

Nomenclature

Naming Organic Compounds

The increasingly large number of organic compounds identified with each passing day, together with the fact that many of these compounds are isomers of other compounds, requires that a systematic nomenclature system be developed. Just as each distinct compound has a unique molecular structure which can be designated by a structural formula, each compound must be given a characteristic and unique name. As organic chemistry grew and developed, many compounds were given trivial names, which are now commonly used and recognized. Some examples are:

Name	Methane	Butane	Acetone	Toluene	Acetylene	Ethyl Alcohol
Formula	CH ₄	C ₄ H ₁₀	CH ₃ COCH ₃	CH ₃ C ₆ H ₅	C ₂ H ₂	C ₂ H ₅ OH

Such **common names** often have their origin in the history of the science and the natural sources of specific compounds, but the relationship of these names to each other is arbitrary, and no rational or systematic principles underlay their assignments.

The IUPAC Systematic Approach to Nomenclature

A rational nomenclature system should do at least two things. First, it should indicate how the carbon atoms of a given compound are bonded together in a characteristic lattice of chains and rings. Second, it should identify and locate any functional groups present in the compound. Since hydrogen is such a common component of organic compounds, its amount and locations can be assumed from the tetravalency of carbon, and need not be specified in most cases.

The IUPAC nomenclature system is a set of logical rules devised and used by organic chemists to circumvent problems caused by arbitrary nomenclature. Knowing these rules and given a structural formula, one should be able to write a unique name for every distinct compound. Likewise, given a IUPAC name, one should be able to write a structural formula. In general, an IUPAC name will have three essential features:

- A root or base indicating a major chain or ring of carbon atoms found in the molecular structure.
- A suffix or other element(s) designating functional groups that may be present in the compound.
- Names of substituent groups, other than hydrogen, that complete the molecular structure.

As an introduction to the IUPAC nomenclature system, we shall first consider compounds that have no specific functional groups. Such compounds are composed only of carbon and hydrogen atoms bonded together by sigma bonds (all carbons are sp³ hybridized).

Alkanes

Alkanes

Hydrocarbons having no double or triple bond functional groups are classified as **alkanes** or **cycloalkanes**, depending on whether the carbon atoms of the molecule are arranged only in chains or also in rings. Although these hydrocarbons have no functional groups, they constitute the framework on which functional groups are located in other classes of compounds, and provide an ideal starting point for studying and naming organic compounds. The alkanes and cycloalkanes are also members of a larger class of compounds referred to as **aliphatic**. Simply put, aliphatic compounds are compounds that do not incorporate any [aromatic rings](#) in their molecular structure.

The following table lists the IUPAC names assigned to simple continuous-chain alkanes from C-1 to C-10. A common "**ane**" suffix identifies these compounds as alkanes. Longer chain alkanes are well known, and their

names may be found in many reference and text books. The names **methane** through **decane** should be memorized, since they constitute the root of many IUPAC names. Fortunately, common numerical prefixes are used in naming chains of five or more carbon atoms.

Examples of Simple Unbranched Alkanes							
Name	Molecular Formula	Structural Formula	Isomers	Name	Molecular Formula	Structural Formula	Isomers
methane	CH ₄	CH ₄	1	hexane	C ₆ H ₁₄	CH ₃ (CH ₂) ₄ CH ₃	5
ethane	C ₂ H ₆	CH ₃ CH ₃	1	heptane	C ₇ H ₁₆	CH ₃ (CH ₂) ₅ CH ₃	9
propane	C ₃ H ₈	CH ₃ CH ₂ CH ₃	1	octane	C ₈ H ₁₈	CH ₃ (CH ₂) ₆ CH ₃	18
butane	C ₄ H ₁₀	CH ₃ CH ₂ CH ₂ CH ₃	2	nonane	C ₉ H ₂₀	CH ₃ (CH ₂) ₇ CH ₃	35
pentane	C ₅ H ₁₂	CH ₃ (CH ₂) ₃ CH ₃	3	decane	C ₁₀ H ₂₂	CH ₃ (CH ₂) ₈ CH ₃	75

Some important behavior trends and terminologies:

- (i) The formulas and structures of these alkanes increase uniformly by a CH₂ increment.
- (ii) A uniform variation of this kind in a series of compounds is called **homologous**.
- (iii) These formulas all fit the **C_nH_{2n+2}** rule. This is also the highest possible H/C ratio for a stable hydrocarbon.
- (iv) Since the H/C ratio in these compounds is at a maximum, we call them **saturated** (with hydrogen).

Beginning with butane (C₄H₁₀), and becoming more numerous with larger alkanes, we note the existence of alkane isomers. For example, there are five C₆H₁₄ isomers, shown below as abbreviated line formulas (**A** through **E**):



Although these distinct compounds all have the same molecular formula, only one (**A**) can be called hexane. How then are we to name the others?

For the above isomers of hexane the IUPAC names are: **B 2-methylpentane** **C 3-methylpentane** **D 2,2-dimethylbutane** **E 2,3-dimethylbutane**

The **IUPAC** system requires first that we have names for simple unbranched chains, as noted above, and second that we have names for simple alkyl groups that may be attached to the chains. Examples of some common **alkyl groups** are given in the following table. Note that the "ane" suffix is replaced by "**yl**" in naming groups. The symbol **R** is used to designate a generic (unspecified) alkyl group.

Group	CH ₃ –	C ₂ H ₅ –	CH ₃ CH ₂ CH ₂ –	(CH ₃) ₂ CH–	CH ₃ CH ₂ CH ₂ CH ₂ –
Name	Methyl	Ethyl	Propyl	Isopropyl (2-methylethyl)	Butyl
Group	(CH ₃) ₂ CHCH ₂ –	CH ₃ CH ₂ CH(CH ₃)–	(CH ₃) ₃ C–	R–	
Name	Isobutyl (3-methylpropyl)	sec-Butyl (1-methylpropyl)	2,2,dimethylethyl	Alkyl	

IUPAC Rules for Alkane Nomenclature

1. Find and name the longest continuous carbon chain.
2. Identify and name groups attached to this chain.
3. Number the chain consecutively, starting at the end nearest a substituent group.
4. Designate the location of each substituent group by an appropriate number and name.
5. Assemble the name, listing groups in alphabetical order using the full name (e.g. cyclopropyl before isobutyl).

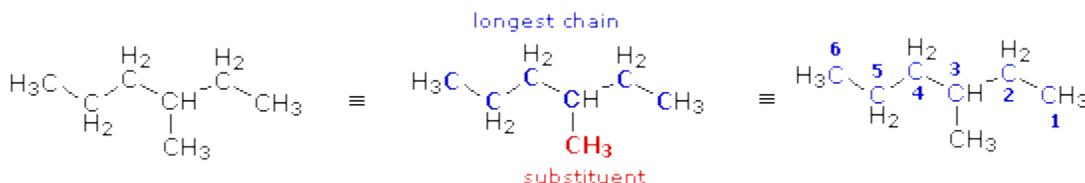
The prefixes di, tri, tetra etc., used to designate several groups of the same kind, are not considered when alphabetizing.

Halogen substituents are easily accommodated, using the names: fluoro (F-), chloro (Cl-), bromo (Br-) and iodo (I-). For example, $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{Br}$ would be named 1-bromo-3-methylbutane. If the halogen is bonded to a simple alkyl group an alternative "alkyl halide" name may be used. Thus, $\text{C}_2\text{H}_5\text{Cl}$ may be named chloroethane (no locator number is needed for a two carbon chain) or ethyl chloride. Halogenated alkyl substituents such as bromomethyl, BrCH_2- , and trichloromethyl, CCl_3- , may be listed and are alphabetized according to their full names.

Practice Problems

Illustration 1. $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$

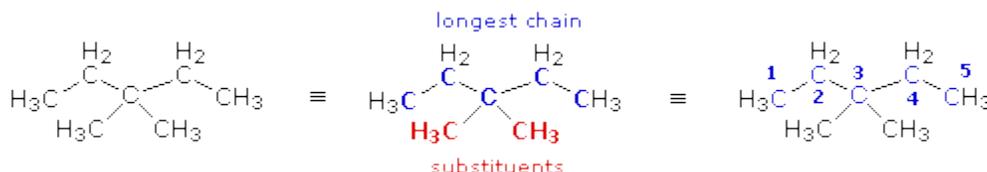
When viewing a condensed formula of this kind, one must recognize that parentheses are used both to identify repeating units, such as the two methylene groups on the left side, and substituents, such as the methyl group on the right side. This formula is elaborated and named as follows:



The condensed formula is expanded on the left. By inspection, the longest chain is seen to consist of six carbons, so the root name of this compound will be **hexane**. A single methyl substituent (colored red) is present, so this compound is a **methylhexane**. The location of the methyl group must be specified, since there are two possible isomers of this kind. Note that if the methyl group were located at the end of the chain, the longest chain would have seven carbons and the root name would be heptane not hexane. To locate the substituent the hexane chain must be numbered consecutively, starting from the end nearest a substituent. In this case it is the right end of the chain, and the methyl group is located on carbon #3. The IUPAC name is thus: **3-methylhexane**

Illustration 2. $(\text{CH}_3)_2\text{C}(\text{C}_2\text{H}_5)_2$

Again, the condensed formula is expanded on the left, the longest chain is identified (five carbons) and substituents are located and named. Because of the symmetrical substitution pattern, it does not matter at which end of the chain the numbering begins.



When two or more identical substituents are present in a molecule, a numerical prefix (di, tri, tetra *etc.*) is used to designate their number. However, **each substituent must be given an identifying location number**.

Thus, the above compound is correctly named: **3,3-dimethylpentane**.

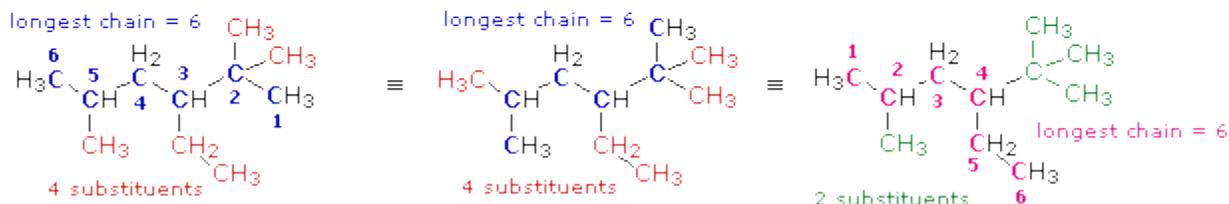
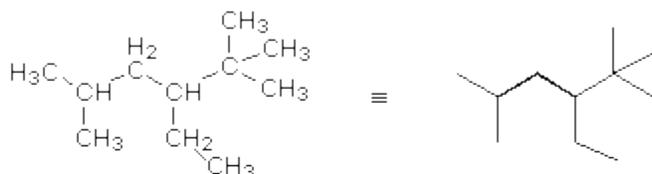
Note that the isomer $(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)_2$ would be named 2,4-dimethylpentane.

Illustration 3. $(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{C}_2\text{H}_5)\text{C}(\text{CH}_3)_3$

This example illustrates some sub-rules of the IUPAC system that must be used in complex cases. The expanded and line formulas are shown below.

Sub-Rules for IUPAC Nomenclature

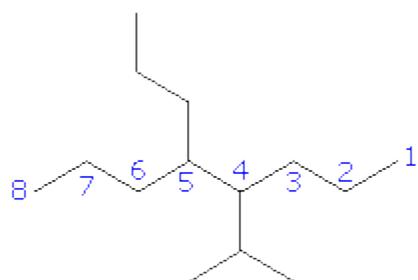
1. If there are two or more longest chains of equal length, the one having the largest number of substituents is chosen.
2. If both ends of the root chain have equidistant substituents:
 - (i) begin numbering at the end nearest a third substituent, if one is present.
 - (ii) begin numbering at the end nearest the first cited group (alphabetical order).



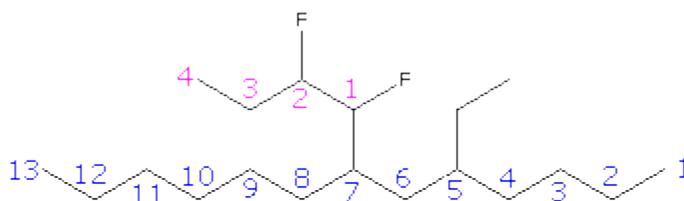
In this case several six-carbon chains can be identified. Some (colored blue) are identical in that they have the same number, kind and location of substituents. The IUPAC name derived from these chains will not change. Some (colored magenta) differ in the number, kind and location of substituents, and will result in a different name. From rule 1 above the blue chain is chosen, and it will be numbered from the right hand end by application of rule (i). Remembering the alphabetical priority, we assign the following IUPAC name: **3-ethyl-2,2,5-trimethylhexane**.

Illustration 4.

The following are additional examples of more complex structures and their names.



4-isopropyl-5-propyloctane



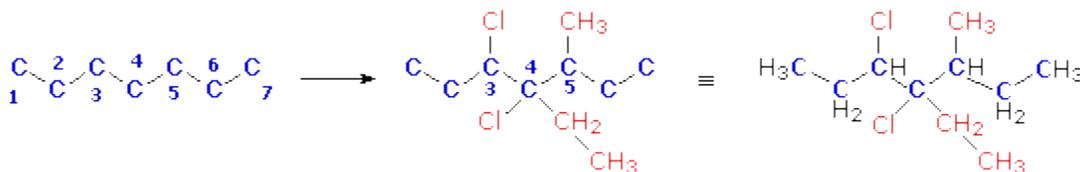
7-(1,2-difluorobutyl)-5-ethyltridecane

The formula on the right shows how a complex substituent may be given a supplementary numbering. In such cases the full substituent name is displayed within parenthesis and is alphabetized including numerical prefixes such as 'di'.

Illustration 5.

Write a structural formula for the compound **3,4-dichloro-4-ethyl-5-methylheptane**.

First, we draw a chain of seven carbon atoms to represent the root name "heptane". This chain can be numbered from either end, since no substituents are yet attached. From the IUPAC name we know there are two chlorine, one ethyl and one methyl substituents. The numbers tell us where the substituents are located on the chain, so they can be attached, as shown in the middle structure below. Finally, hydrogen atoms are introduced to satisfy the tetravalency of carbon. The structural formula on the right can then be written in condensed form as: $\text{CH}_3\text{CH}_2\text{CHClCl}(\text{C}_2\text{H}_5)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ or $\text{C}_2\text{H}_5\text{CHClCl}(\text{C}_2\text{H}_5)\text{CH}(\text{CH}_3)\text{C}_2\text{H}_5$



In naming this compound it should be noted that the seven carbon chain is numbered from the end nearest the chlorine by applying rule (ii) above.

Illustration 6. Questions

In the box following each question enter one or more letters designating formulas displayed at the bottom of the page. If there is no formula that fits the conditions enter **X** for **none**.

1. Which two line formulas (A to G) are the same? Enter two letters or **X** for **none**

2. Which if any of the line formulas (A to G) is not a constitutional isomer of the others? Enter the appropriate letter or **X** for **none**.

3. From the list of condensed formulas (H to O) pick that which corresponds to **A**.

4. From the list of condensed formulas (H to O) pick that which corresponds to **B**.

5. From the list of condensed formulas (H to O) pick that which corresponds to **C**.

6. From the list of condensed formulas (H to O) pick that which corresponds to **D**.

7. Which if any of the line formulas (A to G) is 2,4-dimethylpentane?

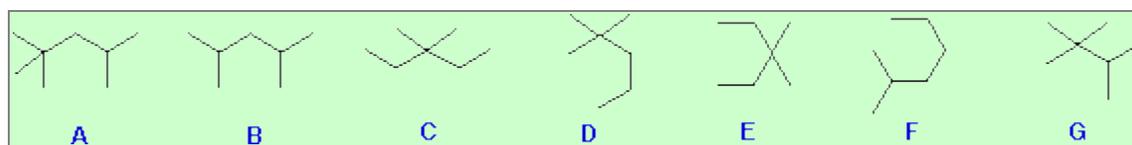
8. Which if any of the line formulas (A to G) is 2,2,3-trimethylbutane?

9. Which if any of the line formulas (A to G) is 2,2-dimethylpentane?

10. Which if any of the line formulas (A to G) is 2,2,4-trimethylpentane?

11. Which if any of the line formulas (A to G) is 3-ethylpentane?

12. Which if any of the line formulas (A to G) is 2-methylhexane?



H



I



J



K



L



M



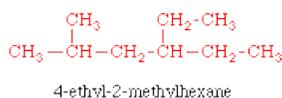
N



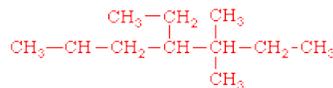
O



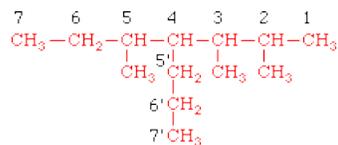
Here are some more examples:



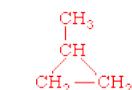
4-ethyl-2-methylhexane



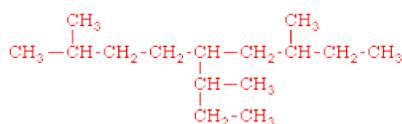
4-ethyl-3,3-dimethylheptane



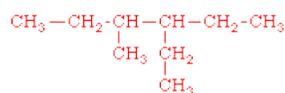
2,3,5-trimethyl-4-propylheptane
(NOT: 2,3-dimethyl-4-sec-butylheptane)



methylcyclopropane



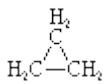
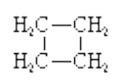
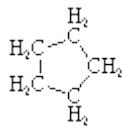
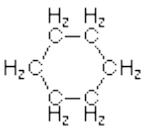
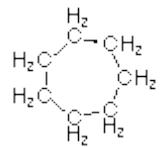
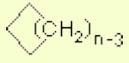
5-sec-butyl-2,7-dimethylnonane



3-ethyl-4-methylhexane

Cycloalkanes

Cycloalkanes have one or more rings of carbon atoms. The simplest examples of this class consist of a single, unsubstituted carbon ring, and these form a homologous series similar to the unbranched alkanes. The IUPAC names of the first five members of this series are given in the following table. The last (yellow shaded) column gives the general formula for a cycloalkane of any size. If a simple unbranched alkane is converted to a cycloalkane two hydrogen atoms, one from each end of the chain, must be lost. Hence the general formula for a cycloalkane composed of n carbons is C_nH_{2n} . Although a cycloalkane has two fewer hydrogens than the equivalent alkane, each carbon is bonded to four other atoms so such compounds are still considered to be **saturated** with hydrogen.

Examples of Simple Cycloalkanes						
Name	Cyclopropane	Cyclobutane	Cyclopentane	Cyclohexane	Cycloheptane	Cycloalkane
Molecular Formula	C_3H_6	C_4H_8	C_5H_{10}	C_6H_{12}	C_7H_{14}	C_nH_{2n}
Structural Formula						$(CH_2)_n$
Line Formula						

Substituted cycloalkanes are named in a fashion very similar to that used for naming branched alkanes. The chief difference in the rules and procedures occurs in the numbering system. Since all the carbons of a ring are equivalent (a ring has no ends like a chain does), the numbering starts at a substituted ring atom.

IUPAC Rules for Cycloalkane Nomenclature

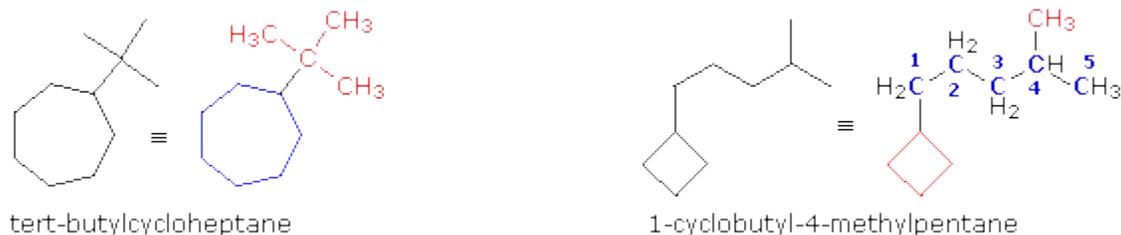
1. For a monosubstituted cycloalkane the ring supplies the root name (table above) and the substituent group is named as usual. A location number is unnecessary.
2. If the alkyl substituent is large and/or complex, the ring may be named as a substituent group on an alkane.
3. If two different substituents are present on the ring, they are listed in alphabetical order, and the first cited substituent is assigned to carbon #1. The numbering of ring carbons then continues in a direction (clockwise or counter-clockwise) that affords the second substituent the lower possible location number.
4. If several substituents are present on the ring, they are listed in alphabetical order. Location numbers are assigned to the substituents so that one of them is at carbon #1 and the other locations have the lowest possible numbers, counting in either a clockwise or counter-clockwise direction.
5. The name is assembled, listing groups in alphabetical order and giving each group (if there are two or more) a location number. The prefixes di, tri, tetra etc., used to designate several groups of the same kind, are not considered when alphabetizing.

Small rings, such as three and four membered rings, have significant angle strain resulting from the distortion of the sp^3 carbon bond angles from the ideal 109.5° to 60° and 90° respectively. This angle strain often

enhances the chemical reactivity of such compounds, leading to ring cleavage products. It is also important to recognize that, with the exception of cyclopropane, cycloalkyl rings are not planar (flat).

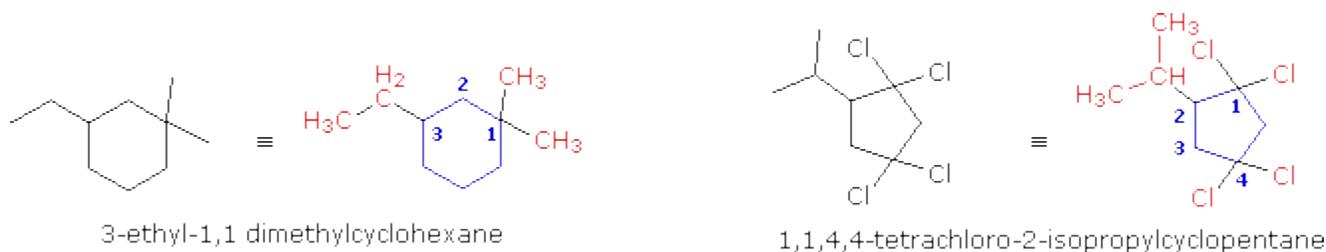
Examples

The following two cases provide examples of monosubstituted cycloalkanes.



In the first case, on the left, we see a seven-carbon ring bearing a C_4H_9 substituent group. Earlier this substituent was identified as the tert-butyl group, so a name based on the cycloheptane root is easily written. In the second case, on the right, a four-carbon ring is attached to a branched six-carbon alkyl group. This C_6H_{13} group could be named "isohexyl", but a better approach is to name this compound as a disubstituted pentane. The four-membered ring substituent is called a cyclobutyl group.

More highly substituted cycloalkanes are named in a similar fashion, but care must be taken in numbering the ring.



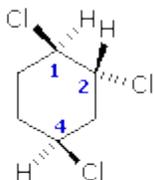
In the example on the left, there are three substituents on the six-membered ring and two are on the same carbon. The disubstituted carbon becomes #1 because the total locator numbers are thereby kept to a minimum. The ethyl substituent is then located on carbon #3 (counter-clockwise numbering), not #5 (clockwise numbering). Alphabetical listing of the substituents then leads to the name "3-ethyl-1,1-dimethylcyclohexane", being careful to assign a locator number to each substituent. Note that if only one methyl substituent was present, the alphabetical citation rule would assign the ethyl group to carbon #1 and the methyl to #3. The second example, on the left, has five substituents, and the numbering is assigned so that the first, second and third arbitrarily chosen substituents have the lowest possible numbers (1,1 & 2 in this case).

There's a little bit of hand waving going on here because stereochemistry is not being accounted for.

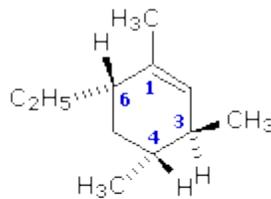
These just illustrate the hand waving I alluded to. We will discuss an alternative system in class which specifies the absolute configuration of substituted carbon atoms may also be used. This system, known as the Cahn-Ingold-Prelog rules, uses and elaborates the priority rules developed earlier (E and Z system – discussed in text and class). The below is for illustration, we will usually avoid *cis* and *trans* (gets round the problem of name a reference group).

When one substituent and one hydrogen atom are attached at each of more than two positions of a monocycle, the steric relations of the substituents may be expressed by first identifying a reference substituent

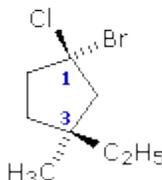
(labeled **r**) followed by a hyphen and the substituent locator number and name. The relative configuration of other substituents are then reported as *cis* (**c**) or *trans* (**t**) to the reference substituent.



r-1,1,2,2-tetrachlorocyclohexane



t-6-ethyl-1,3,4-trimethylcyclohexane



r-1-bromo-1-chloro-3-ethyl-3-methylcyclopentane

When two different substituents are attached at the same position of a monocycle, then the lowest-numbered substituent named as a suffix is selected as reference group. If none of the substituents is named as a suffix, then that substituent of the pair of substituents having the lowest number, and which is preferred by the sequence rule, is chosen as the reference group. The relationship of the sequence-rule-preferred substituent at geminally substituted positions, relative to the reference group, is cited as **c-** or **t-**, as appropriate.

Alkenes & Alkynes

Alkenes and Alkynes

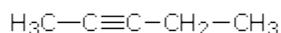
Alkenes and alkynes are hydrocarbons which respectively have **carbon-carbon double bond** and **carbon-carbon triple bond** functional groups. The molecular formulas of these **unsaturated** hydrocarbons reflect the multiple bonding of the functional groups:

Alkane $R-CH_2-CH_2-R$ C_nH_{2n+2} This is the maximum H/C ratio for a given number of carbon atoms.

Alkene $R-CH=CH-R$ C_nH_{2n} Each double bond reduces the number of hydrogen atoms by 2.

Alkyne $R-C\equiv C-R$ C_nH_{2n-2} Each triple bond reduces the number of hydrogen atoms by 4.

As noted earlier in the [Analysis of Molecular Formulas](#) section, the molecular formula of a hydrocarbon provides information about the possible structural types it may represent. For example, consider compounds having the formula C_5H_8 . The formula of the five-carbon alkane pentane is C_5H_{12} so the difference in hydrogen content is 4. This difference suggests such compounds may have a triple bond, two double bonds, a ring plus a double bond, or two rings. Some examples are shown here, and there are at least fourteen others!



IUPAC Rules for Alkene and Cycloalkene Nomenclature

1. The **ene** suffix (ending) indicates an alkene or cycloalkene.
2. The longest chain chosen for the root name must include both carbon atoms of the double bond.
3. The root chain must be numbered from the end nearest a double bond carbon atom. If the double bond is in the center of the chain, the nearest substituent rule is used to determine the end where numbering starts.
4. The smaller of the two numbers designating the carbon atoms of the double bond is used as the double bond locator. If more than one double bond is present the compound is named as a diene, triene or equivalent prefix indicating the number of double bonds, and each double bond is assigned a locator number.
5. In cycloalkenes the double bond carbons are assigned ring locations #1 and #2. Which of the two is #1 may be determined by the nearest substituent rule.
6. Substituent groups containing double bonds are:
 - $\text{H}_2\text{C}=\text{CH}-$ Vinyl group
 - $\text{H}_2\text{C}=\text{CH}-\text{CH}_2-$ Allyl group

IUPAC Rules for Alkyne Nomenclature

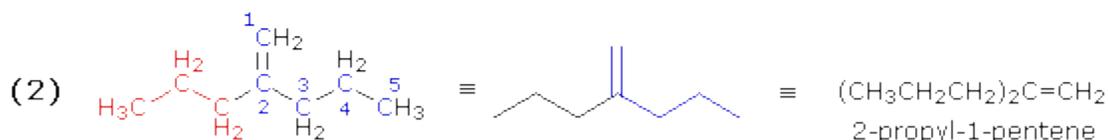
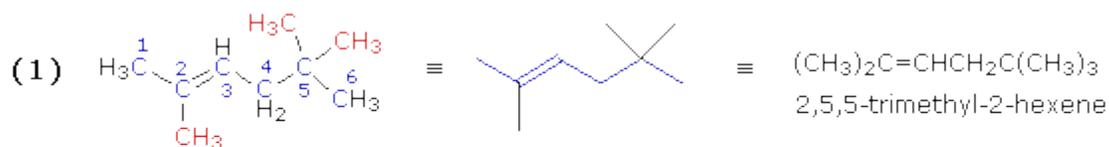
1. The **yne** suffix (ending) indicates an alkyne or cycloalkyne.
2. The longest chain chosen for the root name must include both carbon atoms of the triple bond.
3. The root chain must be numbered from the end nearest a triple bond carbon atom. If the triple bond is in the center of the chain, the nearest substituent rule is used to determine the end where numbering starts.
4. The smaller of the two numbers designating the carbon atoms of the triple bond is used as the triple bond locator.
5. If several multiple bonds are present, each must be assigned a locator number. Double bonds precede triple bonds in the IUPAC name, but the chain is numbered from the end nearest a multiple bond, regardless of its nature.
6. Because the triple bond is linear, it can only be accommodated in rings larger than ten carbons. In simple cycloalkynes the triple bond carbons are assigned ring locations #1 and #2. Which of the two is #1 may be determined by the nearest substituent rule.
7. Substituent groups containing triple bonds are:
 - $\text{HC}\equiv\text{C}-$ Ethynyl group
 - $\text{HC}\equiv\text{CH}-\text{CH}_2-$ Propargyl group

Examples

Illustration 1 $(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{C}(\text{CH}_3)_3$

Illustration 2 $(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{C}=\text{CH}_2$

Expanding these formulas we have:

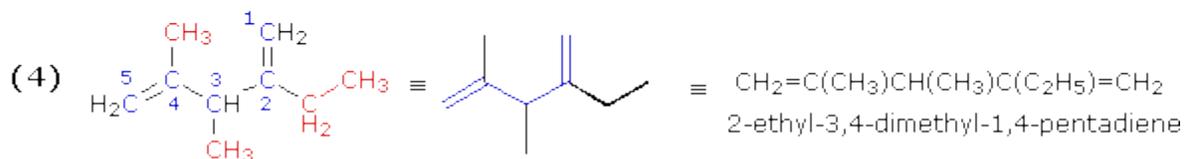
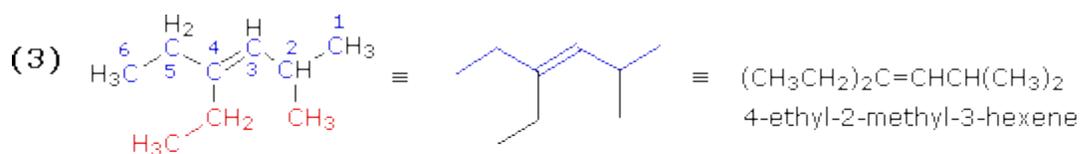


Both these compounds have double bonds, making them alkenes. In example (1) the longest chain consists of six carbons, so the root name of this compound will be **hexene**. Three methyl substituents (colored red) are present. Numbering the six-carbon chain begins at the end nearest the double bond (the left end), so the methyl groups are located on carbons 2 & 5. The IUPAC name is therefore: **2,5,5-trimethyl-2-hexene**. In example (2) the longest chain incorporating both carbon atoms of the double bond has a length of five. There is a seven-carbon chain, but it contains only one of the double bond carbon atoms. Consequently, the root name of this compound will be **pentene**. There is a propyl substituent on the inside double bond carbon atom (#2), so the IUPAC name is: **2-propyl-1-pentene**.

Illustration 3 $(\text{C}_2\text{H}_5)_2\text{C}=\text{CHCH}(\text{CH}_3)_2$

Illustration 4 $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{C}(\text{C}_2\text{H}_5)=\text{CH}_2$

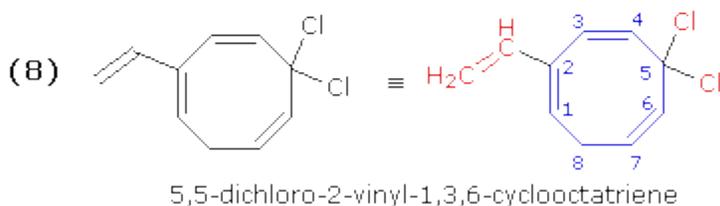
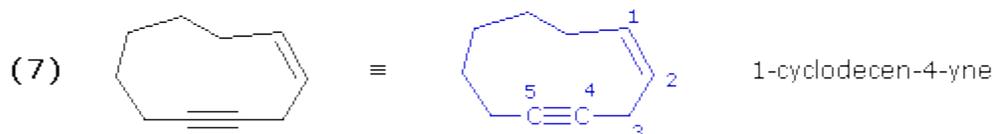
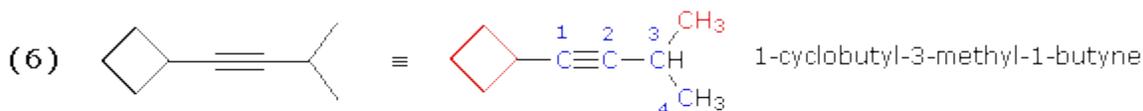
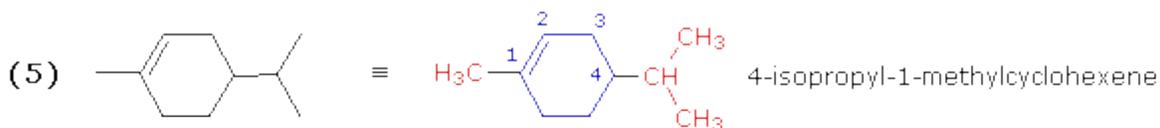
The next two examples illustrate additional features of chain numbering. As customary, the root chain is colored blue and substituents are red.



The double bond in example (3) is located in the center of a six-carbon chain. The double bond would therefore have a locator number of 3 regardless of the end chosen to begin numbering. The right hand end is selected because it gives the lowest first-substituent number (2 for the methyl as compared with 3 for the ethyl if numbering were started from the left). The IUPAC name is assigned as shown.

Example (4) is a diene (two double bonds). Both double bonds must be contained in the longest chain, which is therefore five- rather than six-carbons in length. The second and fourth carbons of this 1,4-pentadiene are both substituted, so the numbering begins at the end nearest the alphabetically first-cited substituent (the ethyl group).

Illustrations 5, 6, 7 & 8



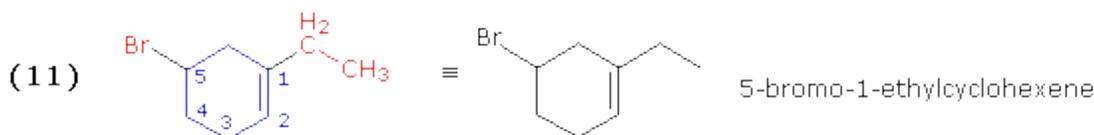
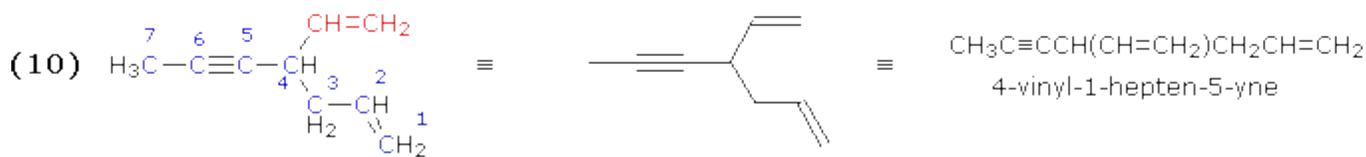
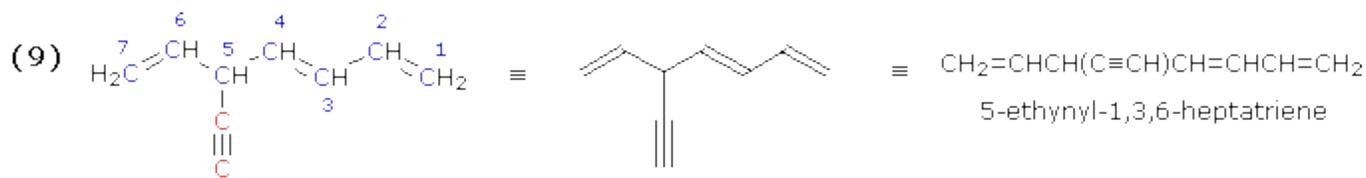
These examples include rings of carbon atoms as well as some carbon-carbon triple bonds. Example (6) is best named as an alkyne bearing a cyclobutyl substituent. Example (7) is simply a ten-membered ring containing both a double and a triple bond. The double bond is cited first in the IUPAC name, so numbering begins with those two carbons in the direction that gives the triple bond carbons the lowest locator numbers. Because of the linear geometry of a triple bond, a ten-membered ring is the smallest ring in which this functional group is easily accommodated. Example (8) is a cyclooctatriene (three double bonds in an eight-membered ring). The numbering must begin with one of the end carbons of the conjugated diene moiety (adjacent double bonds), because in this way the double bond carbon atoms are assigned the smallest possible locator numbers (1, 2, 3, 4, 6 & 7). Of the two ways in which this can be done, we choose the one that gives the vinyl substituent the lower number.

The last three examples, (9), (10) & (11), illustrate some fine points of the nomenclature rules.

Sub-Rules for IUPAC Nomenclature

The root chain is that which contains the maximum number of multiple bonds.

- If more than one such chain is found, the longest is chosen as the root.
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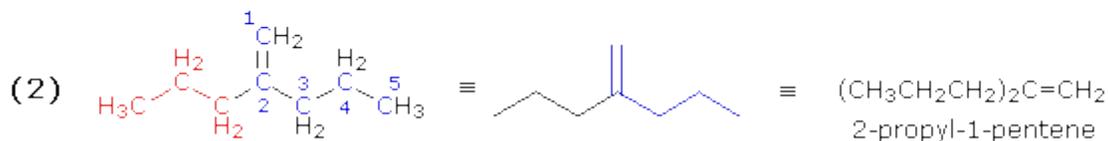
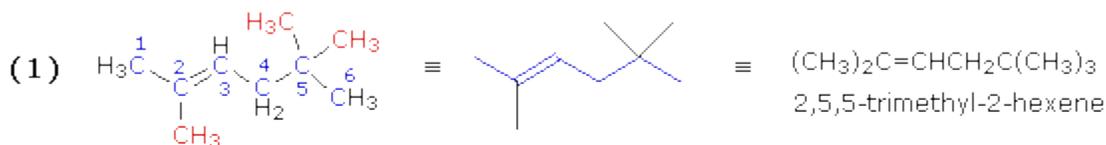


The first two acyclic cases are branched chains containing several multiple bonds. Example (9) has two possible seven-carbon chains, each having three multiple bonds. The one selected has three double bonds and the triple bond becomes a substituent group. In example (10) we find a six-carbon chain containing two double bonds, and a seven-carbon chain with a double and a triple bond. The latter becomes the root chain and the second double bond is a vinyl substituent on that chain. The last example (11) shows that in numbering a cycloalkene one must first consider substituents on the double bond in assigning sites #1 and #2. Here the double bond carbon atom to which the ethyl group is attached becomes #1 and the other carbon of the double bond is necessarily carbon #2. Sometimes this results in other substituents having high locator numbers, as does bromine in this case.

Illustration 1 $(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{C}(\text{CH}_3)_3$

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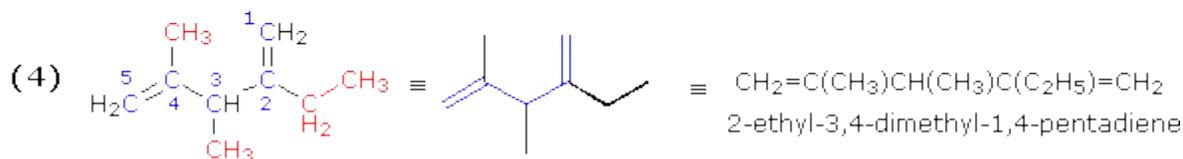
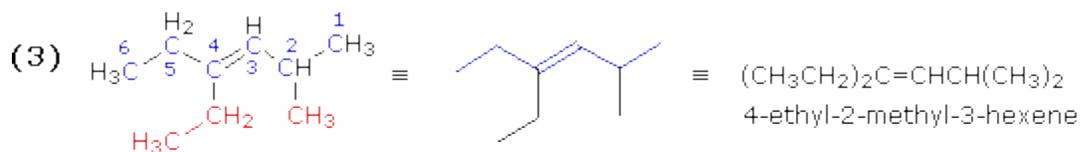
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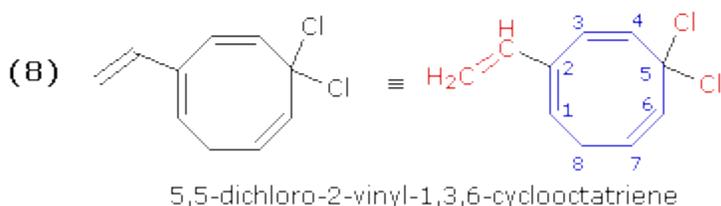
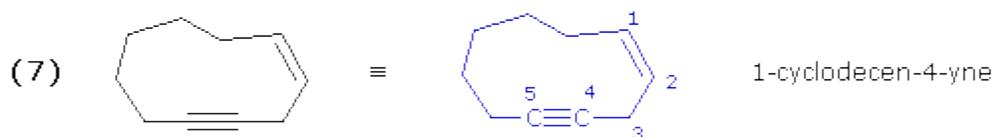
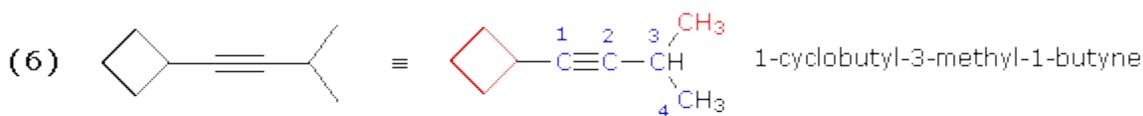
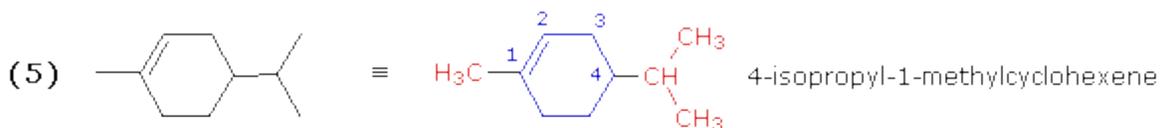
Illustration 3 $(\text{C}_2\text{H}_5)_2\text{C}=\text{CHCH}(\text{CH}_3)_2$ **Illustration 4** $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{C}(\text{C}_2\text{H}_5)=\text{CH}_2$

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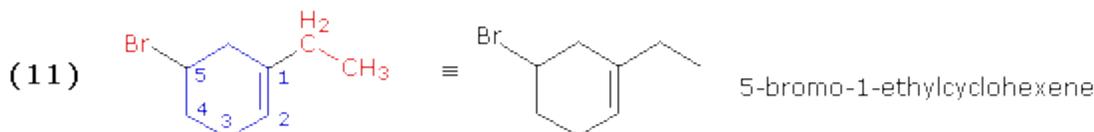
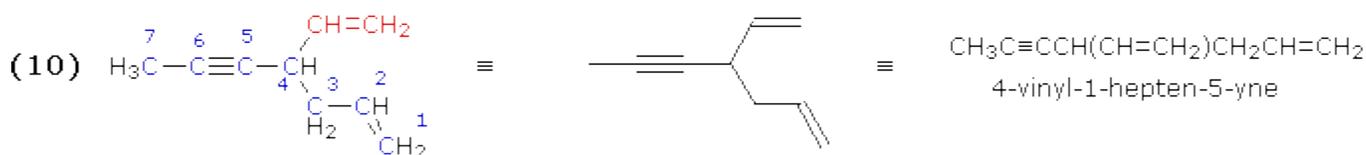
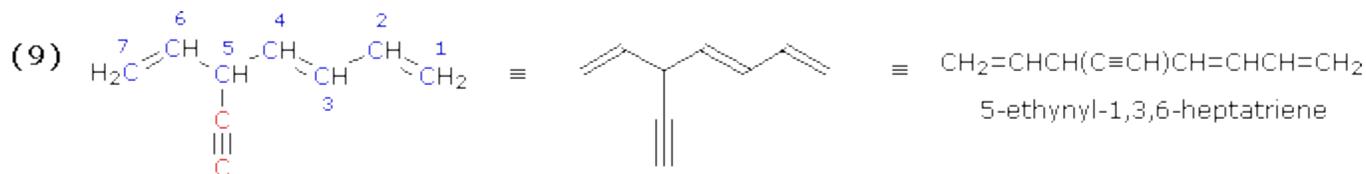
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Sub-Rules for IUPAC Nomenclature

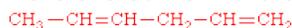
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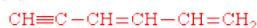


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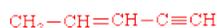
Here are some more examples:



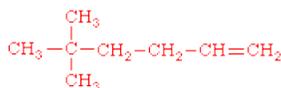
1,4-hexadiene



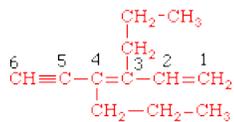
1,3-hexadien-5-yne



3-penten-1-yne



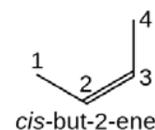
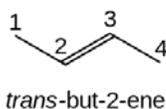
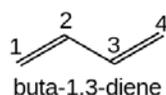
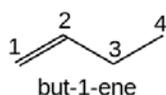
5,5-dimethyl-1-hexene



3,4-dipropyl-1,3-hexadien-5-yne



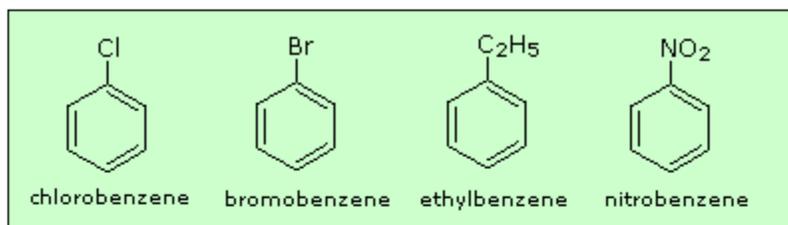
1,4,4-trimethylcyclobutene
(NOT: 2,3,3-trimethylcyclobutene)



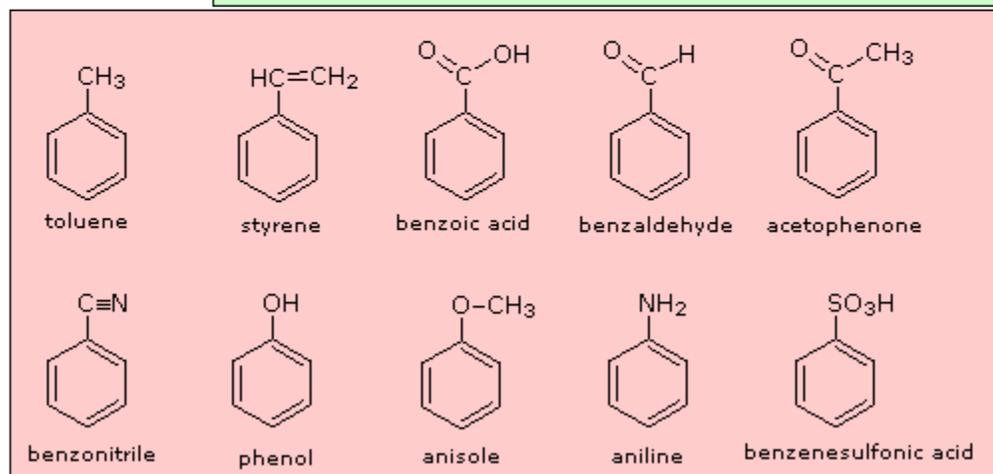
Benzene Derivatives

Benzene Derivatives

The nomenclature of substituted benzene ring compounds is less systematic than that of the alkanes, alkenes and alkynes. A few mono-substituted compounds are named by using a group name as a prefix to "benzene", as shown by the combined names listed below. A majority of these compounds, however, are referred to by singular names that are unique. There is no simple alternative to memorization in mastering these names.

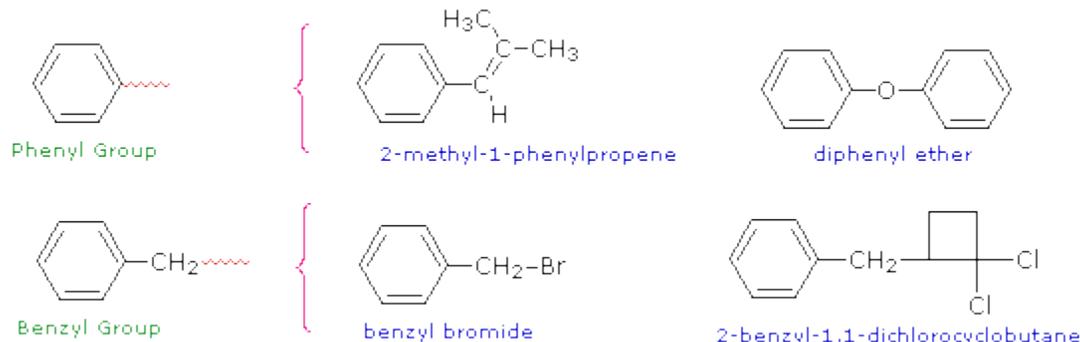


Combined Names

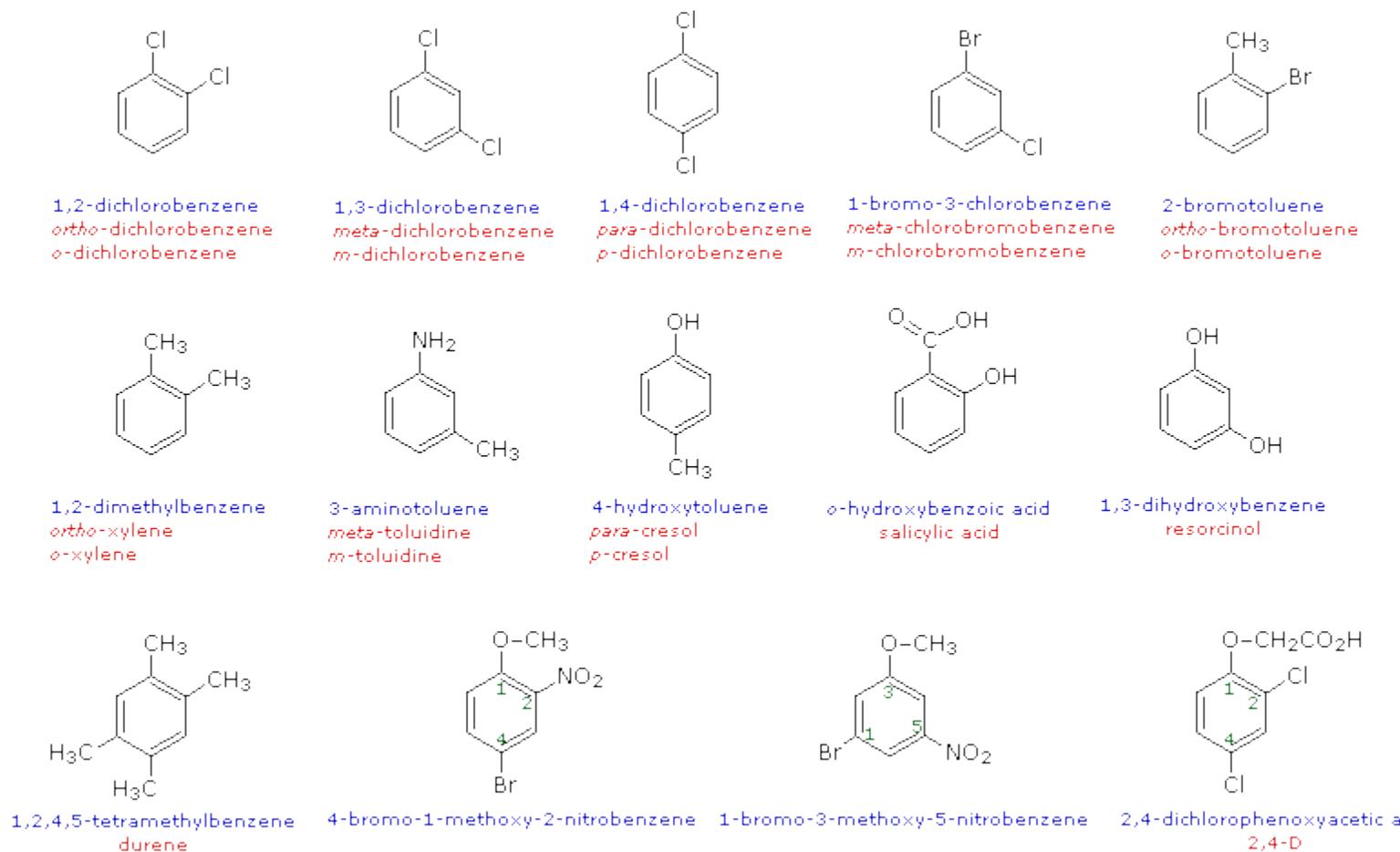


Singular Names

Two commonly encountered substituent groups that incorporate a benzene ring are **phenyl**, abbreviated Ph-, and **benzyl**, abbreviated Bn-. These are shown here with examples of their use. Be careful not to confuse a phenyl (pronounced *fenyl*) group with the compound phenol (pronounced *feenol*). A general and useful generic notation that complements the use of **R-** for an alkyl group is **Ar-** for an aryl group (any aromatic ring).



When more than one substituent is present on a benzene ring, the relative locations of the substituents must be designated by numbering the ring carbons or by some other notation. In the case of disubstituted benzenes, the prefixes *ortho*, *meta* & *para* are commonly used to indicate a 1,2- or 1,3- or 1,4- relationship respectively. In the following examples, the first row of compounds show this usage in red. Some disubstituted toluenes have singular names (e.g. xylene, cresol & toluidine) and their isomers are normally designated by the *ortho*, *meta* or *para* prefix. A few disubstituted benzenes have singular names given to specific isomers (e.g. salicylic acid & resorcinol). Finally, if there are three or more substituent groups, the ring is numbered in such a way as to assign the substituents the lowest possible numbers, as illustrated by the last row of examples. The substituents are listed alphabetically in the final name. If the substitution is symmetrical (third example from the left) the numbering corresponds to the alphabetical order.



Other Functional Groups

The previous discussion has focused on the carbon framework that characterizes organic compounds, and has provided a set of nomenclature rules that, with some modification, apply to all such compounds. An introduction to functional group nomenclature was limited to carbon-carbon double and triple bonds, as well as simple halogen groups. There are, however, many other functional groups that are covered by the IUPAC nomenclature system. A summary of some of these groups and the characteristic nomenclature terms for each is presented in the following table. Specific examples of their nomenclature will be provided as the chemistry of each group is discussed.

Group Names and Suffixes for Some Common Functional Groups

Functional Class	General Formula	Group Name	Suffix
Alcohols	-O-H	hydroxy-	-ol
Ethers	-OR	(R)-oxy-	---
Sulfides	-SR	(R)-sulfanyl-	---
Amines	-NH ₂	amino-	-amine
Carboxylic acids	-CO ₂ H	carboxy-	-carboxylic acid
		---	-oic acid
Carboxylate Salts	-CO ₂ ⁽⁻⁾ M ⁽⁺⁾	---	(cation) ...carboxylate
		---	(cation) ...oate
Amides	-CONH ₂	carbamoyl-	-carboxamide
		---	-amide
Esters (of carboxylic acids)	-COOR	(R)-oxycarbonyl-	(R)...carboxylate (R)...oate
Aldehydes	-CH=O	formyl-	-carbaldehyde
		---	-al
Ketones	C=O	oxo-	-one
Nitriles	-C≡N	cyano-	-carbonitrile
		---	-nitrile

Note that only one functional group suffix, other than "ene" and "yne", may be used in a given name. The following table gives the priority order of suffix carrying groups in arriving at a IUPAC name. When a compound contains more than one kind of group in this list, the principal characteristic group is the one nearest the top. All other groups are then cited as prefixes.

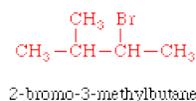
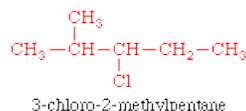
Decreasing Priority Order of Principle Characteristic Groups Identified by a Suffix (Shortened List)

Functional group. (Highest priority determines the type of compound.)
Acids (- COOH)
Esters
Amides
Nitriles
Aldehydes
Ketones
Alcohols and Phenols
Amines
Ethers (in strict IUPAC replace by alkoxys)
Sulfides
Bonds
Arenes
Alkenes
Alkynes
Substituents. Have the lowest precedent, but remember that if there is more than one functional group, the second one etc. is considered a substituent, but the priority list remains the same. This list is impossible to find so may be wrong, but it's close enough.
Halogens (alphabetical),
Alkoxys
Aryle (phenyl, benzyl)
Nitrates (-NO ₂),
Alkyls (alphabetical).

Here are some examples:

Alkyl halides

The halogen is treated as a substituent on an alkane chain. The halo- substituent is considered of equal rank with an alkyl substituent in the numbering of the parent chain. The halogens are represented as follows: F fluoro-, Cl chloro-, Br bromo-, I iodo-

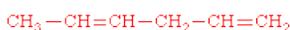


Alkenes and Alkynes - unsaturated hydrocarbons

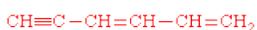
Double bonds in hydrocarbons are indicated by replacing the suffix **-ane** with **-ene**. If there is more than one double bond, the suffix is expanded to include a prefix that indicates the number of double bonds present (**-adiene**, **-atriene**, etc.). Triple bonds are named in a similar way using the suffix **-yne**. The position of the multiple bond(s) within the parent chain is(are) indicated by placing the number(s) of the first carbon of the multiple bond(s) directly in front of the base name.

Here is an important list of rules to follow:

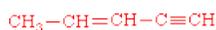
1. The parent chain is numbered so that the multiple bonds have the lowest numbers (double and triple bonds have priority over alkyl and halo substituents).
2. When both double and triple bonds are present, numbers as low as possible are given to double and triple bonds even though this may at times give "-yne" a lower number than "-ene". When there is a choice in numbering, the double bonds are given the lowest numbers.
3. When both double and triple bonds are present, the -en suffix follows the parent chain directly and the -yne suffix follows the -en suffix (notice that the e is left off, -en instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the triple bond(s) is(are) indicated between the -en and -yne suffixes. See below for examples.
4. For a branched unsaturated acyclic hydrocarbon, the parent chain is the longest carbon chain that contains the **maximum number of double and triple bonds**. If there are two or more chains competing for selection as the parent chain (chain with the most multiple bonds), the choice goes to (1) the chain with the greatest number of carbon atoms, (2) the # of carbon atoms being equal, the chain containing the maximum number of double bonds.
5. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.



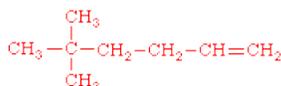
1,4-hexadiene



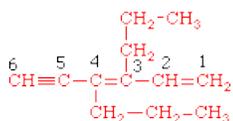
1,3-hexadien-5-yne



3-penten-1-yne



5,5-dimethyl-1-hexene



3,4-dipropyl-1,3-hexadien-5-yne



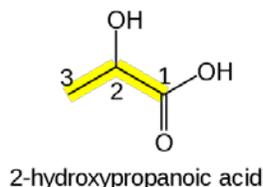
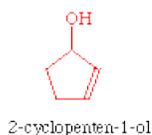
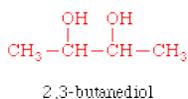
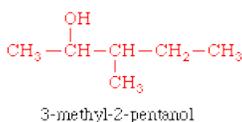
1,4,4-trimethylcyclobutene
(NOT: 2,3,3-trimethylcyclobutene)

Alcohols

Alcohols are named by replacing the suffix **-ane** with **-anol**. If there is more than one hydroxyl group (-OH), the suffix is expanded to include a prefix that indicates the number of hydroxyl groups present (**-anediol**, **-anetriol**, etc.). The position of the hydroxyl group(s) on the parent chain is(are) indicated by placing the number(s) corresponding to the location(s) on the parent chain directly in front of the base name (same as alkenes).

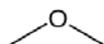
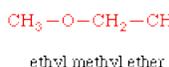
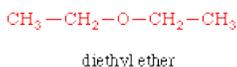
Here is an important list of rules to follow:

6. The hydroxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
7. When both double bonds and hydroxyl groups are present, the -en suffix follows the parent chain directly and the -ol suffix follows the -en suffix (notice that the e is left off, -en instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the hydroxyl group(s) is(are) indicated between the -en and -ol suffixes. See below for examples. Again, the hydroxyl gets priority in the numbering of the parent chain.
8. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

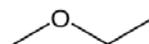


Ethers

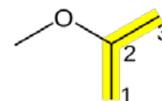
You are only expected to know how to name ethers by their common names. The two alkyl groups attached to the oxygen are put in alphabetical order with spaces between the names and they are followed by the word ether. The prefix di- is used if both alkyl groups are the same.



methoxymethane
(dimethyl ether)



methoxyethane
(ethyl methyl ether)



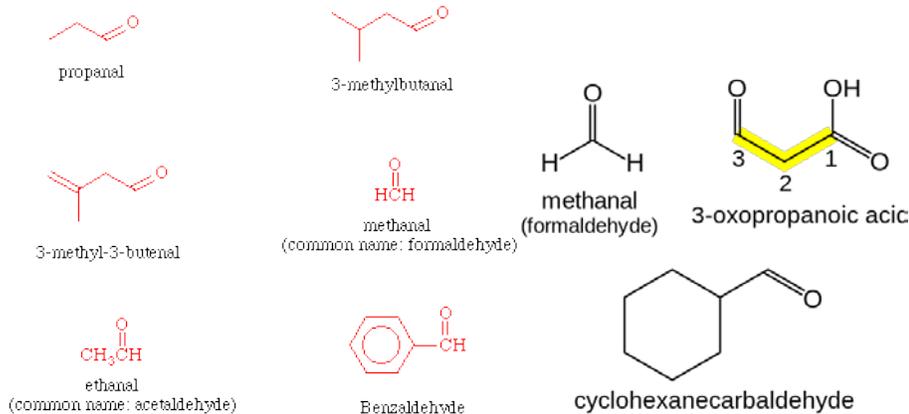
2-methoxypropane
(isopropyl methyl ether)

Aldehydes

Aldehydes are named by replacing the suffix **-ane** with **-anal**. If there is more than one **-CHO** group, the suffix is expanded to include a prefix that indicates the number of **-CHO** groups present (**-anedial** - there should not be more than 2 of these groups on the parent chain as they must occur at the ends). It is not necessary to indicate the position of the **-CHO** group because this group will be at the end of the parent chain and its carbon is automatically assigned as C-1.

Here is an important list of rules to follow:

9. The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
10. When both double bonds and carbonyl groups are present, the **-en** suffix follows the parent chain directly and the **-al** suffix follows the **-en** suffix (notice that the **e** is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the **-al** suffix follows the **-en** suffix directly. Remember it is not necessary to specify the location of the carbonyl group because it will automatically be carbon #1. See below for examples. Again, the carbonyl gets priority in the numbering of the parent chain.
11. There are a couple of common names which are acceptable as IUPAC names. They are shown in the examples at the end of this list but at this point these names will not be accepted by the computer. Eventually they will be accepted.
12. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

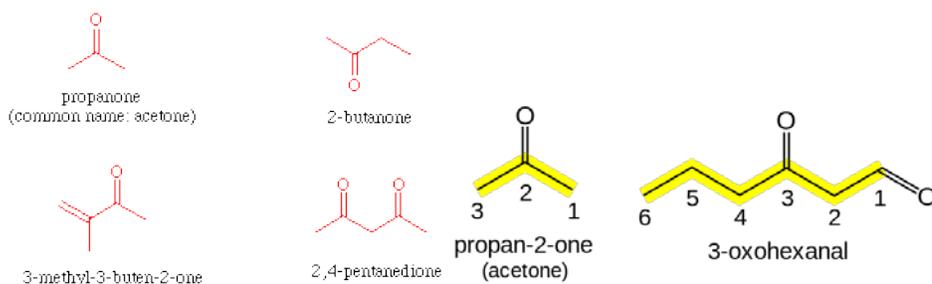


Ketones

Ketones are named by replacing the suffix **-ane** with **-anone**. If there is more than one carbonyl group (C=O), the suffix is expanded to include a prefix that indicates the number of carbonyl groups present (**-anedione**, **-anetrione**, etc.). The position of the carbonyl group(s) on the parent chain is(are) indicated by placing the number(s) corresponding to the location(s) on the parent chain directly in front of the base name (same as alkenes).

Here is an important list of rules to follow:

- The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
- When both double bonds and carbonyl groups are present, the **-en** suffix follows the parent chain directly and the **-one** suffix follows the **-en** suffix (notice that the **e** is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the carbonyl group(s) is(are) indicated between the **-en** and **-one** suffixes. See below for examples. Again, the carbonyl gets priority in the numbering of the parent chain.
- If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

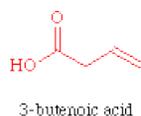
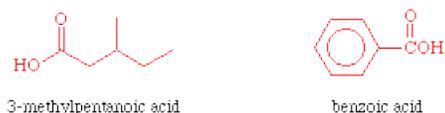


Carboxylic Acids

Carboxylic acids are named by counting the number of carbons in the longest continuous chain including the carboxyl group and by replacing the suffix **-ane** of the corresponding alkane with **-anoic acid**. If there are two **-COOH** groups, the suffix is expanded to include a prefix that indicates the number of **-COOH** groups present (**-anedioic acid** - there should not be more than 2 of these groups on the parent chain as they must occur at the ends). It is not necessary to indicate the position of the **-COOH** group because this group will be at the end of the parent chain and its carbon is automatically assigned as C-1.

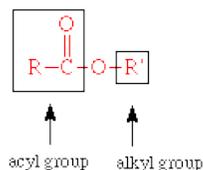
Here is an important list of rules to follow:

16. The carboxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
17. If the carboxyl group is attached to a ring the parent ring is named and the suffix -carboxylic acid is added.
18. When both double bonds and carboxyl groups are present, the -en suffix follows the parent chain directly and the -oic acid suffix follows the -en suffix (notice that the e is left off, **-en** instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the -oic acid suffix follows the -en suffix directly. Remember it is not necessary to specify the location of the carboxyl group because it will automatically be carbon #1. See below for examples. Again, the carboxyl gets priority in the numbering of the parent chain.
19. There are several common names which are acceptable as IUPAC names. They are shown in the examples at the end of this list **but** at this point these names will **not** be accepted by the computer. Eventually they will be accepted.
20. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

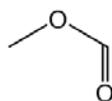
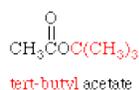
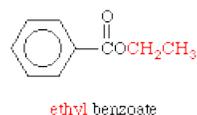
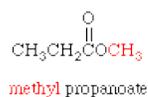


Esters

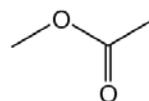
Systematic names of esters are based on the name of the corresponding carboxylic acid. Remember esters look like this:



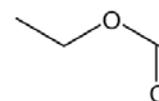
The alkyl group is named like a substituent using the **-yl** ending. This is followed by a space. The acyl portion of the name (what is left over) is named by replacing the **-ic acid** suffix of the corresponding carboxylic acid with **-ate**.



methyl methanoate
(formate)



methyl ethanoate
(acetate)

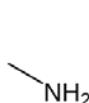


ethyl methanoate
(ethyl formate)

Amines

You are only expected to know how to name amines by their common names. They are named like ethers, the alkyl (R) groups attached to the nitrogen are put in alphabetical order with no spaces between the names and these are followed by the word amine. The prefixes di- and tri- are used if two or three of the alkyl groups are the same.

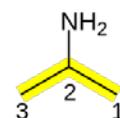
NOTE: Some books put spaces between the parts of the name, but we will not. Follow the examples.



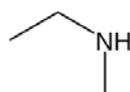
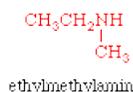
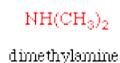
methanamine
(methylamine)



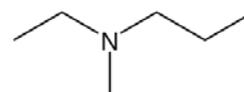
propan-1-amine
(propyl amine)*n*-



propan-2-amine
(isopropyl amine)



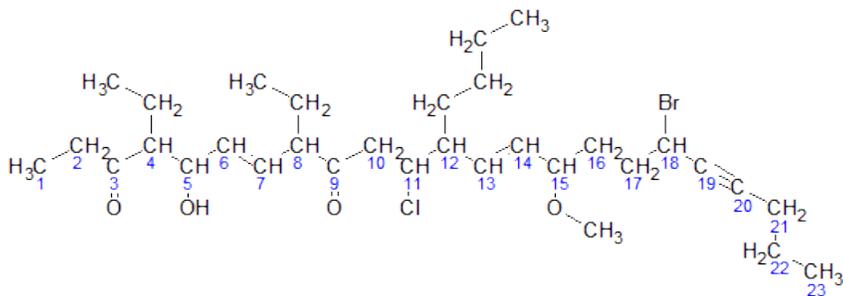
N-methylethanamine



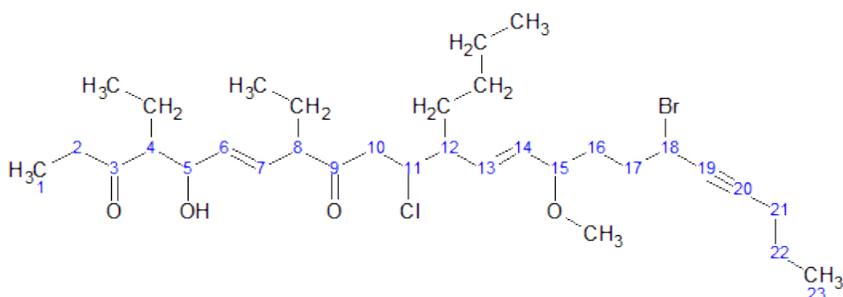
N-ethyl-methylpropanamine

Example: Putting it all together.

Here is a sample molecule with the parent carbons numbered:



For simplicity, here is an image of the same molecule, where the hydrogens in the parent chain are removed and the carbons are shown by their numbers:



Now, following the above steps:

1. The parent hydrocarbon chain has 23 carbons. It is called **tricos-**.
2. The functional groups with the highest precedence are the two ketone groups.
 1. The groups are on carbon atoms 3 and 9. As there are two, we write **3,9-dione**.
 2. The numbering of the molecule is based on the ketone groups. When numbering from left to right, the ketone groups are numbered 3 and 9. When numbering from right to left, the ketone groups are numbered 15 and 21. 3 is less than 15, therefore the ketones are numbered 3 and 9. The **smaller number** is always used, **not the sum** of the constituents numbers.
3. The side chains are: an ethyl- at carbon 4, an ethyl- at carbon 8, and a butyl- at carbon 12.

Note: The -O-CH₃ at carbon atom 15 is not a side chain, but it is a methoxy functional group

 - o There are two ethyl- groups. They are combined to create, **4,8-diethyl**.
 - o The side chains are grouped like this: **12-butyl-4,8-diethyl**. (But this is not the final grouping, as functional groups may be added in between.)
4. The secondary functional groups are: a hydroxy- at carbon 5, a chloro- at carbon 11, a methoxy- at carbon 15, and a bromo- at carbon 18. Grouped with the side chains, this gives **18-bromo-12-butyl-11-chloro-4,8-diethyl-5-hydroxy-15-methoxy**
5. There are two double bonds: one between carbons 6 and 7, and one between carbons 13 and 14. They will be called **6,13-diene**. There is one triple bond between carbon atoms 19 and 20. It will be called **19-yne**
6. The arrangement (with punctuation) is: **18-bromo-12-butyl-11-chloro-4,8-diethyl-5-hydroxy-15-methoxytricos-6,13-diene-19-yne-3,9-dione**

The final name is **18-bromo-12-butyl-11-chloro-4,8-diethyl-5-hydroxy-15-methoxytricos-6,13-diene-19-yne-3,9-dione**.