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НОМЕНКЛАТУРА ОРГАНИЧЕСКИХ СОЕДИНЕНИЙ

HOW TO NAME ORGANIC COMPOUNDS

Методические рекомендации

Минск БГМУ 2024

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Б91

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Содержит рекомендации для подготовки к лабораторному занятию «Introduction. Classification and nomenclature of organic compounds» по биоорганической и органической химии на английском языке. Включает вводную теоретическую часть, глоссарий основных терминов, алгоритмы анализа названий органических соединений с примерами. Приведены задания для самоконтроля и ответы с пояснениями.

Предназначены для студентов 1-го курса медицинского факультета иностранных учащихся, обучающихся на английском языке по специальностям «Лечебное дело», «Стоматология», студентов 2-го курса медицинского факультета иностранных учащихся, обучающихся на английском языке по специальности «Фармация».

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На английском языке

Ответственный за выпуск В. В. Хрусталёв
Компьютерная вёрстка Н. М. Федорцовой

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INTRODUCTION

Nomenclature of organic compounds is the starting point when considering chemical transformations and the structures of the biologically important organic compounds. All subsequent topics contain consideration of the organic compounds' structures based on the various names.

The tasks of studying the discipline are to develop the students' academic competences, based on the ability to classify the organic compounds on the carbon skeletal structure and on the functional groups nature; to build the formulas on the IUPAC name and give the IUPAC name according to the representatives structural formula of the biological important compounds and remedies; to determine the functional groups and substituents in the molecules for prediction of the organic compounds chemical reactivity and classification.

The course of Bioorganic chemistry in medical education is based on the study of the structure and functions of organic compounds that have a biological effect and participate in the biological processes. These effects are caused by the unique structure and the presence of a variety of groups and substituents that influence each other and provide binding to other molecules and the chemical reactions. By the presence of these groups, as well as various types of carbon-carbon bonds, organic compounds can be cyclic, acyclic, carbocyclic, heterocyclic, homo- and heterofunctional compounds etc.

The important classes of organic compounds have specific features in their names. For example, specific suffixes -ol in the name of alkohols, -al in the name of aldehydes, -one in the name of ketones, -oic acid in the name of carboxylic acids, -oate in the name of esters.

Introduction into bioorganic compounds and nomenclature of organic compounds starts bioorganic chemistry course. And part of this topic about nomenclature is closely related with all subsequent topics. Actually why it's so important to name organic compounds?

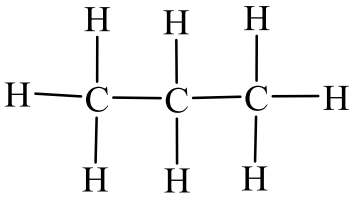
First of all, let's give definition to them. Organic compounds are any chemical compounds that contain carbon-hydrogen bonds. Due to carbon's ability to form chains with other carbon atoms, millions of organic compounds are known. That's why it's necessary to apply approaches to combine structure and properties of organic compounds with naming them correctly.

There are different types of **nomenclature** (from Latin "nomen" means "name"). Let's fix on the most logical nomenclature naming rules known as **IUPAC nomenclature**, abbreviation is derived from the **I**nternational **U**nion of **P**ure and **A**pplied **C**hemistry that is the world authority on chemical nomenclature. It's also named systematic or substitutive nomenclature. Knowing systematic name we can also predict chemical properties of compounds.

There are a number of ways to represent organic compounds. It is useful to know all of these so that you can recognise a molecule regardless of how it is shown.

There are four ways of representing a compound in two dimensions (on your page of workbook or computer screen):

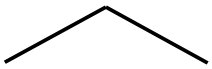
– **structural formula** shows every bond between every atom in the molecule. Each bond is represented by a line. Example,



– **semi-structural formula** without writing out all the carbon-hydrogen bonds, like

$$CH_3–CH_2–CH_3$$

– **skeletal formula** (or stick) means that the omitted atoms when each dot means a carbon atom, hydrogens are not written



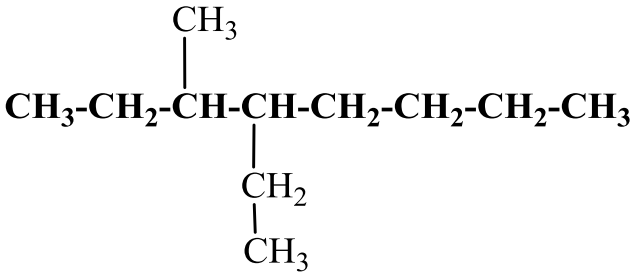
– **condensed formula** (without showing any bonds between atoms at all). As for a semi-structural representation, the carbon atoms are grouped with the hydrogen atoms bonded directly to it. The bonds between these groups are not shown. Branched or substituent groups are shown in brackets after the carbon atom to which they are bonded ($CH_3CH_2CH_3$). In the most cases of naming exercises we use semi-structural and skeletal formulas.

Before consideration of naming rules it’s necessary to discuss the following terms and definitions that will be used.

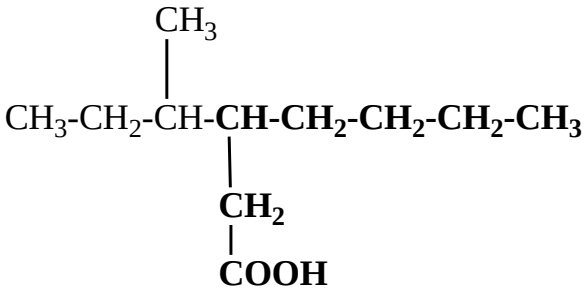
GLOSSARY

Main carbon chain is the longest chain of carbons in the molecule (or largest ring) in the case of absence functional groups and chain of carbons connected with the principal functional group.

e.g. Compare choice of main carbon chain in the cases:



and



Functional groups are collections of atoms that have a common pattern of chemical reactivity.

Principal functional group is a group of the highest priority (seniority). See Table.

Substituents are carbon fragments branching off the main chain. See Table.

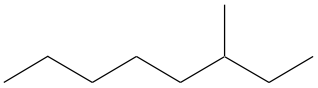
Locants are numbers of carbons in the carbon chain.

Multiplying prefixes are prefixes of the same groups.

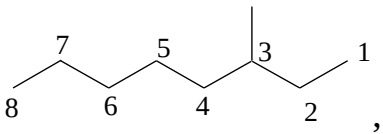
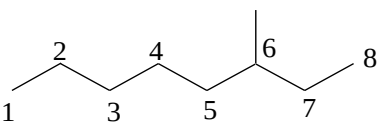
Multiple bonds are double and triple bonds.

The lowest locant rule determines which end is chosen as carbon #1: "Number the chain such as to provide the lowest possible locants for the chain."

e.g. Find the main carbon chain and put locants in the structure



Numbering from the left to the right is not correct because locant of methyl should be

lower (3 less 6)  , but not 

STEPS TO NAME ORGANIC COMPOUNDS

Generally, there are main steps to make a name according to the IUPAC nomenclature rules (Fig. 1).

1. Analyze the structure of the compound. Are there any functional groups, substituents, multiple bonds in the molecule?

2. Find the main carbon chain and count the number of carbons in this chain. Determine the root name for this parent chain due to amount of carbons.

Amount of carbons	**Name**
1 carbon atom	Meth-
2 carbon atoms	Eth-
3 carbon atoms	Prop-
4 carbon atoms	But-
5 carbon atoms	Pent-
6 carbon atoms	Hex-
7 carbon atoms	Hept-
8 carbon atoms	Oct-
9 carbon atoms	Non-
10 carbon atoms	Dec-

3. Put locants in the main carbon chain beginning from the side of the highest priority group

4. The principle functional group will give the suffix of compound according to the Tables 3, 5

5. Remaining functional groups and substituents are named by their prefixes in alphabetical order

6. Collect all parts in the IUPAC name of compound in the following order:
PREFIX – ROOT – SUFFIX

Fig. 1. Steps to name organic compounds

We will now look at each step in more detail and consider cases and notes. To carry out analysis of the molecule's structure means to answer the questions: Does compound cyclic (ring structure) or acyclic (chain structure)? Does it contain just single bond (alkane) or also double/triple (alkene/alkyne) bonds? Does it contain aromatic rings, any substituents and functional groups? This inspection is needed to sort components in naming. Which of them will determine the parent chain, the suffix and, if any, prefix of name. The next important step is how to find main carbon chain (Fig. 2)?

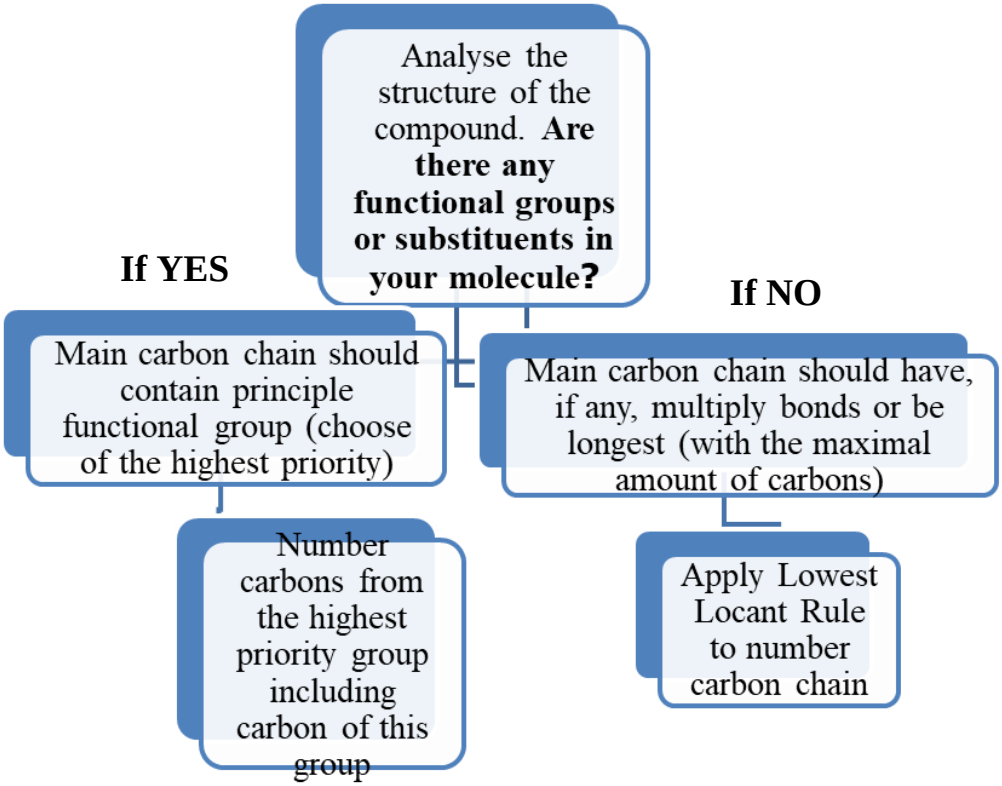


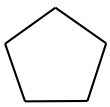
Fig. 2. Analysis of the structure of the compound

If hydrocarbon chain contains just single bonds the name of this molecule will be ended with suffix -ane. And the choice of root will depend on the name of corresponding alkane (Table 1).

If hydrocarbon chain with only single bonds is cyclic it's necessary to use prefix **cyclo**.

 cyclopropane (three carbons are connected into cycle)

 cyclobutane (four carbons are connected into cycle)

 cyclopentane (five carbons are connected into cycle)

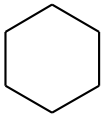
 cyclohexane (six carbons are connected into cycle)

Table 1

Hydrocarbon chain names

Amount of carbons in the chain	**Formula of C_nH_{2n+2}**	**Hydrocarbon chain with only single bonds**	**Name**
1	CH_4		methane
2	C_2H_6	$H_3C–CH_3$	ethane
3	C_3H_8	$H_3C–CH_2–CH_3$	propane
4	C_4H_{10}	$H_3C–CH_2–CH_2–CH_3$	butane
5	C_5H_{12}	$H_3C–CH_2–CH_2–CH_2–CH_3$	pentane
6	C_6H_{14}	$H_3C–CH_2–CH_2–CH_2–CH_2–CH_3$	hexane
7	C_7H_{16}	$H_3C–CH_2–CH_2–CH_2–CH_2–CH_2–CH_3$	heptane
8	C_8H_{18}	$H_3C–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–CH_3$	octane
9	C_9H_{20}	$H_3C–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–CH_3$	nonane
10	$C_{10}H_{22}$	$H_3C–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–CH_3$	decane

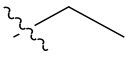
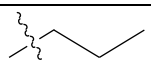
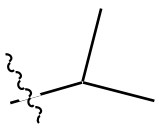
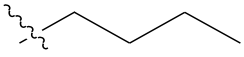
Substituents are formed that replaces (one or more) hydrogen atoms on the parent chain of a hydrocarbon and classified according to length of carbon chain and the suffix **“yl”** is attached. Like methyl from methane, ethyl from ethane etc. The suffix -yl is used when naming organic compounds that contain a single bond replacing one hydrogen (Table 2).

Multiples of the same substituent are given the following prefixes:

“di” (two identical substituents),
“tri” (three identical substituents),
“tetra” (four identical substituents),
“penta” (five identical substituents),
“hexa” (six identical substituents

Table 2

Name of substituents

Amount of carbons	**Complete form**	**Skeletal form (short)**	**Name of Substituent (radical)**
1	$–CH_3$		methyl
2	$–CH_2–CH_3$		ethyl
3	$–CH_2–CH_2–CH_3$		propyl
	$CH_3–CH(CH_3)$		iso-propyl
4	$–H_2C–CH_2–CH_2–CH_3$		butyl

Example. Let's analyze the structure and write the formula according to the IUPAC name of 2,2-dimethylpropanal.

First of all, let's find root prop (carbon chain from 3 carbon atoms) in the middle of name, after root suffix al (indicates class Aldehydes), before root prefix methyl (CH_3 is side substituent), di means 2 identical methyls from second carbon atom (it's necessary to double 2,2 — di) (Fig. 3).

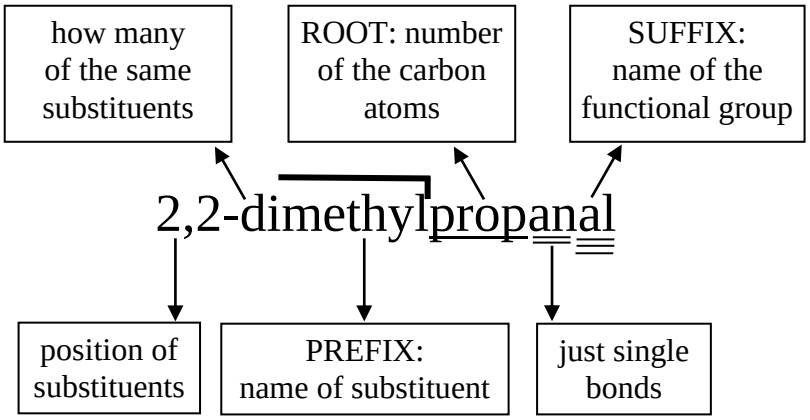


Fig. 3. IUPAC name structure

NAMING OF HYDROCARBON MOLECULES WITH SINGLE BONDS AND SUBSTITUENTS ONLY (WITHOUT FUNCTIONAL GROUP): ALKANES AND CYCLOALKANES CASES

Step 1. Find the *longest carbon chain*. Determine the root name for this parent chain. In cyclic compounds, the ring is usually considered the parent chain, unless it is attached to a longer chain of carbons; indicate a ring with the prefix “cyclo” before the root name. (When there are two longest chains of equal length, use the chain with the greater number of substituents.)

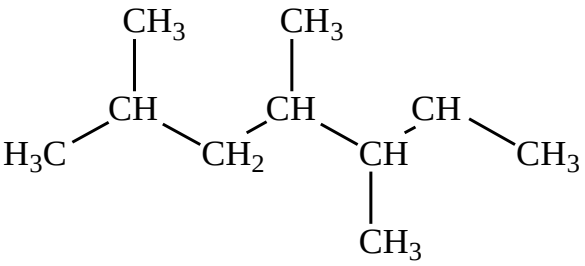
Step 2. Number the chain in the direction such that the position number of the first substituent is the smaller number.

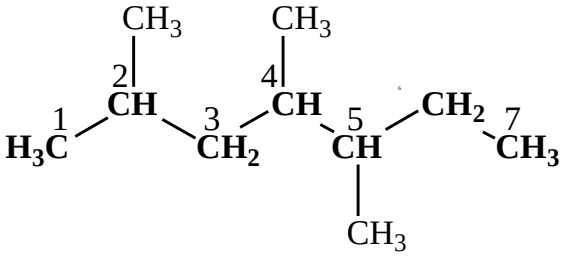
Step 3. Determine the name and position number of each substituent.

Step 4. Indicate the number of identical groups by the prefixes di, tri, tetra, etc.

Step 5. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like sec-, tert-, di, tri, etc., but include iso and cyclo. Always include a position number for each substituent.

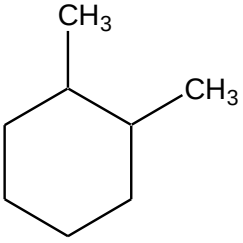
Example. Give the name of the following molecule.



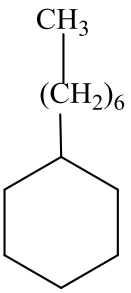


2,4,5-trimethylheptane (not 3,4,6-trimethylheptane)

Example. Compare naming of the structures 1 and 2 with ring:

1 

1,2-dimethylcyclohexane

2 

1-cyclohexylheptane

Note in the example 2 main carbon chain has more carbons than the ring.

NAMING OF HYDROCARBON MOLECULES WITH 1 OR MORE DOUBLE BONDS (WITHOUT FUNCTIONAL GROUP): ALKENES AND ALKADIENES

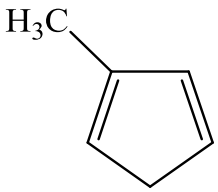
Step 1. Find and name main carbon chain containing double bond.

Step 2. Change the -ane of the alkane name to -ene. If 2 double bonds change to diene.

Step 3. Number the main carbon chain giving the double bond the lowest possible location number.

Step 4. Name sustituents.

Example. Name the following case:



Name is 2-methyl-cyclopenta-1,3-diene

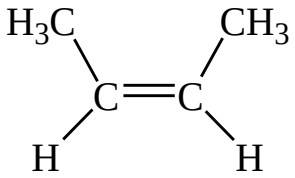
Example. How to name the following structure?

$$CH_3–CH=CH-CH_3$$

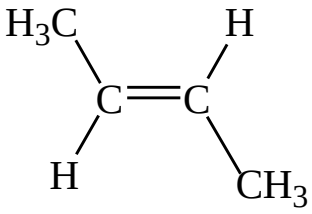
Its name is but-2-ene.

Note! In the naming of alkenes *cis-/trans*-nomenclature is still used to differentiate the isomers. *Cis* is used to indicate the isomer in which the substituents are on the same side of the double bond, trans is used when they are on opposite sides.

For example, *cis*-but-2-ene:



and compare with *trans*-but-2-ene



NAMING OF AROMATIC HYDROCARBON COMPOUNDS

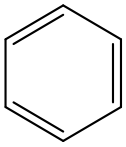
The use of numbers to indicate the position of substituents in aromatic rings is supplemented in the case of disubstituted derivatives of benzene by the terms:

Ortho- abbreviated ***o-*** means 1,2-disubstitution

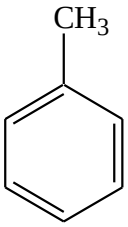
Meta- abbreviated ***m-*** means 1,3-disubstitution

Para- abbreviated ***p-*** means 1,4-disubstitution

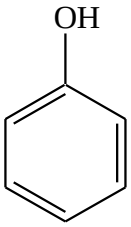
The following aromatic compounds and derived (aryl) groups have special names that should be memorized.



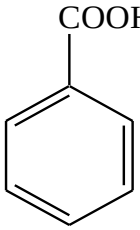
Benzene



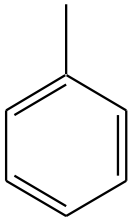
Toluene



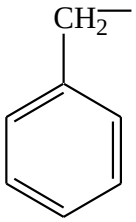
Phenol



Benzoic acid



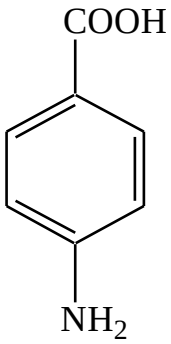
or C_6H_5-
Phenyl
(abbreviated –Ph)

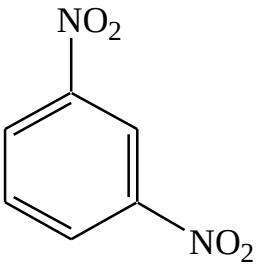


Benzyl
(abbreviated –Bz)

Example. Draw structures due to the names of the *p*-aminobenzoic acid and *m*-dinitrobenzene.

Using prefixes and suffixes of functional groups and meanings for *para* (1,4 — positions) and *meta* (1,3 — positions) in the benzene ring the formulas are drawn.





NAMING OF COMPOUNDS WITH FUNCTIONAL GROUPS CASES

The systematic name of every organic molecule containing a functional group may be made up of the “bricks” (Fig. 4).

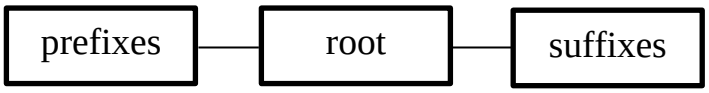


Fig. 4. Naming of compounds with functional groups

Prefixes are names for substituents or remaining functional groups (Tables 3, 4, 5).

Root is name of the main carbon chain.

Suffix identifies the principal functional group (Tables 3 and 5).

Locants (or numbers) show localization of substituents in the molecule. Locants may be before prefixes or suffixes.

Priorities of Substituents and Functional Groups listed here from highest to lowest priority

Table 3

Functional groups indicated by prefix or suffix

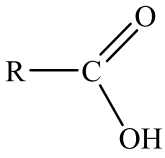
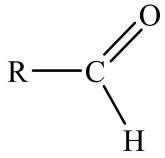
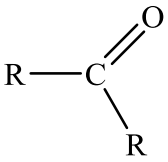
Class of compound	Structure	Prefix	Suffix
Carboxylic acid		Carboxy-	-oic acid (carboxylic acid)
Aldehyde		Oxo- (formyl-)	-al (carbaldehyde)
Ketone		Oxo-	-one
Alcohol	R-OH	Hydroxy-	-ol
Thiol	R-SH	Mercapto-	-thiol
Amine	R-NH_2	Amino-	-amine

Table 4

Functional groups indicated by suffix only

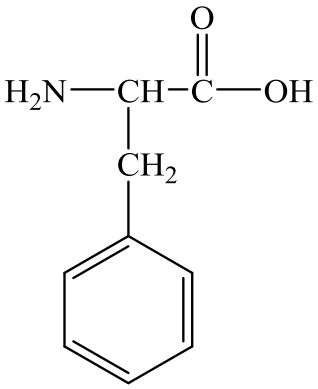
Class of compound	Structure	Suffix
Alkene	C═C	-ene
Alkyne	C≡C	-yne

Table 5

Substituents indicated by prefix only

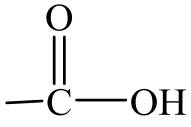
Substituent	Structure	Prefix
Alkyl (see list above)	R-	Alkyl-
Alkoxy-	R-O-	Alkoxy- Methoxy- Ethoxy- , etc
Halogen	-F -Cl -Br -I	Fluoro- Chloro- Bromo- Iodo-
Nitro	$-NO_2$	Nitro-
Other substituents and their prefixes		
Vinyl	$H_2C{=}CH^-$	
Allyl	$H_2C{=}CH{-}CH_2{-}$	

Example. The following case of amino acid illustrates the basic approach to name:



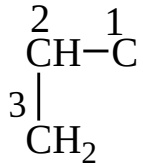
There are the following fragments in the case.

Principle group from Table 3



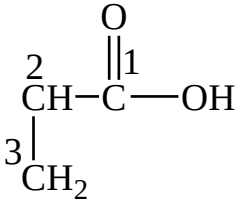
gives suffix -oic acid.

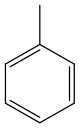
Main carbon chain contains 3 carbon atoms because it with principle group



with just single bonds therefore root is propane.

Main carbon chain plus principle group is propanoic acid.

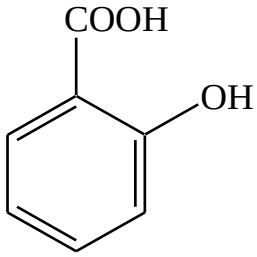


Prefixes (see Table 3) $–NH_2$ (amino) from carbon atom #2 and  (naming is phenyl) from carbon #3.

Locants plus prefixes only in alphabetical order: 2-amino-3-phenyl.

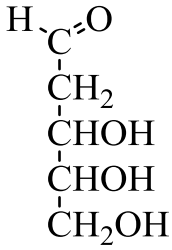
Complete name is 2-amino-3-phenylpropanoic acid.

Example. There are 2 functional groups in the following case



Principal group is COOH (gives suffix) that attached with the ring therefore benzene ring is main carbon chain. Numeration of ring starts from carbon connected with COOH to the direction of the next group OH (gives prefix). Complete name is 2-hydroxybenzoic acid.

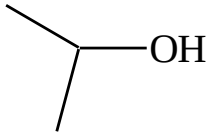
Example. There are many functional groups in the following case



But aldehyde group has higher priority (See Table 3) than hydroxyl group (three identical hydroxyls). Put locants from the aldehyde group side and give the name 3,4,5-trihydroxypentanal.

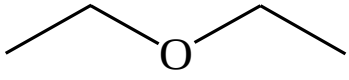
RADICOFUNCTIONAL NAMING

An alternative system of naming which is still very common in many books consists of naming the alkyl or aryl groups attached to a functional group as separate words followed by the functional group name. The following examples illustrate the basic approach to naming:

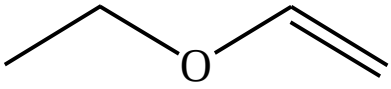


According to the radicofunctional nomenclature this is isopropyl alcohol. Ease to see class of alkohols and branched substituent. Compare with IUPAC name propan-2-ol.

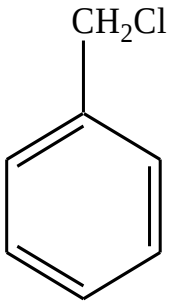
Structure of “spider” contains etheric group (class ether) connected with 2 ethyls (C_2H_5) therefore name is diethyl ether.



Structure of similar contains different substituents ethyl and vinyl therefore in alphabetical order name will be ethylvinylether.



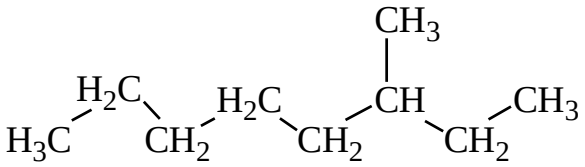
Structure of the following aromatic compound is named benzylchloride.



SELF-CHECK EXERCISES

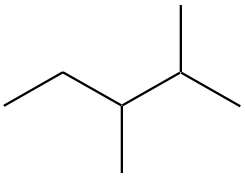
1. There are 7 carbon atoms in the longest carbon chain for an organic compound. What is the correct parent name for this compound?

2. Give IUPAC name for the structure

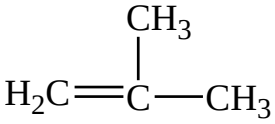


3. Put skipped word. The di- in propan-1,2-diol tells us that there are ___ branched groups or functional groups of the same type in the compound.

4. Give the IUPAC name for the structure

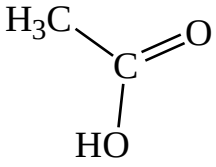


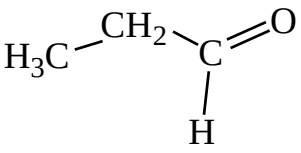
5. Give IUPAC name for the structure



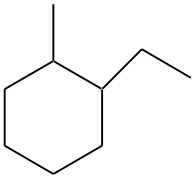
6. What is the correct suffix for a/an aldehyde?

7. Find main carbon chains in the following molecules and name them:

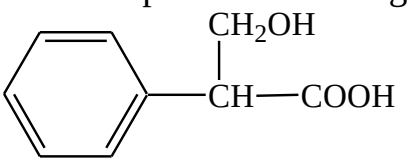
a) 

b) 

8. Give IUPAC name for the structure



9. Choose the correct name for tropic acid according to the IUPAC nomenclature



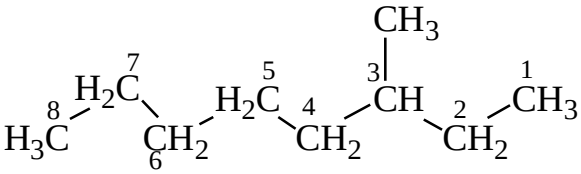
a) α-phenyl-β-oxypropionic acid
b) 2-phenyl-3-hydroxypropanoic acid
c) 3-hydroxy-2-phenylpropanoic acid
d) α-phenyl-3-hydroxypropanoic acid
e) 3-hydroxy-β-phenylpropanoic acid

10. Give IUPAC name for menthol structure.

ANSWERS AND EXPLANATIONS

1. Parent name for 7 carbon atoms is called heptyl (see Table 1).

2. There are just single bonds in carbon chain and one carbon substituent methyl.

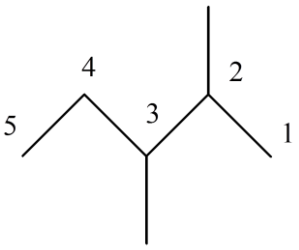


Using Lowest Locant Rule to number carbon chain, name is 3-methyloctane.

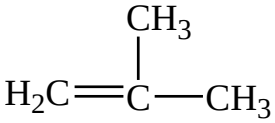
3. The di- tells us that there are 2 branched groups or functional groups of the same type in the compound.

4. Suffix -al is used for aldehydes (see Table 3).

5. This molecule doesn't contain any functional groups therefore the main carbon chain is the longest (5 carbon atoms in the chain with just single bonds gives root pentane). Due to Lowest Locant Rule put numbers of any substituents should be the lowest. It's possible if numeration goes from the right to the left (locants 2 and 3), not from the left to the right (locants 3 and 4). The same substituents methyls are indicated with multiplying prefix di-. The correct name is 2,3-dimethyl pentane.



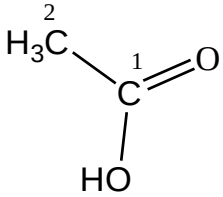
6. This molecule contains double bond



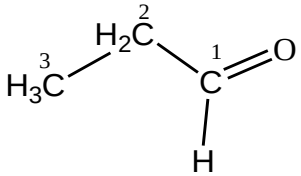
and in this case main carbon chain (3 carbon atoms give root prop) must have double bond (by suffix -ene-) and numeration must be from the nearest carbon to double bond C=C, e.g. from left to right. Substituent methyl is going from second carbon and to finish name pick up together in 2-methylpropene. Pay your attention that in this case double bond is indicated without locant 1 ($C^{\mathbf{1}}=C^{2}$) because it's on the end of molecule and locant 1 should be omitted. In another cases it's necessary to indicate locant for all double or triple bonds in the molecule. For example, butadiene-1,3 contains 2 double bonds between ($C^{1}=C^{2}$) and ($C^{3}=C^{4}$): $CH_2=CH-CH=CH_2$. In this case no matter for numbering direction.

7. You should be attentive in this case **a** there no 2 groups but only one –COOH (carboxy group). Main carbon chain includes carbon of carboxy group (case **a** is ethanoic acid) and aldehyde group (case **b** is propanal).

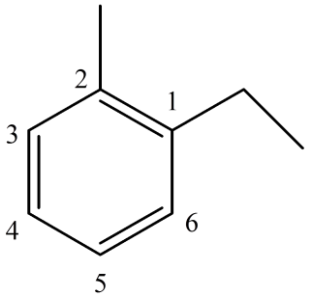
a.



b.

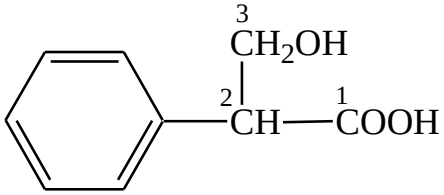


8. Main carbon chain is ring of cyclohexane with two branches of ethyl and methyl, number ring beginning from the carbon connected with ethyl to the direction to the nearest substituent.



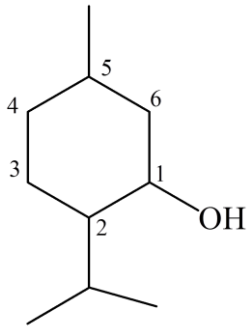
Name both of them in alphabetical order. The name is 1-ethyl-2-methylcyclohexane.

9. Correct answer is C. Main carbon chain contains 3 carbons (is called prop) including functional groups COOH and OH and just single carbon-carbon bonds (propan-).



Numeration starts from carbon of the highest priority COOH group that gives suffix -oic acid. OH-group (is called by prefix hydroxy) and ring phenyl should be indicated with number position only in alphabetical order. Hydroxy is going from number 3, Phenyl is going from second carbon atom. Pick up together all parts in the name: 3-hydrohy-2-phenylpropanoic acid.

10. In menthol structure one functional group OH and substituents CH_3 (methyl) and isopropyl (branched substituent from 3 carbons). OH is principal group immediately connected with ring therefore ring is main carbon chain. Numbering should be started from carbon attached with OH to the direction due to low locator rule.



Don’t forget about alphabetical order for prefixes! Complete name is 2-isopropyl-5-methylcyclohexanol.

LITERATURE

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