Naming Rules for Organic Compounds

The names of organic molecules are divided into three parts;

1. the 'root' name, indicative of the number of carbon atoms in the longest continuous chain, which includes the highest priority functional group.

2. the suffix name, which indicates the position and identity of the highest priority functional group.

3. the prefix name, indicative of the position and identity of substituent groups.

Root Names for Hydrocarbons

# Carbons	Root Name	Alkane (add "ane")	Alkyl Substituent (add "yl")
1	meth	methane	methyl
2	eth	ethane	ethyl
3	prop	propane	propyl
4	but	butane	butyl
5	pent	pentane	pentyl
6	hex	hexane	hexyl
7	hept	heptane	heptyl
8	oct	octane	octyl
9	non	nonane	nonyl
10	dec	decane	decyl
11	undec	undecane	undecyl
12	dodec	dodecane	dodecyl
20	eicos	eicosane	eicosyl

Suffixes for Functional Groups

Alkenes (contain C=C): Add "ene" to the **root name**
Alkynes (contain C≡C): Add "yne" to the **root name**
Alcohols (contain -OH): Add "anol" to the **root name**
Aldehydes (contain terminal C=O): Add "anal" to the **root name**
Ketones (contain C=O): Add "anone" to the **root name**
Amides (contain -CONR): Add "anamide to the **root name**
Esters (contain $-CO_2R$): Add "anoate" to the **root name**
Carboxylic Acids (contain $-CO_2H$): Add "anoic acid" to the **root name**

IUPAC Nomenclature for Hydrocarbons

Alkanes

1) Identify the "parent" chain by counting the longest number of carbon atoms which are continuously bonded in the molecule.

2) Using this number, choose the corresponding **root name** and add "ane". This is the parent chain name.

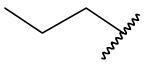
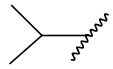
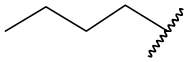
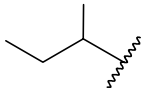
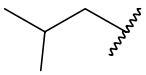
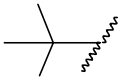
3) Identify substituent groups attached to the parent chain and place them in front of the parent name in alphabetical order. Substituent (or side group) names are based on the total # of carbon atoms in the group and the position of attachment (i.e., *n*-butyl, *sec*-butyl, *tert*-butyl). The *n*-, *sec*-, *tert*-, are used to indicate the whether the position of attachment is *normal* (meaning primary, 1°), *secondary* (2°), or *tertiary* (3°). The prefix "iso" is used to indicate a methyl branching at the end of a side group chain (i.e., isopentyl is $(CH_3)_2CH_2CH_2CH_2$- . Note isopropyl is equivalent to *sec*-propyl but the latter is rarely used). When placing substituent groups in alphabetical order, the prefixes *n* -, *sec*- and *tert*- are ignonored. However, the prefix "iso" is included. Remember, alkyl substituent names must end in "yl".

4) Number the carbon atoms in the parent chain. Assign a number to each of the substituent groups to indicate where it is attached. Start the numbering from whichever end of the parent chain will give rise to the lowest set of numbers. The lowest set is selected on the basis of the lowest number at the first point of difference.

5) If identical substituents are present, then combine them using di, tri, tetra etc. as prefixes. These prefixes are **not** included in the alphabetizing. A list of numbers are separated from each other by commas and the substituent name by a hyphen (i.e., 2,3,3-trimethylhexane).

Notes:

(1) Common Substituent Groups

methyl	CH_3—	
ethyl	CH_3CH_2—	
propyl	$CH_3CH_2CH_2$—	
isopropyl	$(CH_3)_2CH$—	
butyl	$CH_3CH_2CH_2CH_2$—	
sec-butyl	$CH_3CH_2\underset{\vert}{C}HCH_3$	
isobutyl	$(CH_3)_2CHCH_2$—	
tert-butyl	$(CH_3)_3C$—	

(2) Cyclic compounds are named with the prefix "cyclo" directly before parent name (i.e., cyclopentane). Substituents on a cyclic compound may have different geometric orientations *with respect to the plane of the ring*. Groups on the same side of a cyclic molecule are distinguished with the prefix *cis*-, whereas those on opposite sides are denoted *trans*-**.**

Alkenes - compounds containing carbon-carbon double bonds

1) Identify the parent structure with the longest continuous carbon chain that <u>contains</u> the C=C bond. Add "ene" after the appropriate **root name**.

2) Number the parent chain such that carbon starting the double bond has the lowest numerical value. This number is added as a prefix directly in front of the parent alkene name separated by a hyphen (i.e., 2-butene).

3) Treat substituent groups as with alkanes.

4) Use *cis-*/*trans-* or **E**/**Z** to distinguish between geometric isomers where applicable.

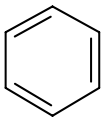
Note: Geometric isomers exist whenever there are two different groups attached on both sides of a double bond. Consider 2-butene; the two methyl groups may be directed on the same side of the double bond (*cis*-or **Z**) or they may be directed away from one another (*trans*- or **E**). (The terms *cis-* and *trans-* are still used but this usage is being phased out).

Alkynes - compounds containing carbon-carbon triple bonds

1) Are named and numbered like alkenes. Add "yne" to **root name**.

Aromatic Hydrocarbons - Compounds containing benzene-like rings

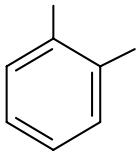
1) Benzene is the simplest aromatic compound containing cyclic structure of six carbons with a total of three double bonds.



benzene

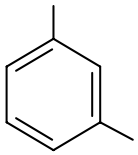
NOT

1,3,5-cyclohexatriene



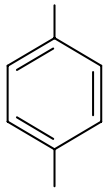
1,2-

ortho



1,3-

meta



1,4-

para

2) Substituents are treated as before.

Notes:

(1) As a substituent, benzene is referred to as a phenyl group.

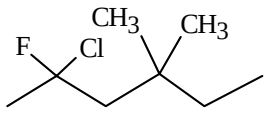
(2) 1,2-disubstituted benzenes are also known as *ortho*-substituted
1,3-disubstituted benzenes are also known as *meta*-substituted
1,4-disubstituted benzenes are also known as *para*-substituted

Nomenclature for Other Functional Groups

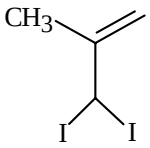
Alkyl Halides (R-X)

- name halogen substituents F, Cl, Br and I as "fluoro", "chloro", "bromo" and "iodo" respectively.

eg.



2-chloro-2-fluoro-4,4-dimethylhexane

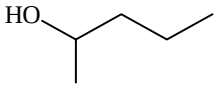


3,3-diiodo-2-methylpropene

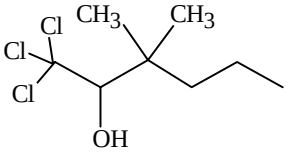
Alcohols (R-OH)

- identify the longest continuous carbon chain that <u>contains</u> the carbon attached to the alcohol group. Add "anol" to the appropriate root name.
- number the parent chain such that the carbon attached to the -OH group has the lowest possible number. Prefix the name with this number.
- treat side groups as before.

eg.

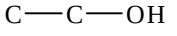


2-pentanol



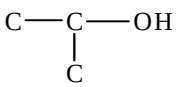
1,1,1-trichloro-3,3-dimethyl-2-hexanol

Note: Coumpounds such as alcohols may be classified as being primary (1^o), secondary (2^o) or tertiary (3^o) depending on the number of carbons bonded to the carbon attached to the -OH group. For example;



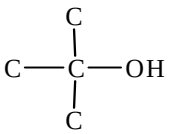
primary ($_1$o)

CH_3CH_2OH



secondary ($_2$o)

$(CH_3)_2CHOH$



tertiary ($_3$o)

$(CH_3)_3COH$

Amines (RNH_2, R_2NH, R_3N)
-many common names are still in usage
-for simple primary amines, name as follows

eg.

$CH_3CH_2CH_2CH_2NH_2$ 2-butanamine

-for simple 2^o and 3^o amines, name the substituents as N-alkyl groups

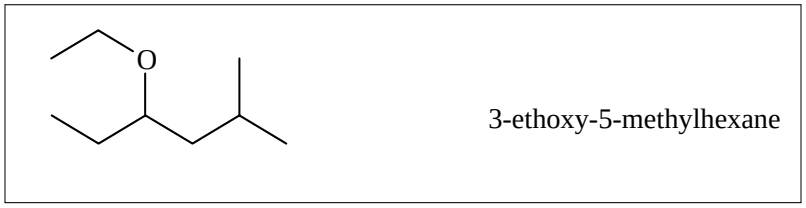
eg. $CH_3CH_2NHCH_3$

N-methylethanamine

-for molecules where the $-NH_2$ group is treated as a substituent, it is referred to as an amino group

Ethers (R-O-R')
-identify the largest alkyl group as the parent name
-treat the remaining R-O- group as an alkoxy side group. Add "oxy" to the root name.

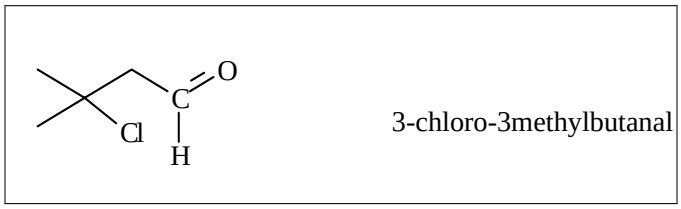
eg.



3-ethoxy-5-methylhexane

Aldehydes (R-CHO)
-identify the longest continuous carbon chain <u>containing</u> the terminal carbon-oxygen double bond. Add "anal" to the root name.
-number the chain such that the aldehyde carbon is atom number one (the number "1" need not appear in the name)

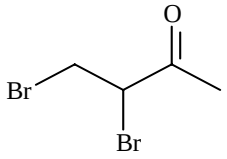
eg.



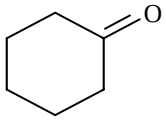
3-chloro-3methylbutanal

Ketones (R-CO-R')
-identify the longest continuous carbon chain containing the carbon-oxygen double bond. Add "anone" to the root name.
-number the chain such that the carbonyl carbon has the lowest possible number. Prefix the name with this number.

eg.



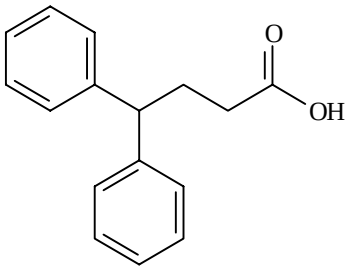
3,4-dibromo-2-butanone



cyclohexanone

Carboxylic Acids (R-CO_2H)
-identify the longest continuous carbon chain containing the acid group (-CO_2H). Add "anoic acid" to the root name.
-number the chain such that the acid carbon is number one (the number "1" need not appear in the name)

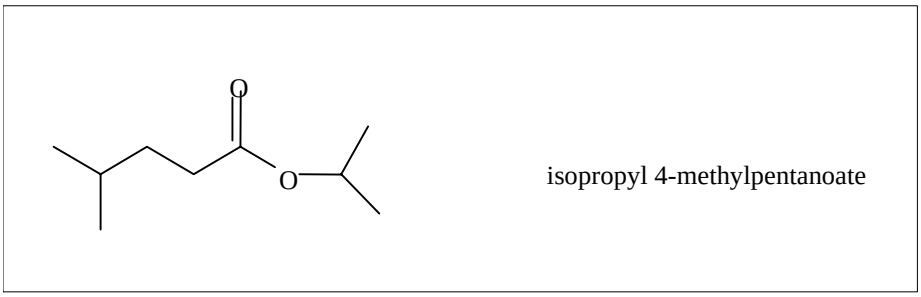
eg.



4,4-diphenylbutanoic acid

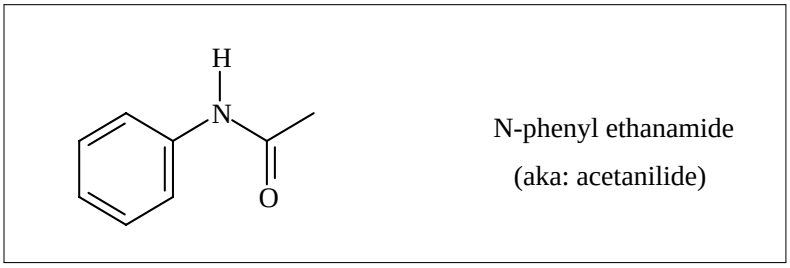
Esters (R-CO_2-R')
-identify longest continuous carbon chain containung the carbonyl carbon. Add "anoate" to root name.
-name R' as an alkyl substituent which preceeds the name with a space.
-number the parent chain such that the carbonyl carbon is number one.

eg.



Amides (R-CONR'$_2$)
-identify longest continuous carbon chain containung the carbonyl carbon. Add "anamide" to root name.
-name R' as an N-alkyl substituent which preceeds the parent name with a space.
-number the parent chain such that the carbonyl carbon is number one.

eg.



Naming Compounds with more than one Functional Group

-use the parent name highest on the priority list

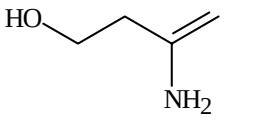
alkane<alkene<alkyne<amine<alcohol<ketone<aldehyde<ester<carboxylic acid
i.e., a compound containing both a C=C and a -OH is regarded as an alcohol derivative
a compound containing an -OH, a C=O and a $-CO_2H$ is regarded as a carboxylic acid

-the numbering system is that for the parent compound

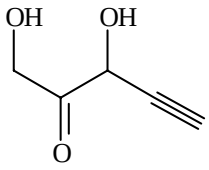
-alcohols can be referred to as hydroxy-side groups, amines as an amino-side group and carbonyls as an oxo-side group.

-when alkenes and alkynes are combined with other functional groups, the root name suffixes are combined.

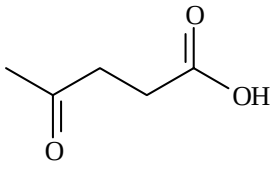
eg.



3-amino-3-buten-1-ol



1,3-dihydroxy-4-pentyne-2-one



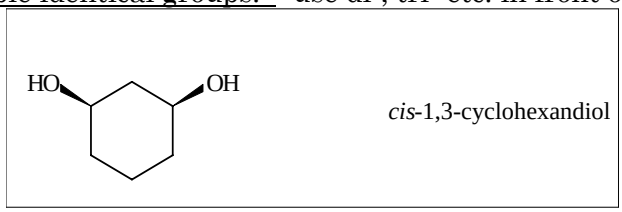
4-oxohexanoic acid

Functional Groups Listed in Decreasing Priority

	Group Name	**Prefix**	**Suffix**
R-CO-OH	carboxylic acid	-	anoic acid
R-CO-Cl	acid chloride	-	anoyl chloride
R-CO-OR	ester	-	anoate
R-CONR'$_2$	amide	-	anamide
R-CHO	aldehyde	oxo	anal
R-CO-R	ketone	oxo	anone
R-OH	alcohol	hydroxy	anol
R-NH_2	amine	amino	amine
-C≡C-	alkyne	-	yne
-C=C-	alkene	-	ene
C_6H_6	aromatic	phenyl	benzene
R-Cl, Br etc	alkyl halide	chloro, bromo	-
R-	alkyl	alkyl	ane

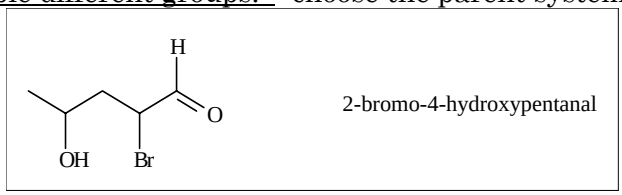
Note: the functional group *prefix* is used when a higher priority group is present in the same molecule (i.e., when both an alcohol and a ketone are present the molecule is named as a ketone, that is an "anone", with a hydroxy substituent).

-multiple identical groups: - use di-, tri- etc. in front of suffix



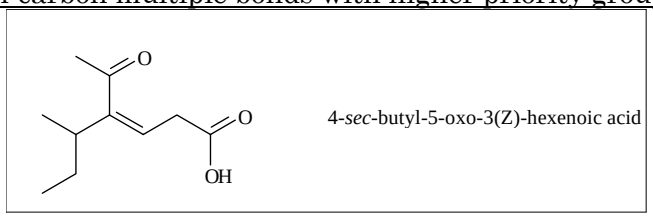
cis-1,3-cyclohexandiol

-multiple different groups: - choose the parent system including the highest priority group



2-bromo-4-hydroxypentanal

-carbon-carbon multiple bonds with higher priority groups: - use the combined suffix name



4-*sec*-butyl-5-oxo-3(Z)-hexenoic acid

Common Names

In many instances, common names are still used. And in some instances the IUPAC system has adopted these. A few common examples follow.

	common	IUPAC
CH_3CO_2H	acetic acid	ethanoic acid
$CH_2=CH_2$	ethylene	ethene
CH_2Cl_2	methylene chloride	dichloromethane
$CHCl_3$	chloroform	trichloromethane
CCl_4	carbon tetrachloride	tetrachloromethane
HO_2CCO_2H	oxalic acid	1,2-ethandioic acid
$C_6H_5CO_2H$	benzoic acid	benzoic acid
C_6H_5OH	phenol	phenol