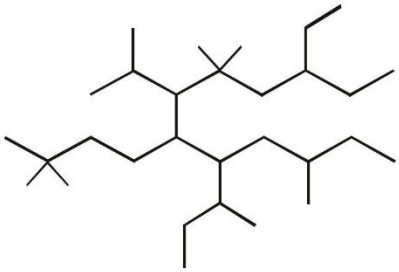


7,7,Bis(2,4-dimethylhexyl)-3-ethyl 5, 9, 11-trimethyl tridecane

(d) The chain having the least branched side chains.

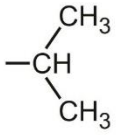
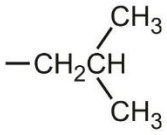
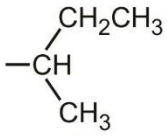
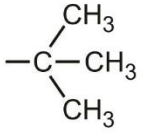
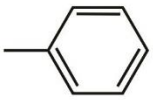
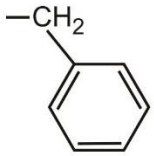
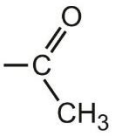
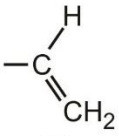
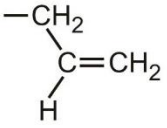


Name That Molecule !



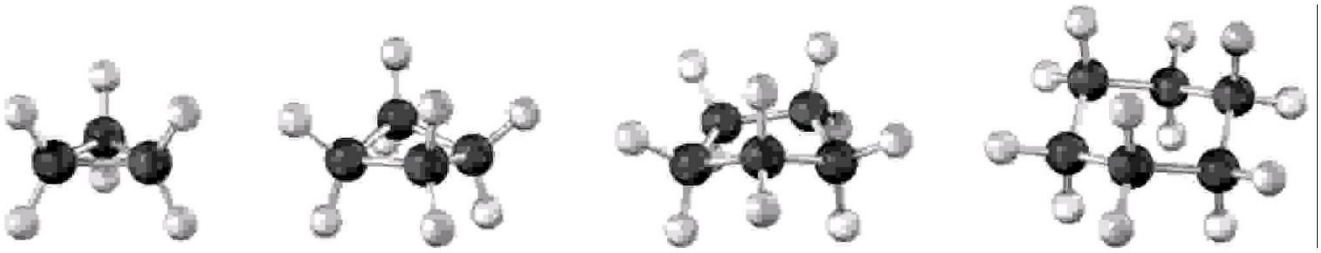
8-sec-butyl-3-ethyl-6-isopropyl-5,5, 10-trimethyl-7-neohexyldodecane
or
8-sec-butyl-7-(3, 3-dimethylbutyl)-3-ethyl-6-(1-methylethyl)-5,5,10-trimethyldodecane

COMMON NAMES AND STRUCTURAL ABBREVIATIONS

Group	Abbreviation	Structure
Alkyl	R	
Aryl	Ar	
Methyl	Me	$-CH_3$
Ethyl	Et	$-CH_2CH_3$
Propyl	Pr or n-Pr	$-CH_2CH_2CH_3$
Butyl	Bu or n-Bu	$-CH_2CH_2CH_2CH_3$
Isopropyl	i-Pr or ^{i}Pr	
Isobutyl	i-Bu or ^{i}Bu	
sec-Butyl	s-Bu or ^{s}Bu	
tert-Butyl	t-Bu or ^{t}Bu	
Phenyl	Ph	
Benzyl	Bn	
Acetyl	Ac	
Vinyl		
Allyl		
Halide	X	–F –Cl –Br –I

NOMENCLATURE OF CYCLIC ALKANE

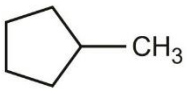
Saturated cyclic hydrocarbons are called cycloalkanes, or alicyclic compounds (aliphatic cyclic). Because cycloalkanes consist of rings of $–CH_2–$units, they have the general formula $(CH_2)_n$, or C_nH_{2n}, and can be represented by polygons in skeletal drawings.



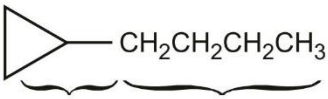
Cyclopropane Cyclobutane Cyclopentane Cyclohexane

Find the parent.

Count the number of carbon atoms in the ring and the number in the largest substituent. If the number of carbon atoms in the ring is equal to or greater than the number in the substituent, the compound is named as an alkyl-substituted cycloalkane. If the number of carbon atoms in the largest substituent is greater than the number in the ring, the compound is named as a cycloalkyl-substituted alkane. For example:



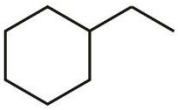
Methylcyclopentane



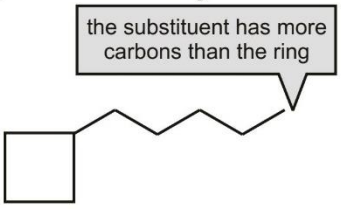
1-Cyclopropylbutane

☞ In a cycloalkane with an attached alkyl substituent, the ring is the parent hydrocarbon unless the substituent has more carbons than the ring. In that case, the substituent is the parent hydrocarbon and the ring is named as a substituent. There is no need to number the position of a single substituent on a ring.

methylcyclopentane



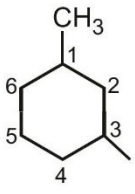
ethylcyclohexane



1-cyclobutylpentane

Number the substituents, and write the name.

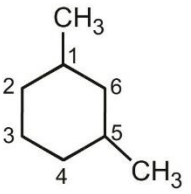
☞ For an alkyl- or halo-substituted cycloalkane, choose a point of attachment as carbon 1 and number the substituents on the ring so that the second substituent has as low a number as possible. If ambiguity still exists, number so that the third or fourth substituent has as low a number as possible, until a point of difference is found.



1,3-Dimethyl cyclohexane

Lower

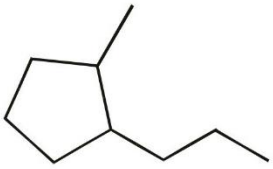
NOT



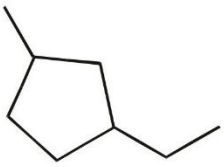
1,5-Dimethyl cyclohexane

Higher

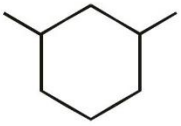
☞ If the ring has two different substituents, they are listed in alphabetical order and the number-1 position is given to the substituent listed first.



1-methyl-2-propylcyclopentane



1-ethyl-3-methylcyclopentane

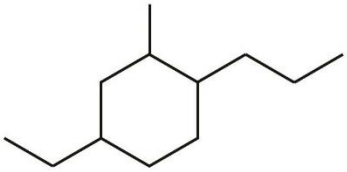


1,3-dimethylcyclohexane

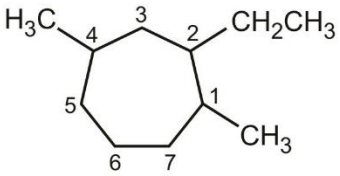
☞ If there are more than two substituents on the ring, they are listed in alphabetical order, and the substituent given the number-1 position is the one that results in a second substituent getting as low a number as possible. If two substituents have the same low numbers, the ring is numbered—either clockwise or counterclockwise—in the direction that gives the third substituent the lowest possible number.

Solved Example

1,1,2-trimethylcyclopentane
not
1,2,2-trimethylcyclopentane
because 1 < 2
not
1,1,5-trimethylcyclopentane
because 2 < 5

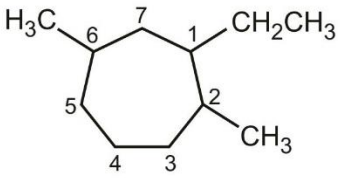


4-ethyl-2-methyl-1-propylcyclohexane
not
1-ethyl-3-methyl-4-propylcyclohexane
because 2 < 3
not
5-ethyl-1-methyl-2-propylcyclohexane
because 4 < 5

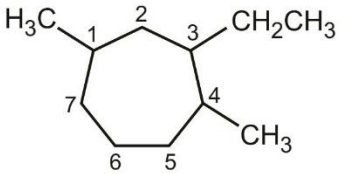


2-Ethyl-1,4-dimethyl cycloheptane
Lower Lower

NOT

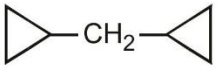


1-Ethyl-2,6-dimethylcycloheptane
Higher

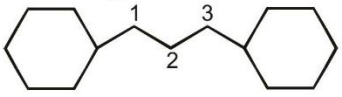


3-Ethyl-1,4-dimethylcycloheptane
Higher

☞ If more than one alicyclic ring is attached to a single chain, the compound is named as a derivative of alkane irrespective of the number of carbon atoms in the ring or the chain. For example,

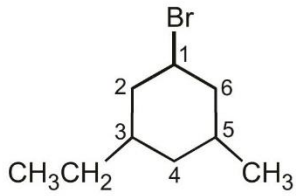


dicyclopropylmethane

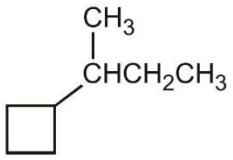


1,3-dicyclohexylpropane

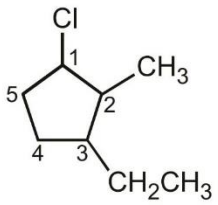
Solved Example



1-Bromo-3-ethyl-5-methyl cyclohexane



(1-Methylpropyl) cyclobutane or sec-butyl cyclobutane



1-Chloro-3-ethyl-2-methyl-cyclopentane

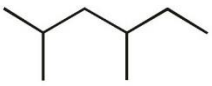
Solved Problems

- Select the correct structure for the IUPAC names given below :

Part 1	Part 2	Part 3
4-methylheptane	2,4-dimethylhexane	2,3-dimethylpentane
Part 4	**Part 5**	**Part 6**
2,2-dimethylhexane	3-ethyl-1,1,2,2-tetramethylcyclopentane	3-ethyl-2-methylpentane
Part 7	**Part 8**	**Part 9**
2,5-dimethylhexane	1,1-dimethylcyclohexane	2,4,6-trimethylheptane

Structures:


A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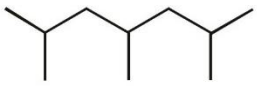
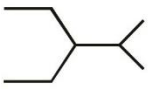
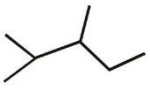
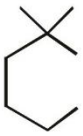
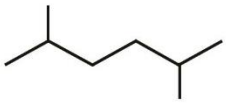

C


D

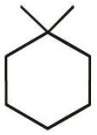

E


F


G


H


I


J


K


L

Sol. Part - 1 $\Rightarrow$ H, Part - 2 $\Rightarrow$ B, Part - 3 $\Rightarrow$ E, Part - 4 $\Rightarrow$ F
Part - 5 $\Rightarrow$ I, Part - 6 $\Rightarrow$ D, Part - 7 $\Rightarrow$ G, Part - 8 $\Rightarrow$ J
Part - 9 $\Rightarrow$ C

Solved Example

- Deduce structural formulas and give IUPAC names for the nine isomers of C_7H_{16}. (b) Why is 2-ethylpentane not among the nine ?

(a) seven-C chain

1. $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ — Heptane

six-C chain

2. $CH_3CH(CH_3)CH_2CH_2CH_2CH_3$ — 2-Methylhexane

3. $CH_3CH_2CH(CH_3)CH_2CH_2CH_3$ — 3-Methylhexane

five-C chain

4. $CH_3CH(CH_3)CH_2CH_2CH_3$ — 2,3-Dimethylpentane

5. $CH_3CH(CH_3)CH_2CH(CH_3)z$ — 2,4-Dimethylpentane

6. $CH_3C(CH_3)_2CH_2CH_2CH_3$ — 2,2-Dimethylpentane

☑ SPECIAL TOPIC

OCTANE NUMBER

In addition to being volatile, gasoline must resist the potentially damaging explosive combustion known as knocking. The antiknock properties of gasoline are rated by an octane number that is assigned by comparing the gasoline to a mixture of *n*-heptane (which knocks badly) and isooctane (2,2,4-trimethylpentane, which is not prone to knocking). The gasoline being tested is used in a test engine with a variable compression ratio. Higher compression ratios induce knocking, so the compression ratio is increased until knocking begins. Tables are available that show the percentage of isooctane in an isooctane/heptane blend that begins to knock at any given compression ratio. The octane number assigned to the gasoline is simply the percentage of isooctane in an isooctane/heptane mixture that begins to knock at that same compression ratio.

$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$

n-heptane (0 octane)
prone to knocking

$CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$

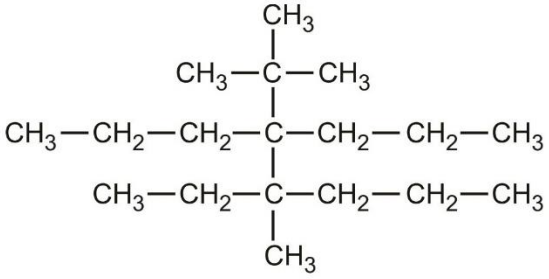
2,2,4-trimethylpentane (100 octane)
"isooctane," resists knocking

The octane number of a gasoline is determined by comparing its knocking with the knocking of mixtures of heptane and 2,2,4-trimethylpentane. The octane number given to the gasoline corresponds to the percent of 2,2,4-trimethylpentane in the matching mixture. Thus, a gasoline with an octane rating of 91 has the same "knocking" property as a mixture of 91% 2,2,4-trimethylpentane and 9% heptane. The term octane number originated from the fact that 2,2,4-trimethylpentane contains eight carbons. Because slightly different methods are used to determine the octane number, gasoline in Canada and the United States will have an octane number that is 4 to 5 points less than the same gasoline in Europe and Australia.

EXERCISE

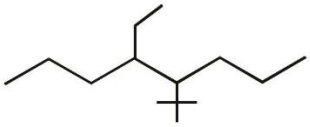
SINGLE CHOICE QUESTIONS

1. Total number of carbon atoms present in parent chain is :



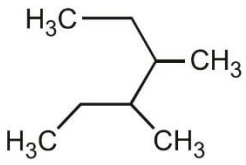
(A) 5 (B) 6 (C) 7 (D) None of these

2. Correct IUPAC name of the following compound is :

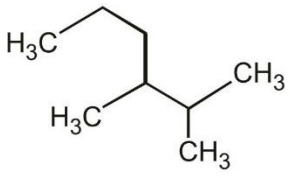


(A) 4-(1,1-dimethylethyl)-5-ethyloctane
(B) 5-ethyl-4-(1,1-dimethylethyl)octane
(C) 5-(1,1-dimethylethyl)-4-ethyloctane
(D) 5-ethyl-5-(1,1-dimethylethyl)octane

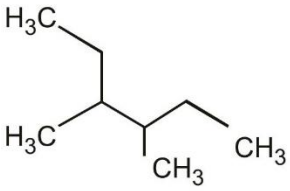
3. Among the following compounds



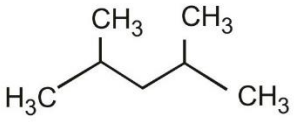
(i)



(ii)



(iii)

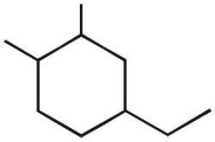


(iv)

2,3-dimethylhexane is :

(A) (i) (B) (ii) (C) (iii) (D) (iv)

4. What would be the best name for the following compound ? (Neglect any cis-trans isomerism that is possible.)



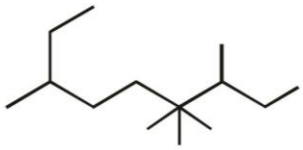
(A) 1-ethyl-3,4-dimethylcyclohexane
(B) 3-ethyl-1,6-dimethylcyclohexane
(C) 1-ethyl-4,5-dimethylcyclohexane
(D) 5-ethyl-1,2-dimethylcyclohexane
(E) 4-ethyl-1,2-dimethylcyclohexane

5. The correct IUPAC name of $CH_3CH_2CH(CH_3)CH(C_2H_5)_2$ is :

(A) 4-ethyl - 3-methyl hexane
(B) 3-ethyl - 4 methyl hexane
(C) 4-methyl - 3-ethyl hexane
(D) 2, 4-diethylpentane

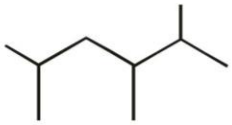
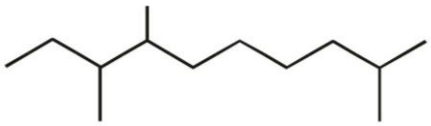
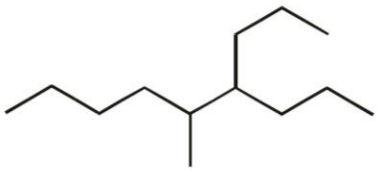
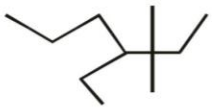
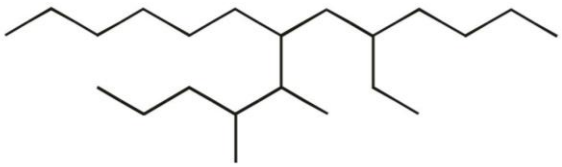
6. What is the parent name for the following alkane ?

(**Note :** The parent name corresponds to the longest continuous chain of carbon atoms.)



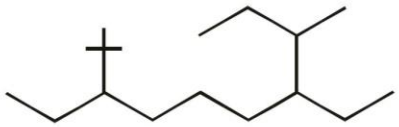
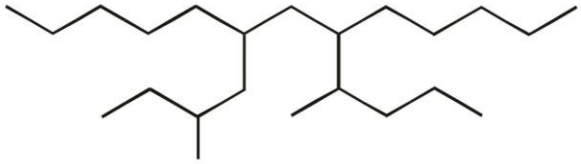
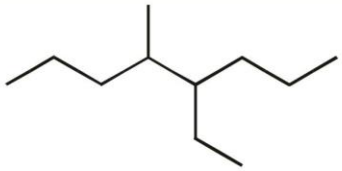
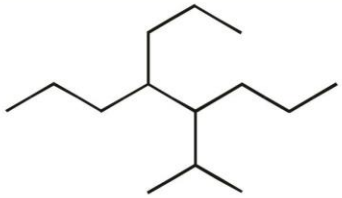
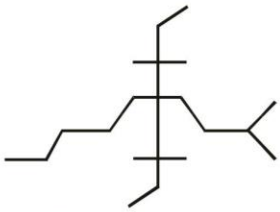
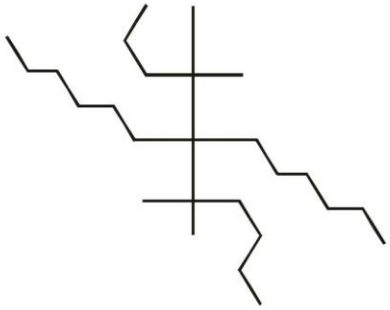
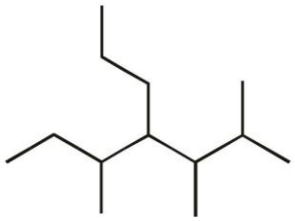
(A) Heptane (B) Octane (C) Nonane (D) Decane

WORK SHEET - 1

S.N.	Compound	Number of carbon atom in Parent chain
1.		
2.		
3.		
4.		
5.	$CH_3CH_2CH_2\underset{\displaystyle CH_2CH_3}{\underset{\vert}{CH}}-CH(CH_3)_2$	
6.	$CH_3-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-CH_2-\underset{\displaystyle CH_2CH_3}{\underset{\vert}{CH}}-CH_3$	
7.	$CH_3-CH_2-\underset{\displaystyle CH_3CH_2}{\underset{\vert}{CH}}-\underset{\displaystyle CH_2CH(CH_3)_2}{\underset{\vert}{CH}}-CH_2-CH_2-CH_3$	
8.		
9.	$CH_3CH_2\underset{\displaystyle C(CH_3)_3}{\underset{\vert}{CH}}\underset{\displaystyle CH(CH_3)_2}{\underset{\vert}{CH}}CH_3$	
10.	$CH_3-\underset{\displaystyle CH_2CH_3}{\underset{\vert}{CH}}-CH_2CH_3$ $(CH_3)_3C-CH-CH_2CH_2CH_3$	

11. $CH_3C(CH_3)_2CH(CH_2CH_3)CH_2CH_2CH(CH_3)_2$

WORK SHEET - 2

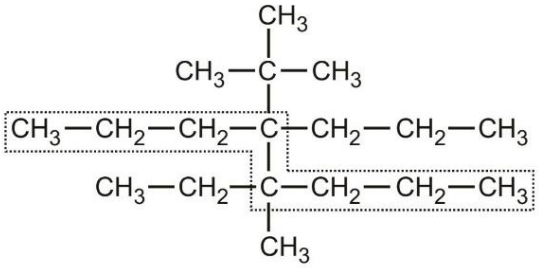
S.N.	Compound	Write IUPAC - Name
1.		
2.		
3.		
4.		
5.		
6.		
7.		

Answer

1. (D) **2.** (A) **3.** (B) **4.** (E) **5.** (B) **6.** (C)

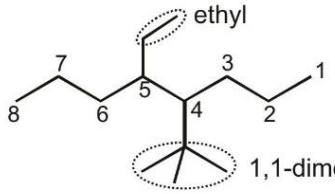
Single Choice Questions

1.



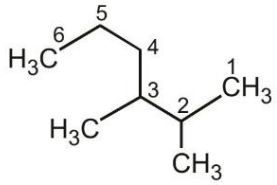
8 Carbons in parent chain

2.



4-(1,1-dimethylethyl)-5-ethyloctane

3.



2, 3-Dimethyl hexane

Work Sheet - 1

1. 6 **2.** 10 **3.** 9 **4.** 7 **5.** 6 **6.** 6 **7.** 7 **8.** 13
9. 6 **10.** 7 **11.** 7

Work Sheet - 2

1. 3, 7-Diethyl - 2, 2,8-trimethyl decane
2. 6-(1-methylbutyl) - 8-(2-methylbutyl) tridecane
3. 4-ethyl - 5 - methyl octane
4. 4-(1-methyl ethyl) - 5-propyl octane **or** 4-isopropyl-5-propyl octane
5. 5, 5-Bis (1, 1-dimethyl propyl)-2-methyl- decane
6. 7-(1,1-dimethyl butyl)-7-(1,1-dimethyl pentyl) tridecane
7. 2, 3, 5-trimethyl - 4-propyl heptane

❑❑❑

CHAPTER
8

Nomenclature of Alkenes & Alkynes

ALKENES

Alkenes are named using a series of rules similar to those for alkanes with the suffix -ene used instead of -ane to identify the functional group. There are two steps.

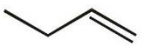
1. **Name the parent hydrocarbon:** Find the longest carbon chain containing the double bond.
2. **Number the carbon atoms in the chain:** Begin at the end nearer the double bond or, if the double bond is equidistant from the two ends, begin at the end nearer the first branch point. This rule ensures that the doublebond carbons receive the lowest possible numbers.

   Functional group suffix = **–ene**

   Substituent name = **alkenyl**

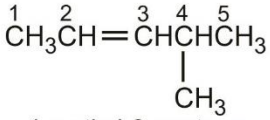
   Structural unit : alkenes contain C = C bonds.

Solved Example



$CH_3CH_2CH=CH_2$

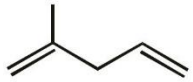
- Functional group is an alkene, therefore suffix = **–ene**
- The longest continuous chain is C4 therefore root = but
- In order to give the alkene the lowest number, number from the right as drawn.
- The C = C is between C1 and C2 so the locant is **but-1-ene** or **1-butene.**



4-methyl-2-pentene

☞ For a compound with two double bonds, the "ne" ending of the corresponding alkane is replaced with "diene."

Solved Example



$CH_3C(CH_3)=CHCH=CH_2$

- Functional group is an alkene, therefore suffix = **–ene.**
- There are two alkenes, so insert the multiplier di.
- The longest continuous chain is C5 therefore root plus "a" = penta.
- The substituent is a C1 alkyl group i.e. a methyl group.
- The first point of difference doesn't distinguish the C = C.
- So, need to apply the first point of difference to the alkyl substituent.
- The first point of difference requires that we number from the left as drawn.
- The methyl group locant is 2-.
- Therefore the locants for C = C units are 1- and 4-

Name : 2-methylpenta-1,4-diene or 2-methyl-1,4-pentadiene

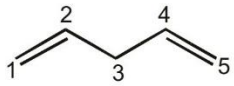
Solved Example

$\overset{1}{C}H_3\overset{2}{C}H=\overset{3}{C}H-\overset{4}{C}H=\overset{5}{C}H\overset{6}{C}H_2\overset{7}{C}H_3$

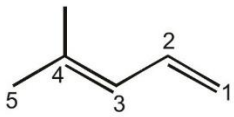
2, 4-heptadiene

$\overset{5}{C}H_3\overset{4}{C}H=\overset{3}{C}H-\overset{2}{C}H=\overset{1}{C}H_2$

1, 3-pentadiene



1,4-pentadiene



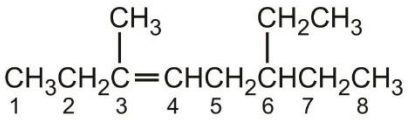
4-methyl-1,3-pentadiene

☞ Groups which always have less priority than multiple bonds :

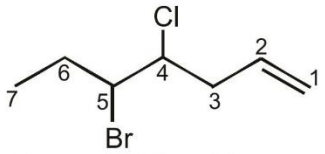
1.	– F	Fluoro	**2.**	– Cl	Chloro
3.	– Br	Bromo	**4.**	– I	Iodo
5.	$-NO_2$	Nitro	**6.**	– NO	Nitroso
7.	– OR	Alkoxy	**8.**	$-OCH_3$	Methoxy
9.	– OEt	ethoxy	**10.**	– OPh	Phenoxy
11.	– R	Alkyl	**12.**	$-N_3$	Azido

Solved Example

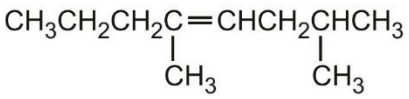
3-bromoprop-1-ene



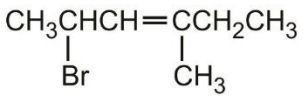
6-ethyl-3-methyl-3-octene



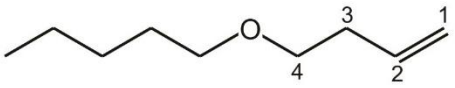
5-bromo-4-chloro-1-heptene



2,5-dimethyl-4-octene
not
4,7-dimethyl-4-octene
because 2 < 4



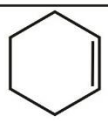
2-bromo-4-methyl-3-hexene
not
5-bromo-3-methyl-3-hexene
because 2 < 3



4-pentoxy-1-butene

NOMENCLATURE OF CYCLIC ALKENE

Solved Example

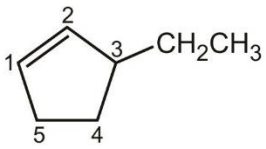


- Functional group is an alkene, therefore suffix = **–ene.**
- The longest continuous chain is C6 therefore root = **hex.**
- The C = C is unambiguously between C1 and C2 therefore the locant isn't required.

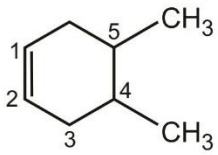
Name: Cyclohexene

☞ A number is not needed to denote the position of the double bond in a cyclic alkene because the ring is always numbered so that the double bond is between carbons 1 and 2. To assign numbers to any substituents, count around the ring in the direction (clockwise or counterclockwise) that puts the lowest number into the name.

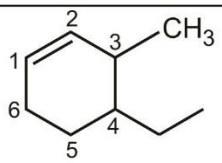
Solved Example



3-ethylcyclopentene



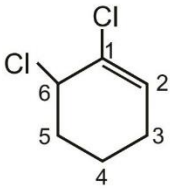
4,5-dimethylcyclohexene



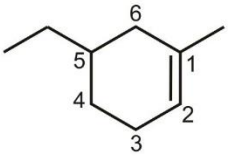
4-ethyl-3-methylcyclohexene

❑ **NOTE :** 1,6-dichlorocyclohexene is not called 2,3-dichlorocyclohexene because the former has the lowest substituent number (1), even though it does not have the lowest sum of substituent numbers (1 + 6 = 7 versus 3 + 2 = 5).

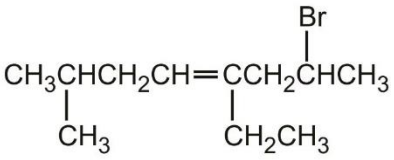
Solved Example



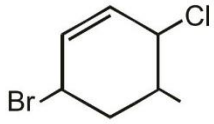
1,6-dichlorocyclohexene
not
2,3-dichlorocyclohexene
because 1 < 2



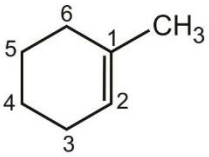
5-ethyl-1-methylcyclohexene
not
4-ethyl-2-methylcyclohexene
because 1 < 2



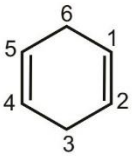
2-bromo-4-ethyl-7-methyl-4-octene
not
7-bromo-5-ethyl-2-methyl-4-octene
because 4 < 5



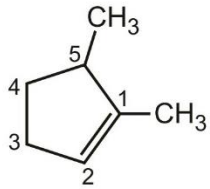
6-bromo-3-chloro-4-methylcyclohexene
not
3-bromo-6-chloro-5-methylcyclohexene
because 4 < 5



1-Methyl cyclohexene



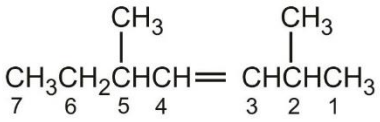
1,4-Cyclohexadiene
(New: Cyclohexa-1,4-diene)

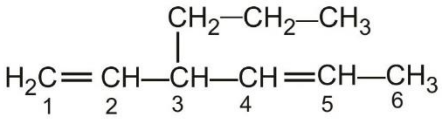


1,5-Dimethylene cyclopent

☞ We should also note that IUPAC changed their naming recommendations in 1993 to place the locant indicating the position of the double bond immediately before the -ene suffix rather than before the parent name: but-2-ene rather than 2-butene, for instance. This change has not been widely accepted by the chemical community in the United States, however, so we'll stay with the older but more commonly used names. Be aware, though, that you may occasionally encounter the newer system.

Solved Example





Older naming system : 2,5-Dimethyl-3-heptene — 3-Propyl-1,4-hexadiene
(Newer naming system: 2,5-Dimethylhept-3-ene — 3-Propylhexa-1,4-diene

Common names of Some Alkenes

Compound	Systematic name	Common name
$H_2C=CH_2$	Ethene	Ethylene
$CH_3CH=CH_2$	Propene	Propylene
$CH_3C(CH_3)=CH_2$	2-Methylpropene	Isobutylene
$H_2C=C(CH_3)-CH=CH_2$	2-Methyl-1,3-butadiene	Isoprene

ALKENES AS SUBSTITUENTS

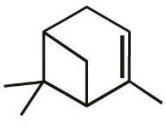
- In some cases, a group containing an alkene may need to be treated as a substituent.
- In these cases the substituent is named in a similar fashion to simple alkyl substituents.

Alkenyl group	Common name	Systematic name
$CH_2=CH-$	Vinyl-	ethenyl
$CH_2=CHCH_2-$	allyl-	2-propenyl
$CH_3CH=CH-$	—	1-propenyl

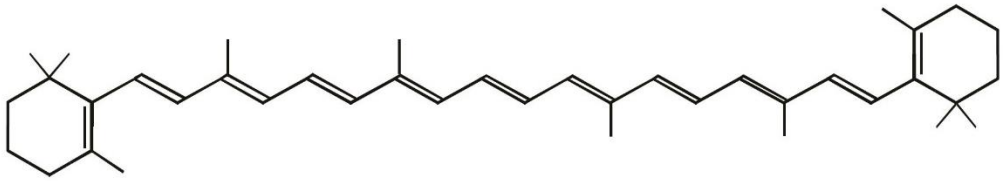
☑ SPECIAL TOPIC

ALKENES (SOMETIMES CALLED OLEFINS) CONTAIN C=C DOUBLE BONDS

It may seem strange to classify a type of bond as a functional group, but you will see later that C=C double bonds impart reactivity to an organic molecule just as functional groups consisting of, say, oxygen or nitrogen atoms do. Some of the compounds produced by plants and used by perfumers are alkenes (see Chapter 1). For example, pinene has a smell evocative of pine forests, while limonene smells of citrus fruits.



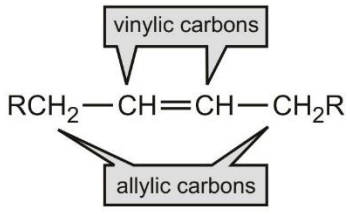
α-pinene



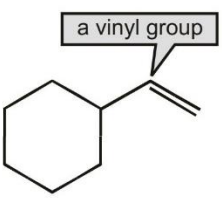
β-carotene

ALLYLIC AND VINYLIC CARBON

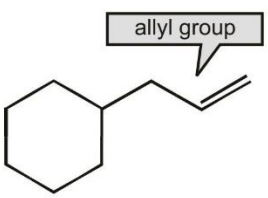
The sp^2 carbons of an alkene are called vinylic carbons . An sp^3 carbon that is adjacent to a vinylic carbon is called an allylic carbon. A hydrogen bonded to a vinylic carbon is called a vinylic hydrogen , and a hydrogen bonded to an allylic carbon is called an allylic hydrogen.



	$CH_2=CHCl$	$CH_2=CHCH_2Br$
common name:	vinyl chloride	allyl bromide
systematic name:	chloroethene	3-bromopropene



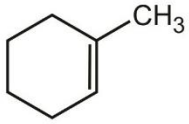
vinylcyclohexane

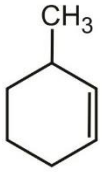


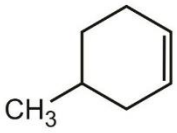
allylcyclohexane

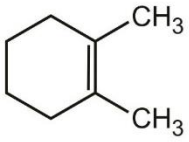
Special Example

- How many carbons are in the planar double-bond system in each of the following compounds?

(a) 

(b) 

(c) 

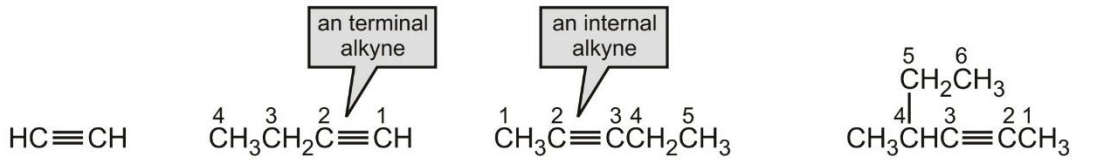
(d) 

Sol. (a) 5 (b) 4 (c) 4 (d) 6

THE NOMENCLATURE OF ALKYNES

Because of its triple bond, an alkyne has four fewer hydrogens than an alkane with the same number of carbons. Therefore, while the general molecular formula for an acyclic alkane is C_nH_{2n+2}, the general molecular formula for an acyclic alkyne is C_nH_{2n-2} and that for a cyclic alkyne is C_nH_{2n-4}.

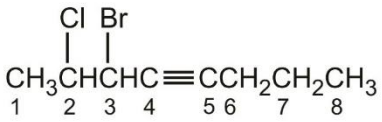
The systematic name of an alkyne is obtained by replacing the "ane" ending of the alkane name with "yne." Analogous to the way compounds with other functional groups are named, the longest continuous chain containing the carbon–carbon triple bond is numbered in the direction that gives the functional group suffix as low a number as possible. If the triple bond is at the end of the chain, the alkyne is classified as a terminal alkyne . Alkynes with triple bonds located elsewhere along the chain are internal alkynes.



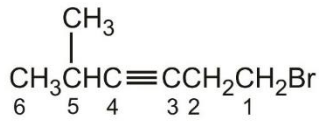
Systematic:	ethyne	1-butyne	2-pentyne	4-methyl-2-hexyne
Common:	acetylene	ethylacetylene	ethylmethylacetylene	*sec*- butylmethylacetylene

☞ If counting from either direction leads to the same number for the functional group suffix, the correct systematic name is the one that contains the lowest substituent number. If the compound contains more than one substituent, the substituents are listed in alphabetical order.

Solved Example

- 

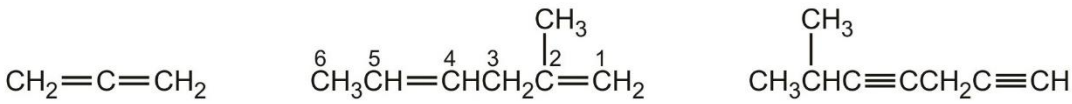
3-bromo-2-chloro-4-octyne
not 6-bromo-7-chloro-4-octyne
because 2 < 6



1-bromo-5-methyl-3-hexyne
not 6-bromo-2-methyl-3-hexyne
because 1 < 2

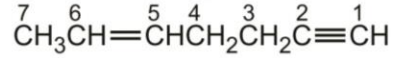
HOW TO NAME A COMPOUND THAT HAS MORE THAN ONE FUNCTIONAL GROUP

The rules for naming compounds with two triple bonds, using the ending "diyne", are similar to the rules for naming compounds with two double bonds.

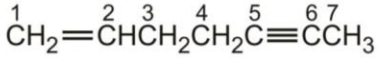


Systematic:	propadiene	2-methyl-1,4-hexadiene	6-methyl-1,4-heptadiyne
Common:	allene	or	or
		2-methylhexa-1,4-diene	6-methylhepta-1,4-diyne

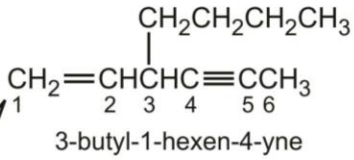
☞ If the two functional groups are a double bond and a triple bond , number the chain in the direction that produces a name containing the lower number. Thus, in the following examples, the lower number is given to the alkyne suffix in the compound on the left and to the alkene suffix in the compound on the right.



5-hepten-1-yne *not* 2-hepten-6-yne
because 1 < 2



1-hepten-5-yne *not* 6-hepten-2-yne
because 1 < 2

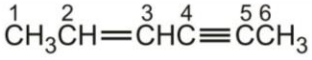


3-butyl-1-hexen-4-yne

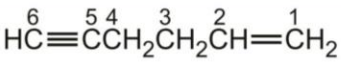
the longest continuous chain has 8 carbons, but the 8-carbon chain does not contain both functional groups; therefore, the compound is named as a hexenyne because the longest continuous chain containing both functional groups has 6 carbons

Solved Example

▸



2-hexen-4-yne
not 4-hexen-2-yne



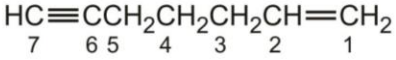
1-hexen-5-yne
not 5-hexen-1-yne

☞ If there is a tie between a double bond and a triple bond, the double bond gets the lower number.

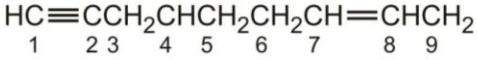
☞ Compounds with more than one triple bond are called diynes, triynes, and so forth; compounds containing both double and triple bonds are called enynes (not ynenes). Numbering of an enyne chain starts from the end nearer the first multiple bond, whether double or triple. When there is a choice in numbering, double bonds receive lower numbers than triple bonds.

Solved Example

▸

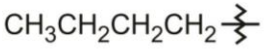


1-Hepten-6-yne
(New : Hept-1-en-6-yne)

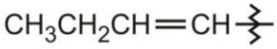


4-Methyl-7-nonen-1-yne
(New : 4-Methyl-7-nonen-1-yne)

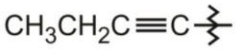
☞ As with alkyl and alkenyl substituents derived from alkanes and alkenes, respectively, alkynyl groups are also possible.



Butyl
(an alkyl group)



1-Butenyl
(a vinylic group)
(New : But-1-enyl)



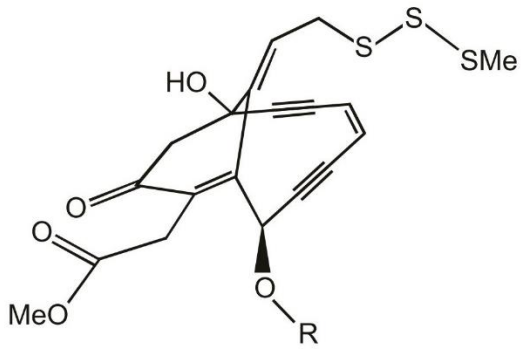
1-Butynyl
(an alkynyl group)
(New : But-1-ynyl)

☑ SPECIAL TOPIC

ALKYNES CONTAIN C ≡ C TRIPLE BONDS

Just like C = C double bonds, C ≡ C triple bonds have a special type of reactivity associated with them, so it's useful to call a C ≡ C triple bond a functional group. Alkynes are linear so we draw them with four carbon atoms in a straight line. Alkynes are not as widespread in nature as alkenes, but one fascinating class of compounds

containing C ≡ C triple bonds is a group of antitumour agents discovered during the 1980s. Calicheamicin is a member of this group. The highreactivity of this combination of functional groups enables calicheamicin to attack DNA and prevent cancer cells from proliferating. For the first time we have drawn a molecule in three dimensions, with two bonds crossing one another—can you see the shape?

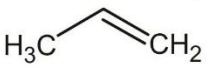
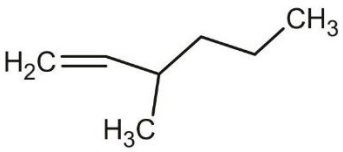
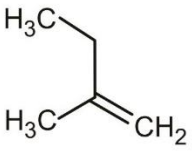
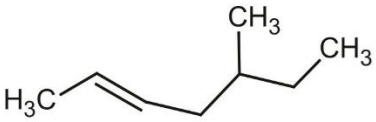
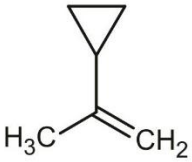
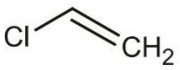
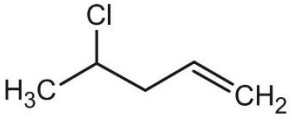


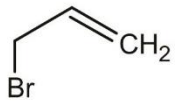
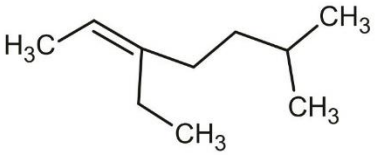
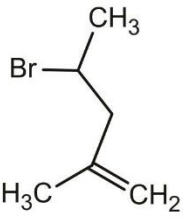
calicheamicin
(R = a string of sugar molecules)

► **Saturated and unsaturated carbon atoms**
In an alkane, each carbon atom is joined to four other atoms (C or H). It has no potential for forming more bonds and is therefore saturated. In alkenes, the carbon atoms making up the C=C double bond are attached to only three atoms each. They still have the potential to bond with one more atom, and are therefore unsaturated. In general, carbon atoms attached to four other atoms are saturated; those attached to three, two, or one are unsaturated.

EXERCISE

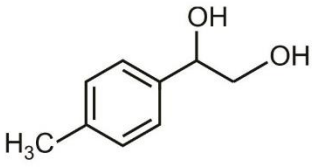
WORK SHEET - 1

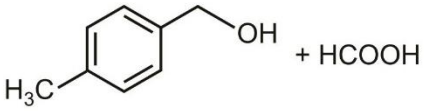
S.No.	Compounds	Write IUPAC - Name
1.		
2.		
3.		
4.		
5.		
6.		
7.		

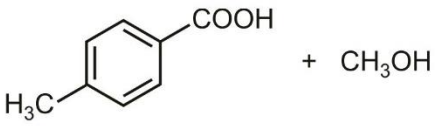
8.		
9.		
10.		

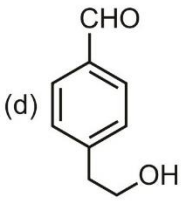
SUBJECTIVE TYPE QUESTIONS

1. The reaction of 50% aq. KOH on an equimolar mixture of 4 -methylbenzaldehyde and formaldehyde followed by acidification gives :

(a) 

(b) 

(c) 

(d) 

Answers

Work Sheet - 1

1. propene **2.** 3-methylhex-1-ene **3.** 2-methylbut-1-ene **4.** 5-methylhept-2-ene
5. 2-cyclopropylpropene **6.** chloroethene **7.** 4-chloropent-1-ene **8.** 3-bromoprop-1-ene
9. 3-ethyl-6-methylhept-2-ene **10.** 4-bromo-2-methylpent-1-ene

Subjective Type Questions

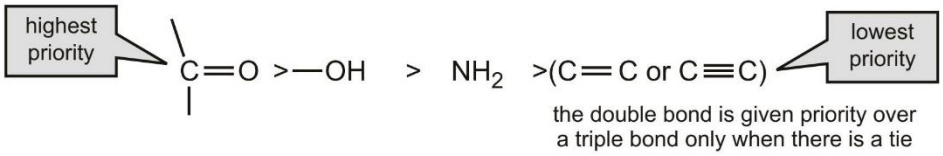
1. (b)

❑❑❑

CHAPTER
9

Nomenclature of Alcohol, Ether, Aldehyde and Ketone

PRIORITIES OF FUNCTIONAL GROUP SUFFIXES



The following rules are used to name a compound that has a functional group suffix :

1. The parent hydrocarbon is the longest continuous chain containing the functional group .
2. The parent hydrocarbon is numbered in the direction that gives the functional group suffix the lowest possible number .

☑ SPECIAL TOPIC

NAME ALCOHOL COMES FROM ?

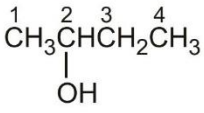
Arabic alchemy has given us a number of chemical terms; for example, alcohol is believed to derive from Arabic al-khwl or al-ghawl whose original meaning was a metallic powder used to darken women's eyelids (Kohl).

Alcohol entered the English language in the 17th Century with the meaning of a "sublimated" substance, then became the "pure spirit" of anything, and only became associated with "spirit of wine" in 1753. finally, in 1852, it become a part of chemical nomenclature that denoted a common class of organic compound. But it's still common practice to refer to the specific substance CH_3CH_2OH as "Alcohol" rather then its systematic name ethanol.

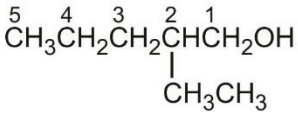
Solved Example

- $CH_3CH(OH)CH_3$
  - Functional groups is an alcohol, therefore suffix = -ol
  - Hydrocarbon structure is an alkane therefore -ane
  - The longest continuous chain is C3 therefore root = prop
  - It doesn't matter which end we number from, the alcohol group locant is 2-

Ans. **Propan-2-ol**

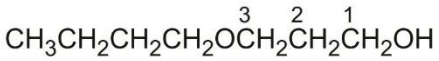


2-butanol
or
butan-2-ol



2-ethyl-1-pentanol
or
2-ethylpentan-1-ol

The longest continuous chain has six carbons, but the longest continuous chain containing the OH functional group has five carbons so the compound is named as a pentanol.

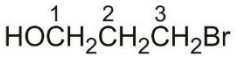


3-butoxy-1-propanol
or
3-butoxypropan-1-ol

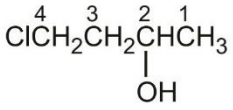
The longest continuous chain has four carbons, but the longest continuous chain containing the OH functional group has three carbons, so the compound is named as a propanol.

☞ If there is a functional group suffix and a substituent, the functional group suffix gets the lowest possible number.

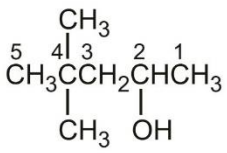
Solved Example



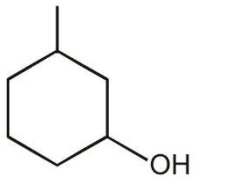
3-bromo-1-propanol



4-chloro-2-butanol



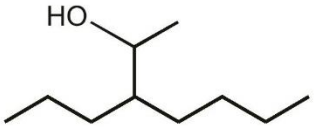
4,4-dimethyl-2-pentanol



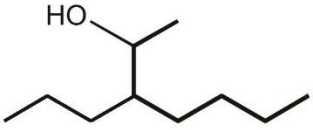
3-methylcyclohexanol
not
5-methylcyclohexanol

Solved Example

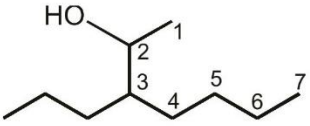
- For the compound below, choose the parent chain and then number it correctly :



Ans. To choose the parent chain, remember that we need to choose the longest chain containing the functional group:



To number it correctly, we need to go in the direction that gives the functional group the lowest number:



NAME: 3-Propyl-2-heptanol

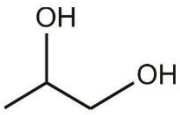
DIOLS (OR POLYOLS)

- Functional group is an alcohol, therefore suffix **= -ol**
- Hydrocarbon structure is an alkane therefore**-ane**
- There are two alcohols, so insert the multiplier **di**
- The longest continuous chain is C2 therefore root **= eth**

ethane-1,2-diol

or

1,2-ethanediol

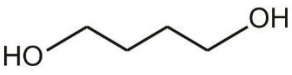


- Hydrocarbon structure is an alkane therefore**-ane**
- There are two alcohols, so insert the multiplier **di**
- The longest continuous chain is C3 therefore root **= prop**
- Locants for -OH units are **1-** and **2-**

Propane-1, 2-diol

or

1,2-propanediol

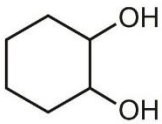


- Hydrocarbon structure is an alkane therefore **-ane**
- There are two alcohols, so insert the multiplier **di**
- The longest continuous chain is C4 therefore root **= but**

butane-1,4-diol

or

1,4-butanediol



- Hydrocarbon structure is an alkane therefore **-ane**
- There are two alcohols, so insert the multiplier **di**
- The ring is C6 therefore root **= cyclohex**
- Locants for –OH units are **1-** and **2-**

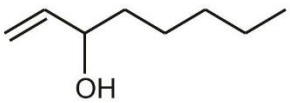
Cyclohexane-1,2-diol

or

1,2-cyclohexanediol

☑ SPECIAL TOPIC

HOW A BANANA SLUG KNOWS WHAT TO EAT



1-octene-3-ol

Many species of mushrooms synthesize 1-octen-3-ol, a repellent that drives off predatory slugs. Such mushrooms can be recognized by small bite marks on their caps, where the slug started to nibble before the volatile compound was released. People are not put off by the release of this compound because to them it just smells like a mushroom. 1-Octen-3-ol also has antibacterial properties that may protect the mushroom from organisms that would otherwise invade the wound made by the slug. Not surprisingly, the species of mushroom that banana slugs commonly eat cannot synthesize 1-octen-3-ol.

Solved Example

▸ (a) $CH_3—CH_2—CH_2—CH_2—OH$
Butan-1-ol

(b) $CH_3—\underset{\displaystyle OH}{\underset{|}{CH}}—CH_3$
Propan-2-ol

(c) $CH_3—\underset{\displaystyle CH_3}{\overset{\displaystyle CH_3}{\overset{|}{\underset{|}{C}}}}—OH$
2-Methylpropan-2-ol

COMMON AND IUPAC NAMES OF SOME ALCOHOLS

Compound	Common name	IUPAC name
$CH_3—OH$	Methyl alcohol	Methanol
$CH_3—CH_2—CH_2—OH$	*n*-Propyl alcohol	Propan-1-ol
$CH_3—\underset{\displaystyle OH}{\underset{|}{CH}}—CH_3$	Isopropyl alcohol	Propan-2-ol
$CH_3—CH_2—CH_2—CH_2—OH$	*n*-Butyl alcohol	Butan-1-ol
$CH_3—\underset{\displaystyle OH}{\underset{|}{CH}}—CH_2—CH_3$	sec-Butyl alcohol	Butan-2-ol
$\overset{\displaystyle CH_3}{\overset{|}{CH_2}}—CH—CH_3$ (OH on CH_2)	Isobutyl alcohol	2-Methylpropan-1-ol
$CH_3—\overset{\displaystyle CH_3}{\overset{|}{\underset{|}{C}}}—OH$ (CH_3)	tert-Butyl alcohol	2-Methylpropan-2-ol
$CH_2(OH)—CH(OH)—CH_2(OH)$	Glycerol	Propan-1,2, 3-triol

☑ SPECIAL TOPIC

ETHERS ($R^1–O–R^2$) CONTAIN AN ALKOXY GROUP (–OR)

The name ether refers to any compound that has two alkyl groups linked through an oxygen atom. 'Ether' is also used as an everyday name for diethyl ether, Et_2O. You might compare this use of the word 'ether' with the common use of the word 'alcohol' to mean ethanol. Diethyl ether is a highly flammable solvent that boils at only 35°C. It used to be used as an anaesthetic. Tetrahydrofuran (THF) is another commonly used solvent and is a cyclic ether.

► Another common laboratory solvent is called 'petroleum ether'. Don't confuse this with diethyl ether! Petroleum ether is in fact not an ether, but a mixture of alkanes. 'Ether', according to the Oxford English Dictionary, means 'clear sky, upper region beyond the clouds', and hence used to be used for anything light, airy, and volatile.

Compound	IUPAC name
CH_3OCH_3	Methoxymethane
$C_2H_5OC_2H_5$	Ethoxyethane
$CH_3OCH_2CH_2CH_3$	1-Methoxypropane

ETHERS

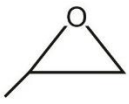
Common names of ethers are derived from the names of alkyl/aryl groups written as separate words in alphabetical order and adding the word 'ether' at the end. For example, $CH_3OC_2H_5$ is ethylmethyl ether.

COMMON AND IUPAC NAMES OF SOME ETHERS

Compound	Common name	IUPAC name
CH_3OCH_3	Dimethyl ether	Methoxymethane
$C_2H_5OC_2H_5$	Diethyl ether	Ethoxyethane
$CH_3OCH_2CH_2CH_3$	Methyl *n*-propyl ether	1-Methoxypropane
$C_6H_5OCH_3$	Methylphenyl ether (Anisole)	Methoxybenzene (Anisole)
$C_6H_5OCH_2CH_3$	Ethylphenyl ether (Phenetole)	Ethoxybenzene
$C_6H_5O(CH_2)_6 - CH_3$	Heptylphenyl ether	1-Phenoxyheptane
$CH_3O-CH(CH_3)-CH_3$	methyl isopropyl ether	2-Methoxypropane

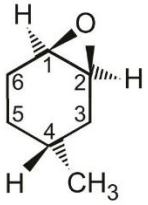
EPOXIDES

- Functional group is an epoxide, therefore suffix = –epoxide.
- The longest continuous chain is C3 therefore root **= prop.**
- Location of "alkene" is unambiguous, so no locant needed.

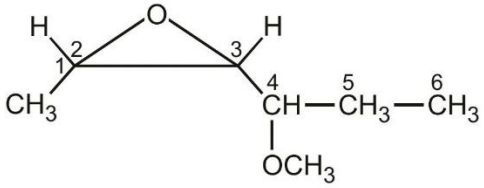


1,2-epoxypropane

One systematic method for naming epoxides is to name the rest of the molecule and use the term “epoxy” as a subsituent, giving the numbers of the two carbon atoms bonded to the epoxide oxygen.

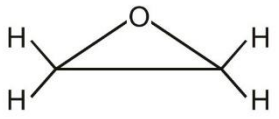


trans-1,2-epoxy-4-methylcyclohexane

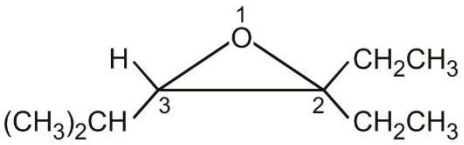


cis-2-3-epoxy-4-methoxyhexane

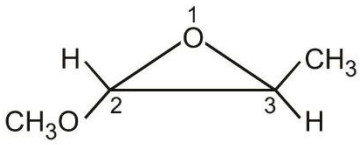
Another systematic method names epoxides as derivatives of the parent compound, ethylene oxide, using “oxirane” as the systematic name for ethylene oxide. In this system, the ring atoms of a heteroxyclic compound are numbered starting with the heteroatom and going the direction to give the lowest substituent numbers. The “epoxy” system names are also listed for comparison. Note that the numbering is different for the “epoxy” system names, which number the longest chain rather than the ring.



oxirane
1,2-epoxyethane



2,2-diethyl-3-isopropyloxirane
3,4-epoxy-4-ethyl-2-methylhexane



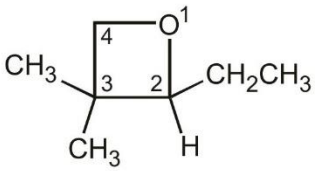
trans-2-methoxy-3-methyloxirane
1,2-epoxy-1-methoxypropane

☑ SPECIAL TOPIC

OXETANES

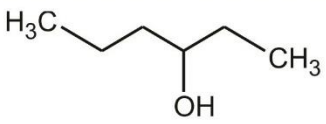
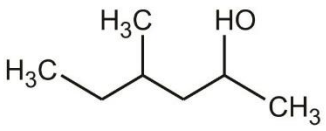
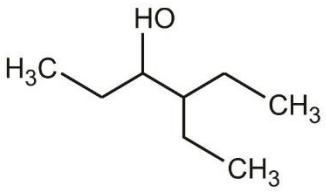
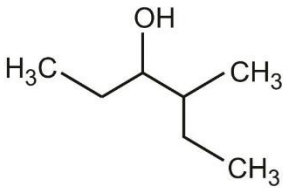
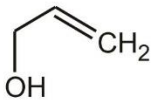
The least common cyclic ethers are the four-membered oxetanes. Because these four-membered rings are strained, they are more reactive than larger cyclic ethers and open-chain ethers. However they are not as reactive as the highly strained oxiranes (epoxides).

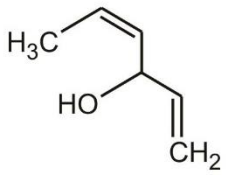
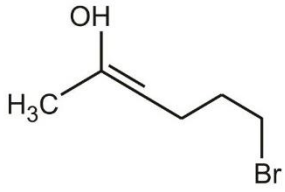
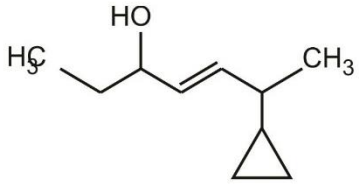
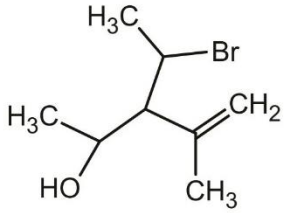
oxetane



2-ethyl-3,3-dimethyloxetane

WORK SHEET

S.No.	Compounds	Write IUPAC - Name
1.		
2.		
3.		
4.		
5.		

6.		
7.		
8.		
9.		
10.		

Answers

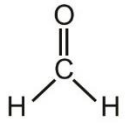
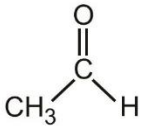
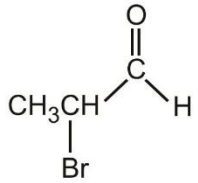
Work sheet

1. hexan-3-ol
2. 4-methylhexan-2-ol
3. 4-ethylhexan-3-ol
4. 4-methylhexan-3-ol
5. prop-2-en-1-ol
6. hexa-1,4-dien-3-ol
7. 6-bromohex-2-en-2-ol
8. hexa-1,5-dien-1-ol
9. 6-cyclopropylhept-4-en-3-ol
10. 3-(1-bromoethyl)-4-methylpent-4-en-2-ol

THE NOMENCLATURE OF ALDEHYDES

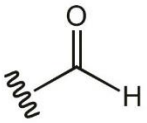
NAMING ALDEHYES

The systematic (IUPAC) name of an aldehyde is obtained by replacing in final “e” on the name of the parent hydrocarbon with “al.” For example. A one-carbon aldehyde is called methanal, and two-carbon aldehyde is called ethanal. The position of the carbonyl carbon does not have to be designated because it is always at the end of the parent hydrocarbon (or else the compound would not be an aldehyde). So it always has the 1-position.

			
systematic name:	methanal	ethanal	2-bromopropanal
common name :	formaldehyde	acetaldehyde	α-bromopropionaldehyde

Points to Remember

- –CHO represents:



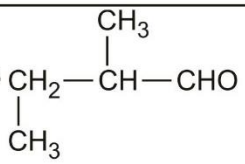
When we write aldehydes as R–CHO, we have no choice but to write in the C and H (because they're part of the functional group).

◎ Mistake to Avoid

- For drawing structures.

  Another point: always write R–CHO and never R–COH, which looks too much like an alcohol.

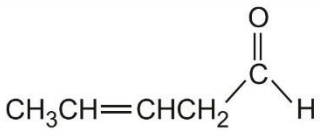
Solved Example

- The IUPAC name of is 

Ans. 2-methyl butanal

☞ If one of the functional groups is an alkene, suffix endings are used for both functional groups and the alkene functional group is stated first, with its "e" ending omitted to avoid two successive vowels.

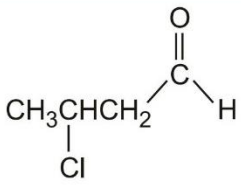
Solved Example

- 

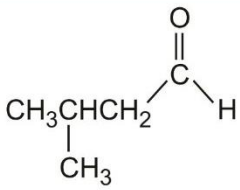
3-pentenal

☞ Note that the terminal "e" of the parent hydrocarbon is not removed in hexanedial (The "e" is removed only to avoid two successive vowels.)

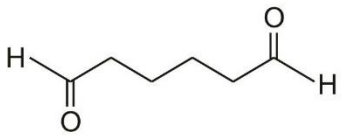
Solved Example



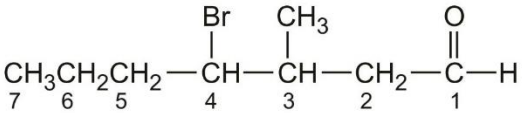
systematic name: 3-chlorobutanal
common name : β-chloropionaldehyde



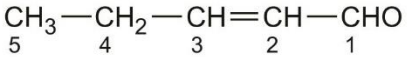
3-methylbutanal
isovaleraldehyde



hexanedial



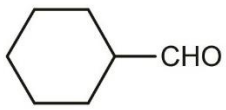
4-bromo-3-methylheptanal



2-pentenal or pent-2-enal

☞ If the aldehydic group is attached to a ring, then the suffix carbaldehyde is added to the full name of cyclohexane.

Example



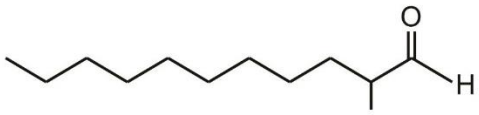
Cyclohexanecarbaldehyde

4-Nitrobenzenecarbaldehyde
or
4-Nitrobenzaldehyde

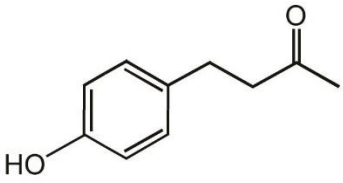
☑ SPECIAL TOPIC

SPECIAL TOPIC: ALDEHYDES (R–CHO) AND KETONES (R^1–CO–R^2) CONTAIN THE CARBONYL GROUP C = O

Aldehydes can be formed by oxidizing alcohols—in fact the liver detoxifies ethanol in the bloodstream by oxidizing it first to acetaldehyde (ethanal, CH_3CHO). Acetaldehyde in the blood is the cause of hangovers. Aldehydes often have pleasant smells—2-methylundecanal is a key component of the fragrance of Chanel No 5™, and 'raspberry ketone' is the major component of the flavour and smell of raspberries.

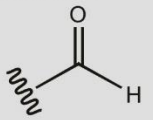


2-methylundecanal



"raspberry ketone"

► **—CHO represents :**



When we write aldehydes as R—CHO, we have no choice but to write in the C and H (because they're part of the functional group) — one important intance where you should ignore Guideline 3 for drawing structures.

Another point : always write R—CHO and never R—CHO, which looks too much like an alcohol.

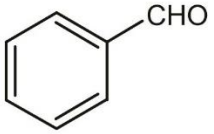
COMMON NAMES OF ALDEHYDE & KETONE ALDEHYDES :

- Often called by their common names instead of IUPAC names.
- Derived from the common names of the carboxylic acids by replacing the ending '–ic' of the acid with aldehyde.
- Location of the substituent in the carbon chain is indicated by the Greek letters $\alpha, \beta, \gamma, \delta$ etc.

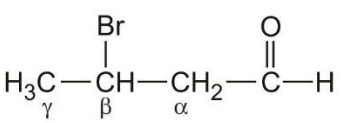
Example

CH_3CHO

Acetaldehyde



Benzaldehyde



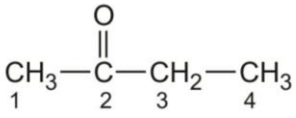
β-Bromobutyraldehyde

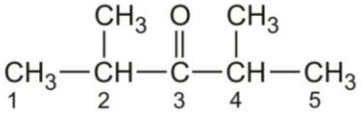
NOMENCLATURE OF KETONES

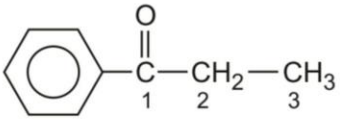
IUPAC NAMES

- For open-chain aliphatic aldehydes and ketones, IUPAC names are derived from the names of the corresponding alkanes by replacing the ending '–e' with '–al' and '–one' respectively.
- In the case of aldehydes, the longest chain is numbered starting from the carbon of the aldehydic group.
- In the case of ketones, the numbering begins from the end nearer to the carbonyl group.
- Substituents are prefixed in the alphabetical order along with the numerals indicating their positions in the carbon chain.
- Same rule is applicable to cyclic ketones.

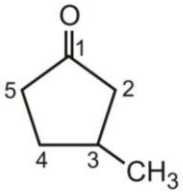
Solved Example



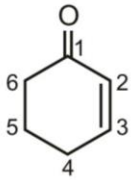




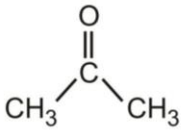
old IUPAC names: 2-butanone | 2,4-dimethyl-3-pentanone | 1-phenyl-1-propanone
new IUPAC names: butan-2-one | 2,4-dimethylpentan-3-one | 1-phenylpropan-1-one

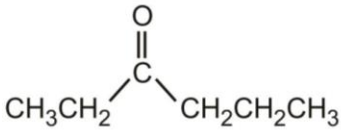


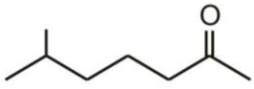
3-methylcyclopentanone



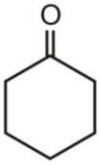
2-cyclohexenone
cyclohex-2-en-1-one

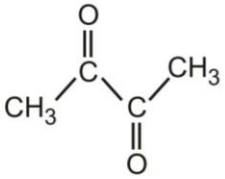


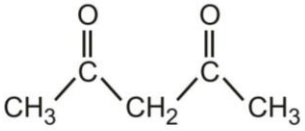


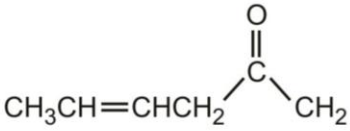


systematic name: propanone | 3-hexanone | 6-methyl-2-heptanone
common name : acetone
derived name : **dimethyl ketone** | **ethyl propyl ketone** | **isohexyl methyl ketone**





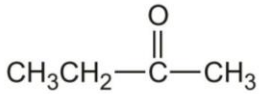




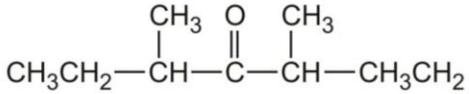
systematic name : cyclohexanone | butanedione | 2,4-pentanedione | 4-hexen-2-one
common name : acetylacetone

COMMON NAMES

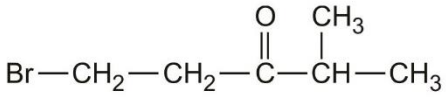
As with other classes of compounds, ketones and aldehydes are often called by common names instead of their systematic IUPAC names. Ketone common names are formed by naming the two alkyl groups bonded to the carbonyl group. Substituent locations are given using Greek letters, beginning with the carbon next to the carbonyl group.



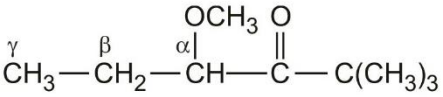
ethyl methylketone



di-sec-butyl ketone



bromoethyl isopropyl ketone

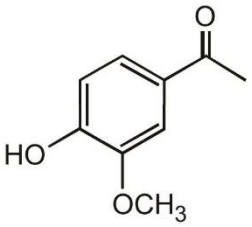


tert-butyl -methoxypropyl ketone

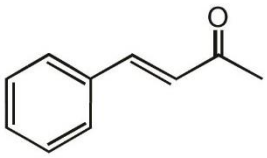
☑ SPECIAL TOPIC

SPECIAL TOPIC: SMELLS OF ALDEHYDE AND KETONES

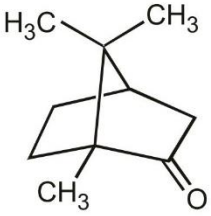
Many compounds found in nature have aldehyde or ketone functional groups. Aldehydes have pungent odors. Whereas ketones tend to smell sweet. Vanillin and cinnamaldehyde are examples of naturally occurring aldehydes. A whiff of vanilla extract will allow you to appreciate the pungent odor of vanillin. The ketones camphor and carvone are responsible for the characteristic sweet odoros of the leaves of camphor trees, spearmint leaves, and caraway seeds.



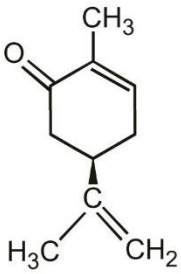
vanillin
vanilla flavoring



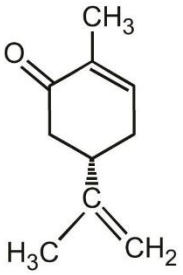
cinnamaldehyde
cinnamon flavoring



camphor

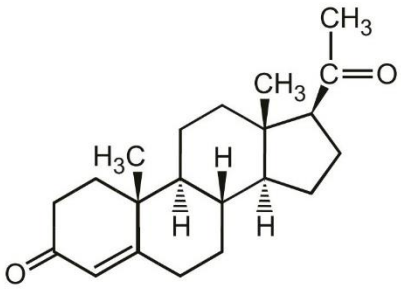


(R)-(–)-carvone
spearmint oil

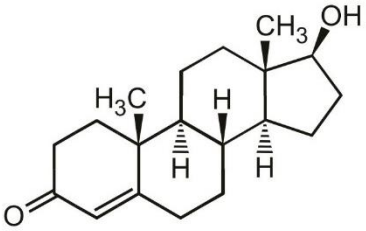


(S)-(+)-carvone
caraway speed oil

Progesterone and testosterone are two biologically important ketones that illustrate how a small difference in structure can be responsible for a large difference in biological activity. Both are sex hormones, but progesterone is synthesized primarily in the ovaries, where testosterone is synthesized primarily in the testes.



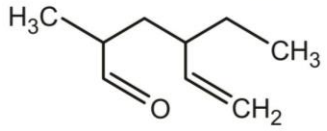
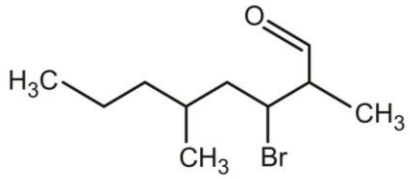
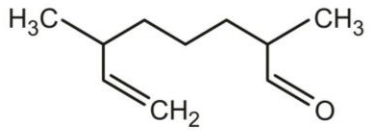
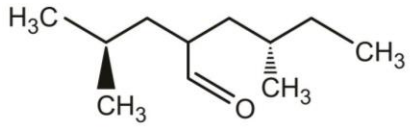
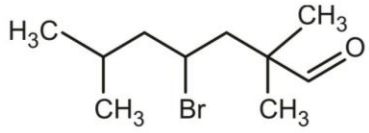
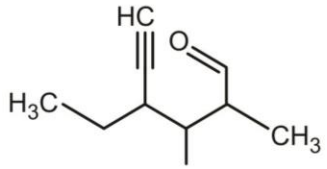
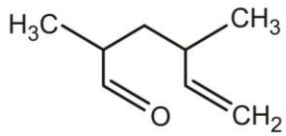
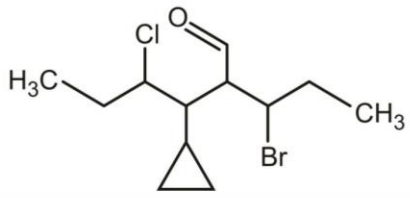
progesterone



testosterone

EXERCISE

WORK SHEET - 1

S.No.	Compounds	Write IUPAC - Name
1.		
2.		
3.		
4.		
5.		
6.		
7.		
8.		

Answers

Work Sheet-1

1. 4-ethyl-2-methylhex-5-enal
2. 3-bromo-2,5-dimethyloctanal
3. 2,6-dimethyloct-7-enal
4. 4-methyl-2-(2-methylpropyl)hexanal
5. 4-bromo-2,2,6-trimethylheptanal
6. 4-ethyl-2,3-dimethylhex-5-ynal
7. 2,4-dimethylhex-5-enal
8. 2-(1-bromopropyl)-4-chloro-3-cyclopropylhexanal

❑❑❑❑