

IUPAC Rules for Naming Organic Molecules

From *J. Chem. Ed.* Article by Stanislaw Skonieczny

To name a compound using the IUPAC system, follow the steps shown (if applicable) in the following order.

Step 1

Determine the principle functional group in the compound. When a compound contains more than one group in Table 1, the principle group is that which has the highest precedence. This group will be cited as a suffix; all other groups are cited as prefixes.

Functional Group	Suffix if Highest Precedence	Prefix if Lower Precedence
-(C) ^a OOH	-oic acid	-
-COOH	-carboxylic acid	carboxy-
-SO ₂ OH	-sulfonic acid	sulfo-
-C(O)OC(O)-	-oic anhydride	-
-(C)OOR	alkyl -oate	alkoxy-oxo-
-COOR	alkyl carboxylate	-
-(C)OX	-oyl halide	halo-oxo-
-COX	-carbonyl halide	halocarbonyl-
-(C)ONH ₂	-amide	amino-oxo-
-CONH ₂	-carboxamide	aminocarbonyl-
-(C)≡N	-nitrile	-
-C≡N	-carbonitrile	cyano-
-(C)HO	-al	oxo-
-CHO	-carbaldehyde	formyl-
>(C)=O	-one	oxo-
-OH	-ol	hydroxy-
-SH	-thiol	sulfanyl-
-NH ₂	-azane (-amine)	azanyl- (-amino)
>NH	-azane (-imine)	azanylidene-
>C=C<	-ene	*
-C≡C-	-yne	**
-X, -R, -OR	-	halo-, alky-l, alkoxy-
-Ar, -NO ₂	-	aryl-, nitro-
-NO, -N ₃	-	nitroso-, azido-
=N ₂ , -SR	-	diazo-, (R)-sulfanyl-

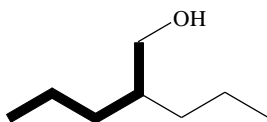
^a (C) designates a carbon atom included in the parent hydrocarbon (part of the longest chain or ring).

* and ** These are always used as a suffix. If a higher priority group is present in the molecule the suffix is changed to -en- or -yn- and is followed by the suffix of the higher priority group.

Step 2

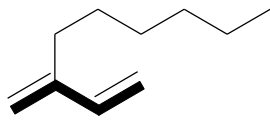
Determine the parent hydrocarbon (principle chain or ring system system):

- (a) If the principle group occurs in a chain, the principle chain is selected as
- the chain containing the functional group of the highest seniority as the parent.



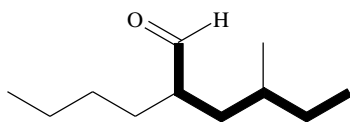
2-(propan-1-yl)pentan-1-ol

- If more than one such choice is possible, select the chain with the maximum number of multiple bonds.



2-(hexan-1-yl)buta-1,3-diene

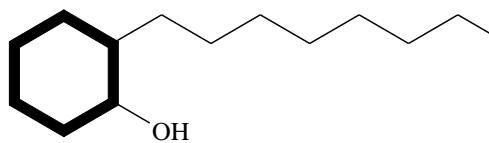
- If (i) and (ii) together are not definitive, then choose the longest chain.
- If two chains of the same length are possible, choose the one with the maximum number of substituent groups.



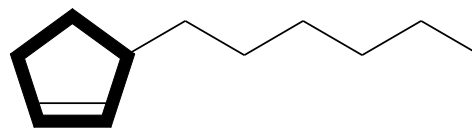
2-(butan-1-yl)-4-methylhexanal

The parent chain here contains six carbon atoms.

- (b) If the principle functional group occurs in a cyclic system, that system forms the parent.



2-(octan-1-yl)cyclohexanol



2-(hexan-1-yl)cyclopentene

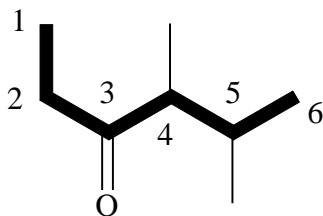
Step 3

Name the parent structure of and the principle group(s). Give the parent name the same name as if it were an alkane, but replace *-ane* with the suffix characteristic of the functional group of the highest priority (Table 1). Note: Multiple unsaturation in hydrocarbons is indicated by the numerical prefixes *di-*, *tri-*, etc. In such cases, however, the ending *-ane* of the parent alkane is replaced with *-adiene*, *-atriene*, etc. leaving the “a” in the root alkane name whenever the first letter of the suffix is a consonant to make the name easier to pronounce. Thus we get alkadienes, alkatrienes, alkadiynes, etc.

Step 4

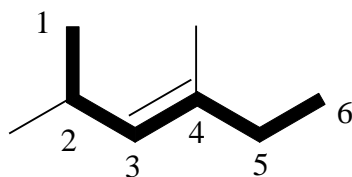
Complete the number system.

- (a) Number the carbon atoms consecutively from the end of the chain nearer the functional group of the highest priority.



4,5-dimethylhexan-3-one

- (b) If the same number for the functional group of highest priority is obtained in both directions, the correct IUPAC name is the one that contains the lowest substituent numbers.

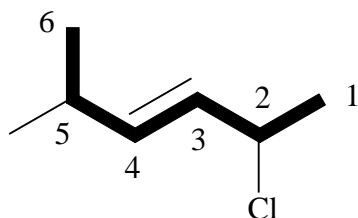


2,4-dimethylhex-3-ene

The substituent numbers are 2 and 4. If we numbered from the other end, the substituent numbers would have been 3 and 5. 2+4 is a lower numbering system than 3+5.

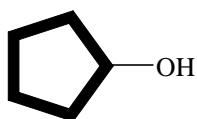
- (c) If the first substituents occur at an equal distance from each end of the chain, number the end nearer a second substituent. If still the same, continue until the first point of difference.

- (d) If numbering for either end gives the same set of numbers, number from the end with the substituent that comes first in alphabetical order.

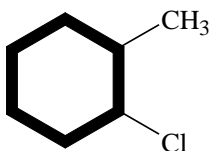


2-chloro-5-methylhex-3-ene

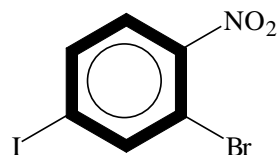
- (e) In monosubstituted cycloalkanes and benzene derivatives. The carbon to which the substituent is bonded is always number 1. If there is only one substituent, the locant number "1" is omitted. However, the number one is required in polysubstituted compounds.



Cyclopentanol



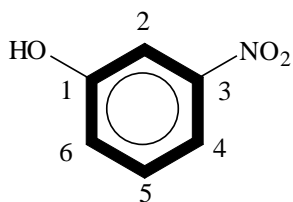
1-chloro-2-methylcyclohexane



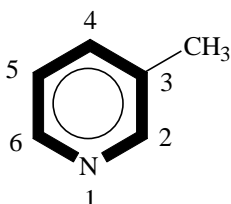
2-bromo-4-iodo-1-nitrobenzene

- (f) In polysubstituted cyclic compounds, the starting point and the direction of numbering are chosen to give the lowest numbering system. The starting point is chosen according to the following factors:

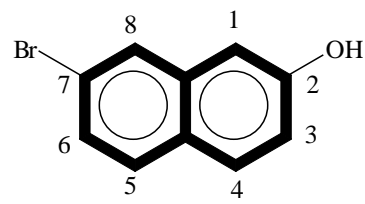
- (i) The principle functional group named as the suffix is always given the lowest possible number. Because certain cyclic systems have fixed numbering systems, it is not always possible to place a substituent on carbon number 1.



IUPAC: 3-nitrobenzen-1-ol
(3-nitrophenol accepted)

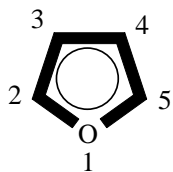


3-methylazabenzene
(3-methylpyridine accepted)

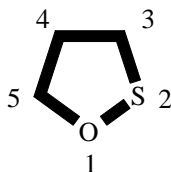


7-bromonaphthalene-2-ol
(7-bromo-2-naphthol accepted)

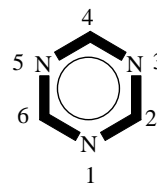
Note: When one heteroatom is present in the ring the number 1 is assigned to that atom. If more than one is present then we use the number 1 on the O, S, or N in that order of priority.



IUPAC: oxole
(Furan accepted)

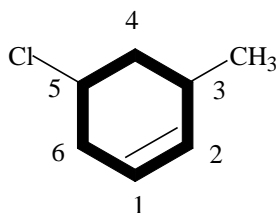


1,2-oxathiolane

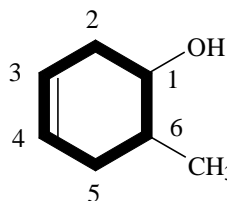


1,3,5-triazine

(ii) Lowest numbering for multiple bonds in cyclic compounds.



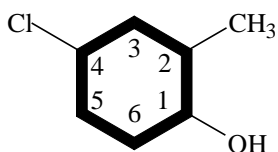
5-chloro-3-methylcyclohexene



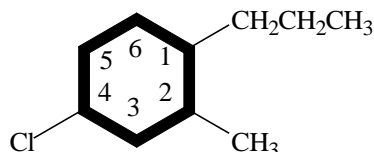
6-methylcyclohex-3-en-1-ol

Note: In naming cycloalkenes, the double bond is located between C1 and C2, and the "1" is usually omitted in the name. The ring is numbered clockwise or counterclockwise to give the first substituent the lower number. However, when functional group with a higher priority than an alkene is present, the carbon bonded to the higher priority group becomes C1 and then multiple bonds are considered for lowest possible numbering.

(iii) Lowest numbering for first substituent (or first point of difference).

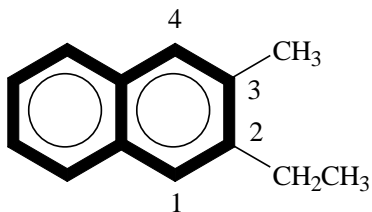


4-chloro-2-methylcyclohexan-1-ol

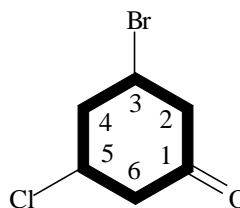


4-chloro-2-methyl-1-(propan-1-yl)cyclohexane

(iv) If the same numbers will result from numbering in either direction, give the lowest number for the substituent that is cited first in the name.



2-ethyl-3-methylnaphthalene



3-bromo-5-chlorocyclohexanone

Step 5

Name alkyl groups, halides, and other substituents and determine their position on the chain by the numbering system established by step 4.

Step 6

Assign the stereochemistry to chiral carbon atoms (stereocenters) and the double bond(s):

- (a) Disubstituted alkenes may be named in two ways: (i) using terms *cis*- and *trans*- or (ii) using terms (*E*) or (*Z*). Note: Use of (*E*) and (*Z*) stereocenters is preferred. However, the *cis-trans* terms are accepted.

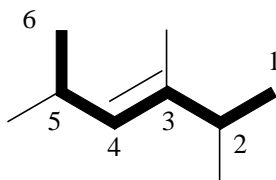


(*E*)-pent-2-ene or *trans*-pent-2-ene



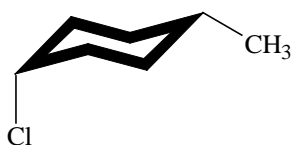
(*Z*)-hex-3-ene or *cis*-hex-3-ene

- (b) Tri- and tetra- substituted alkenes may only be named using the (*E-Z*) system.



(*E*)-2,3,5-trimethylhex-3-ene

- (c) Disubstituted cycloalkanes may be named using the terms *cis-trans* or (*R-S*).

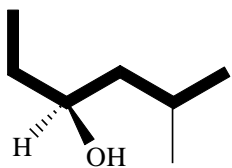


cis-1-chloro-4-methylcyclohexane
(*R-S*) system not applicable here

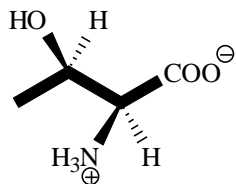


trans-3-methylcyclopentanol
(*1R,3R*)-3-methylcyclopentanol

(d) Chiral carbon atoms are assigned (*R*) or (*S*) configuration.

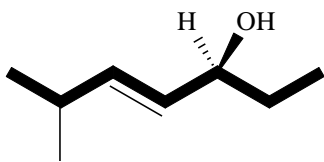


(*S*)-5-methylhexan-3-ol

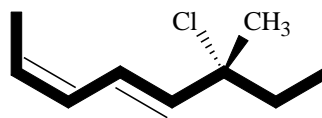


(*2S,3R*)-2-amino-3-hydroxybutanoic acid
common name: threonine

(e) When both (*R-S*) and (*E-Z*) stereodescriptors are present, they are placed in parentheses followed by a hyphen; each stereodescriptor is immediately preceded by its associated number and they are arranged in numerical order.



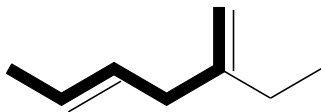
(*3S,4E*)-6-methylhept-4-en-3-ol



(*2Z,4E,6R*)-6-chloro-6-methylocta-2,4-diene

Step 7

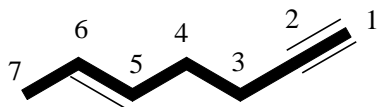
Compounds with multiple bonds and triple bonds have the following suffixes: *-adiene*, *-adiyne*, *-atriene*, *-atetraene*, and so on. Specify the location of each multiple bond by a locant number placed between the “*a*” and *diene*, *diyne*, *triene*, etc.



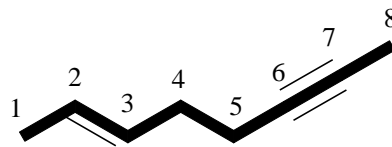
(*E*)-2-ethylhexa-1,4-diene
previously: (*E*)-2-ethyl-1,4-hexadiene

Step 8

Compounds with both double and triple bonds are called enynes. Start the numbering of enynes from the end nearest the first multiple bond, regardless of type. When a double bond is the same distance from one end as a triple bond from the other end, assign the double bond the lower number.



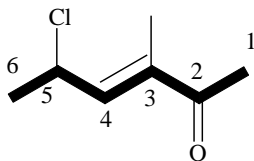
(*E*)-hept-5-en-1-yne



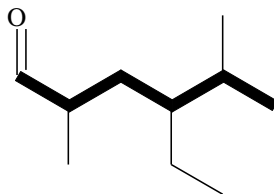
(*E*)-oct-2-en-6-yne

Step 9

Write the complete name of the compound as a single word with the correct locant numbers for all substituents, which are listed in alphabetical order. The prefixes *di*, *tri*, *tetra*, etc. do not alter the alphabetical ordering of the substituents. The stereochemistry is indicated by placing the appropriate prefix within parentheses followed by a hyphen in front of the name.

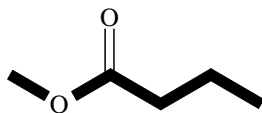


(*E*)-5-chloro-3-methyl-3-en-2-one



4-ethyl-2,5-dimethylhexanal

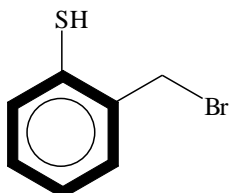
- The numbers indicating locations of substituents are separated by commas.
- The letters and numbers are joined by hyphens.
- When naming esters, no hyphen is placed between the name of the alkyl group derived from the alcohol and the name of the acid from which the ester was derived.



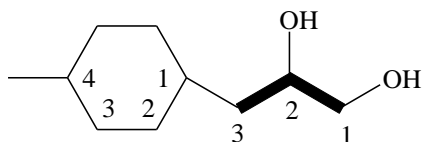
methyl butanoate

Step 10

A complex substituent is named by applying the above steps just as if the substituent were a compound itself. We begin numbering the sidechain at the point of attachment to the parent hydrocarbon giving the carbon at the point of attachment the locant of C1. We then give this substituent the suffix *-yl*. We put this name in parentheses and in front of the parentheses we place the locant number on the parent hydrocarbon.

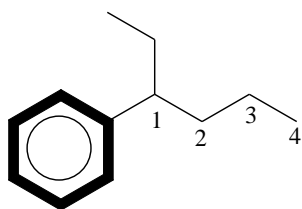


2-(bromomethyl)benzenethiol

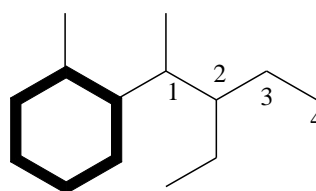


3-(4-methylcyclohexyl)propane-1,2-diol

When a complex sidechain contains a chain that is attached to the parent hydrocarbon at a position other than at the end of the chain, the carbon of attachment is still numbered as C1 and the other part of the chain is named as a substituent group to that chain.

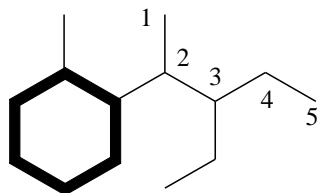


(1-ethylbutyl)benzene



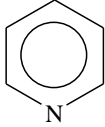
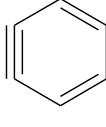
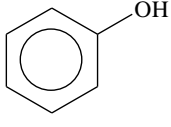
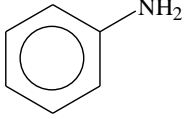
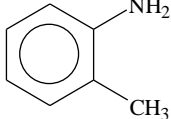
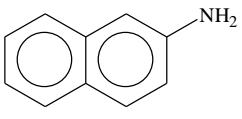
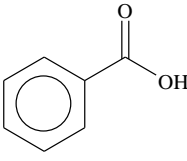
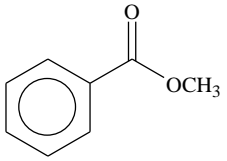
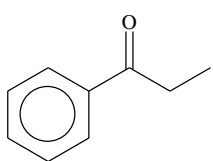
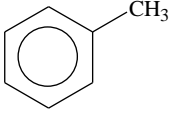
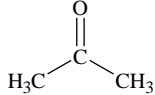
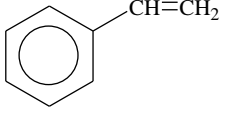
1-(2-ethyl-1-methylbutyl)-2-methylcyclohexane

Note: An alternate method of numbering the sidechain is to find the longest chain and begin numbering at the end closest to its attachment to the parent hydrocarbon. The *-yl* ending is added to the chain parent name and the position of the attachment is placed before the *-yl* ending.



1-(3-ethylpentan-2-yl)-2-methylcyclohexane

Many common names are accepted by IUPAC and retained because of their wide use in organic, biochemistry, and polymer nomenclature. The table below shows some examples of IUPAC names for commonly known compounds. The IUPAC system allows the trivial names of these compounds to be retained as official IUPAC names and, for some, to be used in naming substituted compounds such as 4-bromobenzoic acid. The IUPAC systematic name for this compound would be 4-bromobenzenecarboxylic acid.

IUPAC: Trivial (retained)	 azabenzene pyridine	 1,2-dehydrobenzene benzyne	 benzenol phenol
IUPAC: Trivial (retained)	 phenylazane benzenamine aniline	 2-methylphenylazane 2-methylbenzenamine <i>ortho</i> -toluidine	 naphthalene-2-ylazane naphthalene-2-amine 2-naphthylamine
IUPAC: Trivial (retained)	 benzenecarboxylic acid benzoic acid	 methyl benzenecarboxylate methyl benzoate	 1-phenylpropan-1-one propiophenone
IUPAC: Trivial (retained)	 methylbenzene toluene	 propan-2-one acetone	 (ethenyl)benzene styrene

Many other trivial names are also retained but can only be used for the unsubstituted compound. For example, the names butanoic acid (systematic) and butyric acid (trivial retained) are both approved by the IUPAC. However, $\text{BrCH}_2\text{CH}_2\text{CH}_2\text{COOH}$ must be named systematically as 4-bromobutanoic acid and cannot be named as 4-bromobutyric acid. A list of approved trivial names can be found at http://www.acdlabs.com/iupac/nomenclature/93/r93_671.htm.

