General organic chemistry-II



- Nomenclature of hydrocarbons
- Organic compounds with functional groups
- Nomenclature of aromatic compounds

Nomenclature of bicyclic compounds

Introduction

- The carbon atom is unique in its bonding in that it can form stable molecules consisting of chains of carbon atoms of any length
- Coupled with the observation that each carbon atom forms four bonds to other atoms this leads to incomprehensibly large numbers of possible molecules

How?

Because every organic compound contains carbon, and almost every one contains hydrogen, the names of these two elements do not appear directly in the compound names.

At its simplest, the name for an organic compound contains two parts:

(1) a root indicating the number of carbon atoms in the longest continuous chain of carbon atoms

(2) a prefix and/or suffix to indicate the functional group to which the compound belongs

Example: "ethanol" indicates a carbon chain of length two (ethan-) and an OH functional group (-ol).



Nomenclature of branched alkanes

(i) Locate the longest chain of carbon atoms; this chain determines the parent name for the alkane.

(ii) Number the longest chain beginning with the chain nearer the substituent.



Nomenclature of branched alkanes (iii) Use the number obtained by the application of rule 2 to designate the location of the substituents group. CH₃CH₂CH₂CH₂CH₂CH₃ ² CH₂CH₃ 4-ethyl-2-methylhexane (iv) When two or more substituents are present, give each substituent a number corresponding to its location on the longest chain. CH₃CH—CH₂—CHCH₂CH₃ CH₃ CH₂CH₃ 4-ethyl-2-methylhexane



Nomenclature of branched alkanes

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



 (viii) When branching first occurs at an equal distance from either end of the longest chain, choose the name that gives the lower number at the first point of difference. CH₃CH-CH₂-CH-CH-CH₃

$$CH_3$$
 CH_3 CH_3 CH_3 CH_3 CH_3

(not 2,4,5-trimethylhexane)

Nomenclature of organic compound:Six Step Process

- 1) Find the longest carbon chain
- 2) Name it
- 3) Determine any ending
- 4) Numbering of the carbon atoms
- 5) Separate and name side/substituent groups
- 6) List side/substituent groups alphabetically

Step 1: Find the longest carbon chain

Find the longest, uninterrupted, continuous carbon chain.

It is not required that in the picture or drawing of the carbon chain that atoms all are in line only that it is the longest continuous carbon chain





Step 2: Name it

Name it.

Count the number of carbons in the chain and select the appropriate root name based on the number of carbon atoms on the chain

Butane

Ethane



Root Names									
	Number of	<u>Root</u>	Number of	Root					
	<u>Carbon</u>	<u>Name</u>	<u>Carbon</u>	Name					
	<u>Atoms</u>		<u>Atoms</u>						
	1	meth	11	undec					
	2	eth	12	dodec					
	3	prop	13	tridec					
	4	but	14	tetradec					
	5	pent	15	pentadec					
	6	hex	20	icos					
	7	hept	21	henicos					
	8	oct	22	docos					
	9	non	30	triacont					
	10	dec	40	tetracont					

Step 3: Determine any ending

Determine if any ending needs to be added to the base name

This is determined by the presence of a *functional group* on any of the carbon atoms

A list of functional groups and their structure can be found on next slide

Butane

Ethanol



Compound Class	<u>Ending</u>	Functional	
		<u>Group</u>	
Alkanes	-ane	None	
Haloalkanes	-ane	—X	O.
Alcohols	-ol	—ОН	
Ethers	ether	-0-	
Alkenes	-ene	—C=C—	0
Alkynes	-yne	—C≡C—	Ĭ
Aldehydes	-al	—сно	ĊO
Ketones	-one	—CO—	
Carboxylic Acids	-oic acid	—соон	
Esters	-oate	-CO-O-	CC
Anhydrides	anhydride		
Amides	-ide		
Nitriles	-ile	—C≡N	N
Amines	-amine		

Priority of functional groups

If more than one functional group is present then we decide the the parent functional group on the basis of the following priority basis.

Decreasing priority of the functional group

 $-COOH, -SO_3H, -COOR, -COCI, -CONH_2, -CN, -CHO, >CO, -OH, -NH_2, >C=C<, -C=C-.$

Step 4: Number the carbon atoms

Start at both ends of the carbon chain, naming the first carbon #1, the next #2, and so on

Find which end leads to or arrives at a side group first

That end then becomes the carbon #1 end

Number each carbon continuously through to the other end of the main chain starting with #1



Step 4: Number the carbon atoms

- If both ends of the chain come to a side group with the same number of carbons, then the side with the more complex group (contains more atoms) becomes the end that receives the #1 label on its end carbon
 - If that also is a tie then the next tie breaker is alphabetizing the side groups
 - The higher order or first occurring alphabetical character side group becomes carbon #1

Illustrative example The correct name of the given compound will be



- (a) Cycloethylmethylpentane
- (b) 1-ethyl-3-methylpentane
- (c) 1-ethyl-3-methylcyclopentane
- (d) 1-methyl-3-ethylcyclopentane

Solution

1-ethyl-3-methylcyclopentane

Hence correct option is (c).

Step 5: Separate and name substituent groups

- Separate out and individually name all the substituent side groups or chains, sometimes referred to as pendent groups
- The common names for side groups are
 - CI = chloro
 - F = fluoro
 - Br = bromo
 - OH = hydroxy
 - NH₂ = amino
 - CN = cyano
 - $NO_2 = nitro$



1,3-dibromo-2-butanone

Names of branched alkyl Groups

Structure	Common Name	Systematic Name	Derived From	Designation
н ₃ с — с — Н	Isopropyl	1-Methylethyl	Propane	Secondary
CH ₃ H ₃ CCCH ₂ H	Isobutyl	2-Methylpropyl	2-Methylpropane (Isobutane)	Primary
СН ₃ 	sec-Butyl	1-Metylpropyl	Butane	Secondary
СН ₃ Н ₃ С — С — СН ₃	<u>tert</u> -Butyl	1,1-Dimethylethyl	2-Methylpropane (Isobutane)	Tertiary
CH ₃ H ₃ CCCH ₂ CH ₃	Neopentyl	2,2- Dimethylpropyl	2,2- Dimethylpropane (Neopentane)	Primary

Step 5: Separate and name substituent groups

The presence of a double bond between two carbons gives the *—ene* ending to the root and the number of carbon of the pair is put proceeding the root.

A triple bond gives a *-yne* ending, and the same proceeding number system.

$$2HC == CH == CH_2 \qquad CH_3 - CH_2 - C \equiv C$$
butadiene
$$1 - but yne$$

Step 5: Separate and name substituent groups

- If two of the same atoms appear in a molecule, the word "di" is used to describe it.
- If three similar atoms appear in a molecule, the word "tri" is used to describe it.

-4-tetra

-5-penta

These prefixes are inserted directly before the name of the group.
 F F

buta diene



*tetra*flouroethylene

Illustrative example

The correct name of the given compound will be



(a)5-isopropyl-5-methyl-3-heptanone
(b)3-isopropyl-5-methylheptanone
(c)5,6-dimethyl-5-ethyl-3-heptanone
(d)5-ethyl-5,6-dimethyl-3-heptanone

Correct option is (d).

Illustrative example The correct name of the given compound will be



(a)4-isopropyl-2,5-dimethylhexanol (b)2,5-dimethyl-4-isopropyl-3-hexanol (c)2,5-dimethyl-4-isopropylhexanol (d)4-isopropyl-2,5-dimethyl-3-hexanol solution

4-isopropyl-2,5-dimethyl-3-hexanol

Hence correct option is (d).

Step 6: List substituent chains in alphabetical order

Write in alphabetical order all substituent chains or groups preceded by the carbon atom number where they are attached

$$\begin{array}{c}
H \\
H \\
H \\
H \\
C \\
H \\
H \\
H \\
H \\
H \\
H
\end{array}$$

1,6-Dichloro-2,5-dimethyl-3-hexyne

Step 6: List substituent chains in alphabetical order

The convention requires a parenthesis to be placed around the substituent chains or groups if it is more than a single atom or molecule

Commas are placed between numbers and dashes are placed between numbers and letters and in front of the parenthesis

A group of atoms appearing in the brackets is alphabetized by the real first letter of the group, whereas, normal convention does not treat the di's or tri's as part of the alphabetizing process

Illustrative example

Write the IUPAC name of the following compound.





4,5-Dichloro-2-[4'-chloro-2'-(hydroxymethyl)-5'oxohexyl]cyclohexane-1-carboxylic acid

Nomenclature of substituted **benzene compounds** Substituent is placed as prefix to the word benzene.

Bonobenzene

Ntrob

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





1,3-Dibromobenzene **HAR**

Nomenclature of substituted benzene compounds

In trivial system of nomenclature the terms *ortho*(*o*), *meta*(*m*), and *para*(*p*) are used as prefixes to indicate the relative positions of the substituents.

Nomenclature of bicyclic compounds

Named as bicycloalkanes





Spirocyclic

Condensed

Bridgehead

- First of all we count the total number of carbon atom(name drived from the number of total carbon atom).
- Identify the bridged carbon atomsto decide the number of carbon atoms in each bridge.
- Interpose in the name an expression in bracket that denote the number of carbon atoms in eatch bridge



Nomenclature of bicyclic compounds

If substituents are present, we start numbering from a bridged carbon atom and move in the direction of longest bridge.



8-methylbicyclo[5.3.0]nonane



3- Methylbicyclo[3.2.1]octane

Which is the correct IUPAC name for the following compound?

(a) 3, 4 - Dimethyl 3 - n - propylnonane
(b) 6, 7 - Dimethyle - n - propylnonane
(c) 4-Ethyl - 4, 5 - dimethyldecane
(d) 6, 7 - Dimethyl 7 - ethyldecane

Solution

Correct option is (c).

The IUPAC name of the compound having the structure

$$\begin{array}{c} \mathsf{CH}_3 - \mathsf{CH} - \mathsf{CH}_2 - \mathsf{CHCH}_2\mathsf{CI} \\ | & | \\ \mathsf{C}_2\mathsf{H}_5 & \mathsf{HO} & \mathsf{C}_2\mathsf{H}_5 \end{array}$$

(a)1 - Chloro -4- methylhexanol -2(b)3 - Chloro - 6 - methyl - 2 - octano

Solution

Correct option is (b).

The IUPAC name of the compound having the formula

 CH_3 $CH_3 - C - CH = CH_2$ CH_3 (a)1, 1- Dimethyl-1- butene (b) 3, 3, 3 - Trimethyl - 1 - propene (c) 1, 1, 1 - Trimethyl - 3 - propene (d) 3, 3 - Dimethyl - 1 - butene Solution **Correct option is (d).**

The IUPAC name of

 $\begin{array}{c} \mathsf{CH}_3\\ \mathsf{H}\\ \mathsf{CH}_3-\mathsf{N}-\mathsf{C}-\mathsf{CH}_2\mathsf{CH}_3\\ \mathsf{H}_3 & \mathsf{H}_2\mathsf{CH}_3\\ \mathsf{CH}_3 & \mathsf{CH}_2\mathsf{CH}_3 \end{array}$

(a) 3-Dimethylamino-3-methylpentane (b) 3- N,N- Dimethylamino) -3-ethylbutane (c) 3-Dimelthylamino-3- ethylbutane (d) 3, N,N-Trimethyl -3 pentanamine

Solution

Correct option is (d).



The IUPAC name of

 $CH_3 - CH - CH_2 - CH_3$

(a) 2 - Cyclohexylbutane
 (b) 2 - Phenylbutane
 (c) 3 - Cyclohexylbutane
 (d) 3 - Phenylbutane
 Solution
 Correct option is (a).

Class exercise 7 The IUPAC name of the compound $\begin{array}{c} \mathsf{CH}_3 - \mathsf{CH} - \mathsf{CH}_2 - \mathsf{C} - \mathsf{CH}_3 \\ | & | \end{array}$ OH OH (a)2 - Methyl - 2, 4 - pentanediol (b) 1, 1-Dimethyl -1, 3- butanediol (c) 4 - Methyl - 2, 4 - pentanediol (d) 1, 3, 3 - Trimethyl -1, 3 - propanediol Solution **Correct option is (a).**

The structure of 4 - methylpent -2 -ene is



Solution Correct option is (b).

Class exercise 9 Write the structural formula of

(i) 4 - Ethyl - 5 - methyl - 2 - hexene

(ii) 4 - oxo - pentane - 1 - oic acid

(iii) 1 - Hydroxy - 2 - Propanone

(iv) 3 - Chloro - 5 - yne - hexa - 1 - al Solution

(i)
$$CH_3 - CH = CH - CH - CH - CH_3$$
 (ii) $H_3C - C - CH_2 - CH_2 - CH_2 - COOH$
 $\begin{vmatrix} & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\$



