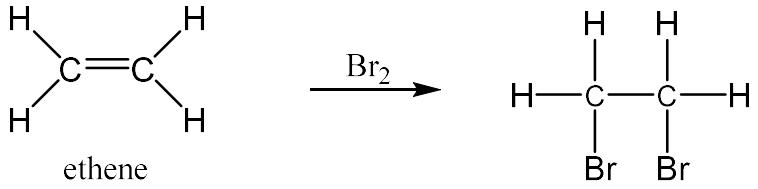
UNIT 2

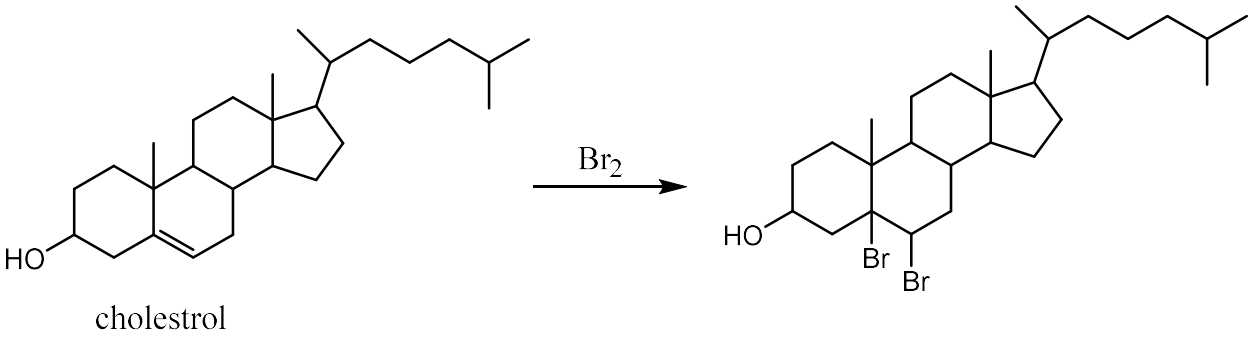
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

2.1 The importance of classification of organic compounds according to their functionality

A functional group is a particular combination of atoms in a molecule that is particularly responsible for characteristic set of reactions that the molecule exhibit.

- The chemistry of every organic molecule, regardless of size and complexity, is determined by the functional group it contains.

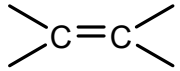
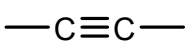
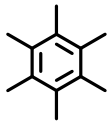
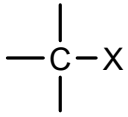
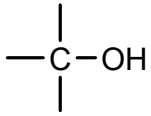
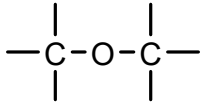
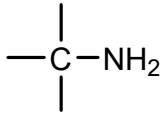
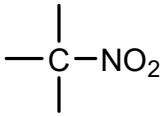
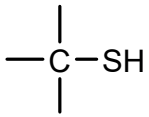
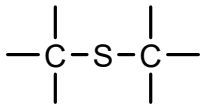


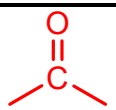
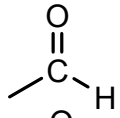
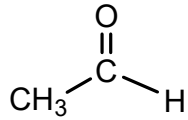
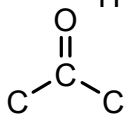
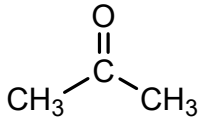
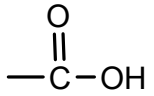
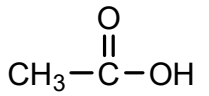
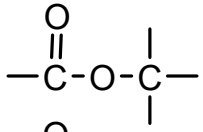
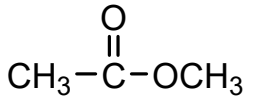
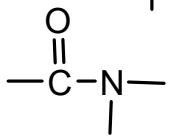
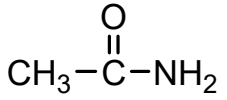
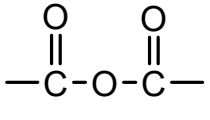
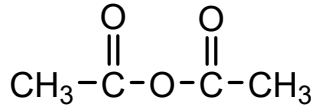
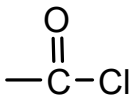
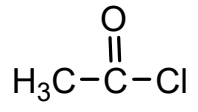


The importance of classification of organic compounds according to their functionality

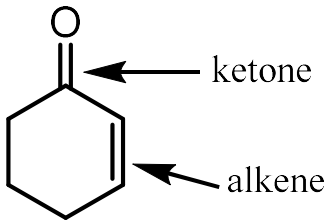
- To study the properties and nature of organic compounds systematically.
- The reactions and physical properties of organic compounds are influenced by the nature of the functional groups present.
- The chemistry of every organic molecule, regardless of size and complexity, is determined by the functional group it contains.

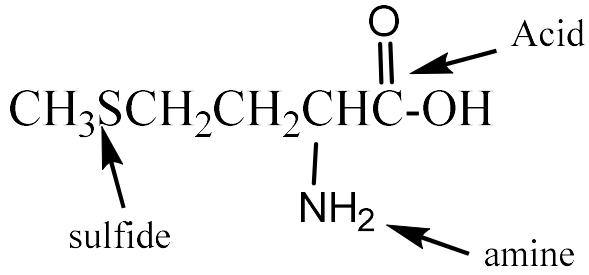
Structure of Some Functional Groups

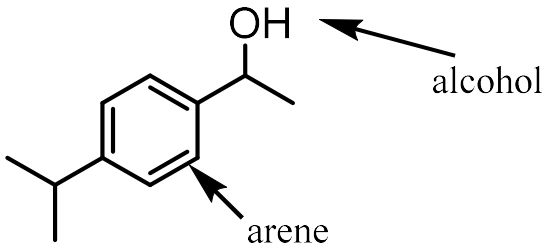
Name	Functional Group Structure	Example
Alkene		$H_2C{=}CH{-}CH_3$
Alkyne		$H{-}C{\equiv}C{-}CH_3$
Arene		 Benzene
Halide	 (X=F,Cl,Br, I)	CH_3CH_2Cl
Alcohol		CH_3CH_2OH
Ether		$H_3C{-}O{-}CH_3$
Amine		$CH_3CH_2NH_2$
Nitrile		$CH_3{-}C{\equiv}N$
Nitro		$CH_3CH_2NO_2$
Thiol		CH_3CH_2SH
Sulfide		$H_3C{-}S{-}CH_3$

Name	Functional Group Structure	Example
Carbonyl		
Aldehyde		
Ketone		
Carboxylic acid		
Ester		
Amide		
Acid anhydride		
Acid chloride		

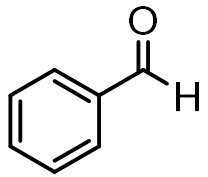
Many compounds contain more than one functional group.

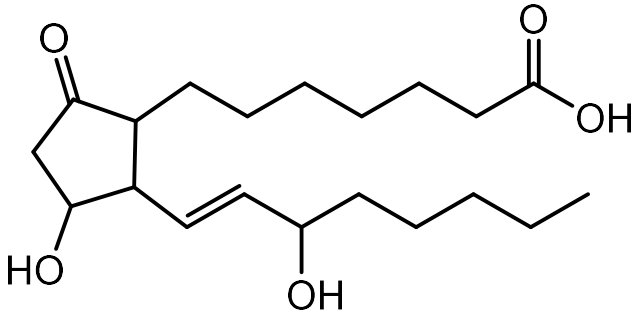




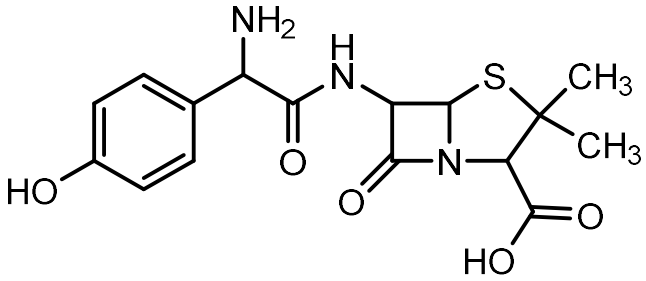


Identify the functional groups found





Prostagladin E_1



amoxicillin

2.2 Nomenclature of organic compounds

- **Common** name

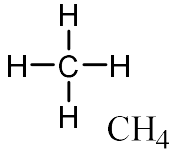
  n-butane, isobutane, n-pentane, isopentane, and neopentane

- **Systematic** name

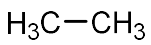
  IUPAC rules

A. Nomenclature of ALKANE

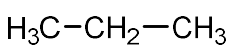
- Alkanes are saturated hydrocarbons with C-C single bond. They are saturated, because contain maximum possible number of H per C.



CH_4



C_2H_6



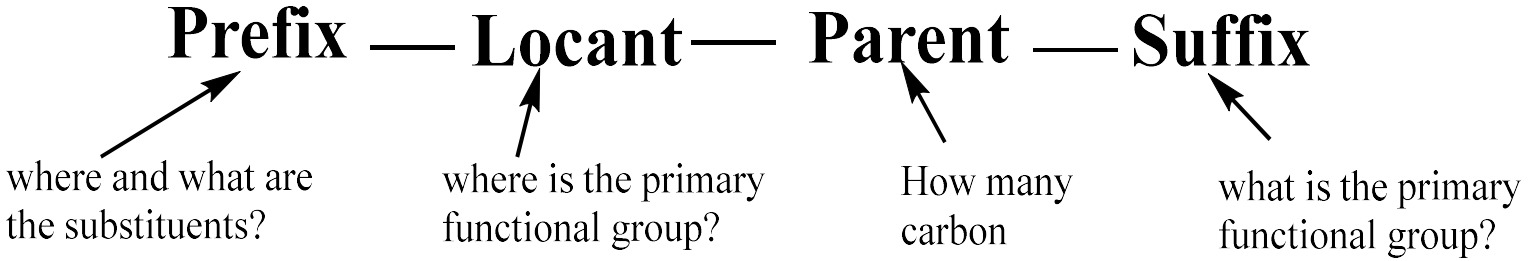
C_3H_8 ..... C_nH_{2n+2}

Molecular Formula	Structural Formula	IUPAC Name
CH_4	CH_4	Methane
C_2H_6	CH_3-CH_3	Ethane
C_3H_8	CH_3-CH_2-CH_3	Propane
C_4H_{10}	CH_3-$(CH_2)_2$-CH_3	Butane
C_5H_{12}	CH_3-$(CH_2)_3$-CH_3	Pentane
C_6H_{14}	CH_3-$(CH_2)_4$-CH_3	Hexane
C_7H_{16}	CH_3-$(CH_2)_5$-CH_3	Heptane
C_8H_{18}	CH_3-$(CH_2)_6$-CH_3	Octane
C_9H_{20}	CH_3-$(CH_2)_7$-CH_3	Nonane
$C_{10}H_{22}$	CH_3-$(CH_2)_8$-CH_3	Decane

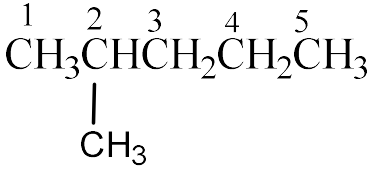
Molecular Formula	Structural Formula	IUPAC Name
$C_{11}H_{24}$	CH_3-$(CH_2)_9$-CH_3	Undecane
$C_{12}H_{26}$	CH_3-$(CH_2)_{10}$-CH_3	Dodecane
$C_{13}H_{28}$	CH_3-$(CH_2)_{11}$-CH_3	Tridecane
$C_{14}H_{30}$	CH_3-$(CH_2)_{12}$-CH_3	Tetradecane
$C_{15}H_{32}$	CH_3-$(CH_2)_{13}$-CH_3	Pentadecane
$C_{20}H_{42}$	CH_3-$(CH_{18}$-CH_3	Icosane
$C_{30}H_{62}$		Triacontane
$C_{40}H_{82}$		Tetracontane
$C_{50}H_{102}$		Tentacontane
$C_{100}H_{202}$		Hectane

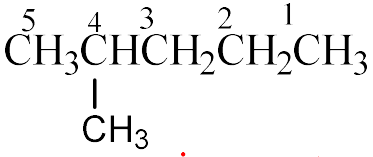
IUPAC rule

IUPAC name typically has four parts: prefix, locant, parent, and suffix.



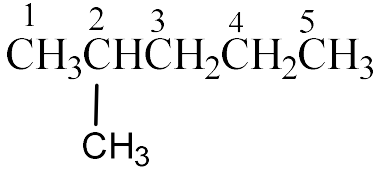
1. Find the parent hydrocarbon-Pick out the longest continuous carbon chain.
2. Number the longest continuous chain in the direction that gives the lowest number to the substituent group at the first point of branching.





incorrect

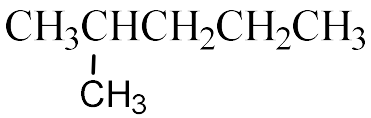
3. Identify and number the substituents.



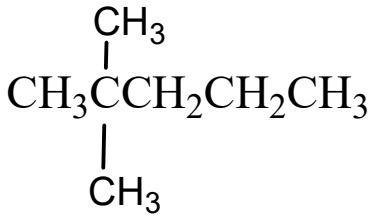
parent name: pentane

substituent: methyl (CH_3) on C-4

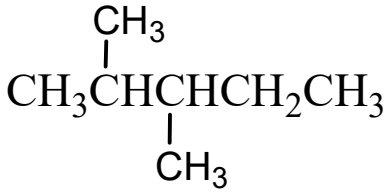
4. Write the name as a single word- use hyphens to separate the locants from words.



IUPAC name: 2-methylpentane



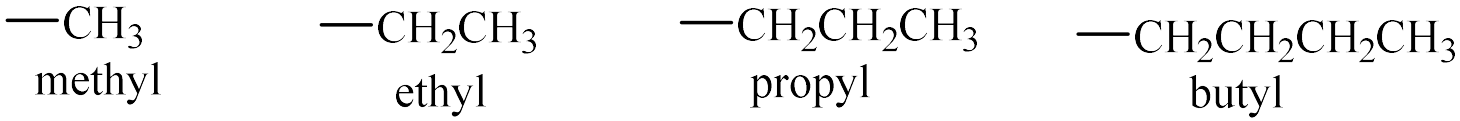
2,2-dimethylpentane



2,3-dimethypentane

ALKYL GROUPS

An alkyl group lacks one of the hydrogens of an alkane.
Replacing the -ane endings -yl.

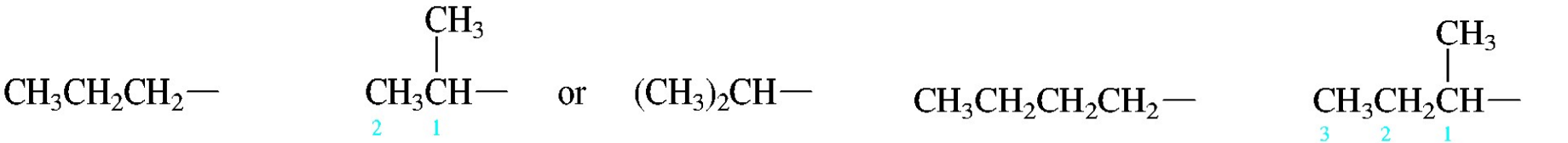


—CH_3 methyl

—CH_2CH_3 ethyl

—$CH_2CH_2CH_3$ propyl

—$CH_2CH_2CH_2CH_3$ butyl

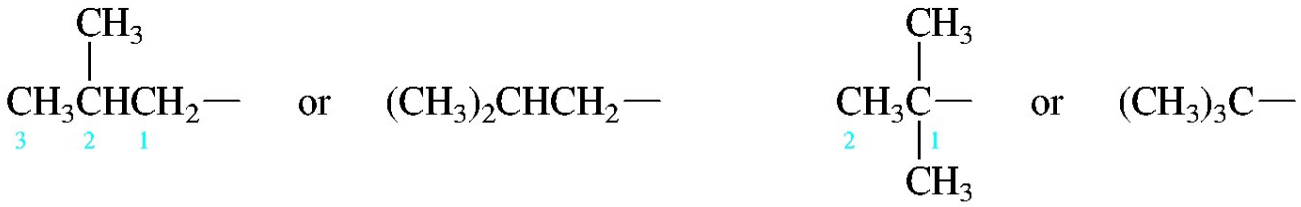


$CH_3CH_2CH_2$— **Propyl** group (common name: *n*-propyl)

CH_3CH— or $(CH_3)_2CH$— **1-Methylethyl** group (common name: isopropyl)

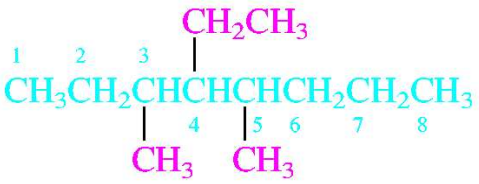
$CH_3CH_2CH_2CH_2$— **Butyl** group (common name: *n*-butyl)

CH_3CH_2CH— **1-Methylpropyl** group (common name: *sec*-butyl)

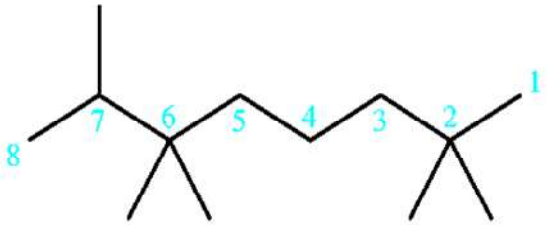


CH_3CHCH_2— or $(CH_3)_2CHCH_2$— **2-Methylpropyl** group (common name: isobutyl)

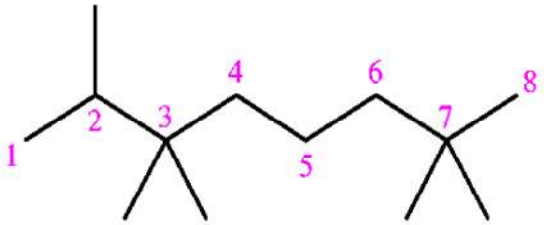
CH_3C— or $(CH_3)_3C$— **1,1-Dimethylethyl** group (common name: *tert*-butyl)



4-ethyl-3,5-dimethyloctane.



2,2,6,6,7-Pentamethyloctane
(correct)



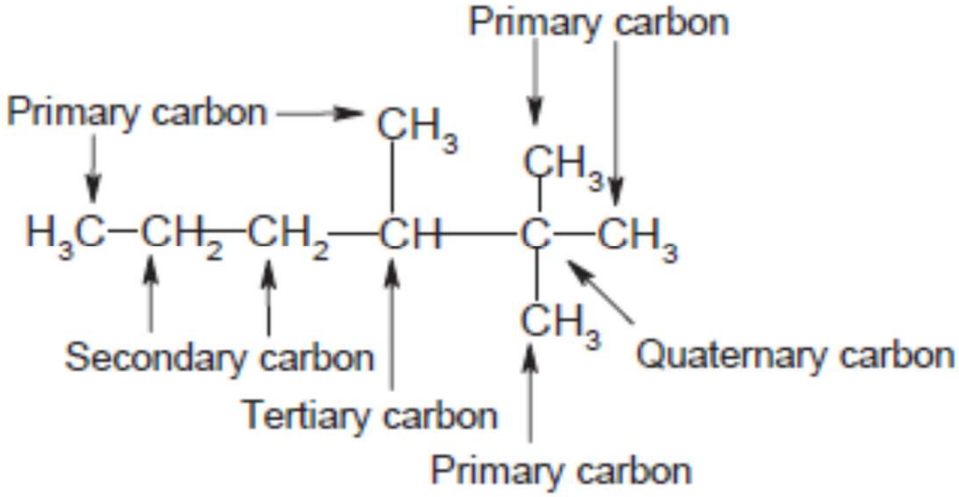
2,3,3,7,7-Pentamethyloctane
(incorrect!)

"first point of difference" rule

- Locants are not added together, but examined one by one.

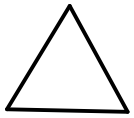
Classification of carbon

- **Primary** carbon (1°) is directly attached to one other carbon.
- **Secondary** carbon (2°) is directly attached to two other carbons
- **Tertiary** carbon (3°) to three
- **Quaternary** carbon (4°) to four.

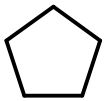


NOMENCLATURE OF CYCLOALKANE

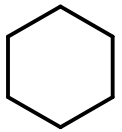
- prefix cyclo- to the name of the unbranched alkane with the same number of carbons as the ring.



cyclopropane

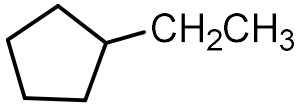


cyclopentane

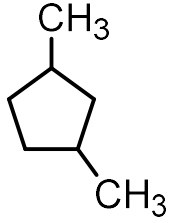


cyclohexane

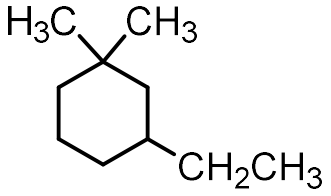
- Choose a point of attachment at C-1 and number the ring in the direction that gives the lowest number to the substituents at the first point of difference



Ethylcyclopentane

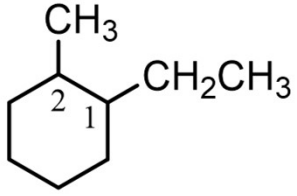


1,3 dimethylcyclopentane



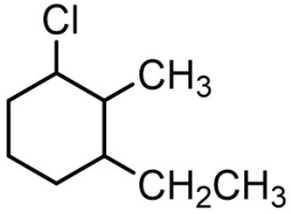
3-Ethyl-1,1-dimethylcyclohexane

not 1-Ethyl-3,3-dimethylcyclohexane

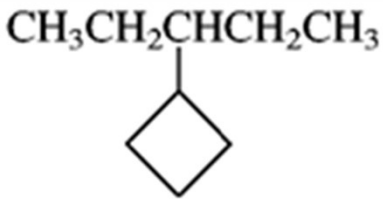


1-Ethyl-2-methylcyclohexane

not 2-Ethyl-1-methylcyclohexane



1-chloro-3-ethyl-2-methylcyclohexane



3-Cyclobutylpentane

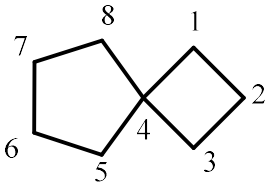
POLYCYCLIC ALKANES

a) Spirocyclic compounds: two rings share one common atom.

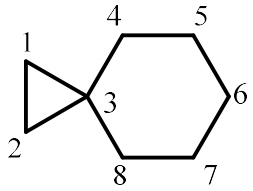
Named as spiro[n,m]alkane. n and m are number of atoms in each bridge (excluding the spiro atom)

Parent name is total number of carbon in the ring.

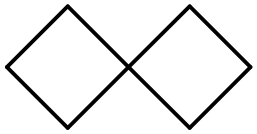
The c-atom in the smaller ring containing the common atom (spiro atom) is assign no. 1



Spiro[3,4]octane



Spiro[2,5]octane

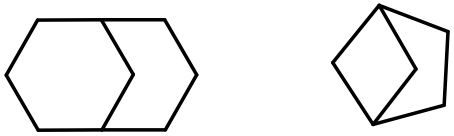


Spiro[3,3]heptane

b) Fused ring compounds: two rings share one common side

c) Bridge-ring compounds: two rings share more than one common side

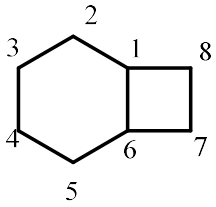
There are more than two common atoms which are adjacent to each other.



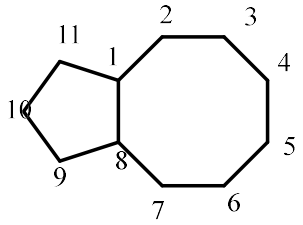
Both Fused ring and Bridge- ring compounds named using the same set of rules.

Use prefix bicyclo-

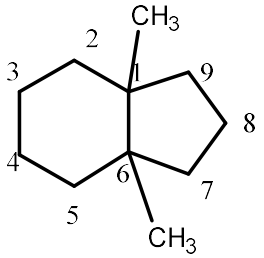
- Number the compound by beginning at one bridgehead, then proceeding around the 2nd longest and then finally to the shortest bridge.
- The number of atoms in each bridges placed in descending order, within brackets.



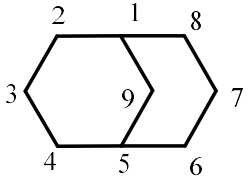
Bicyclo[4,2,0]octane



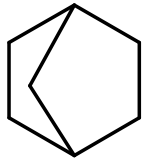
Bicyclo[6,3,0]undecane



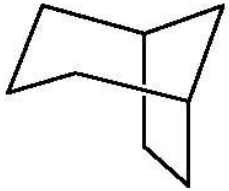
1,6-dimethylbicyclo[4,3,0]nonane



Bicyclo[3,3,1]nonane



Bicyclo[2,2,1]heptane

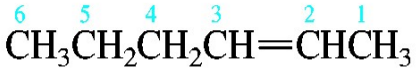


Bicyclo[3.2.1]octane

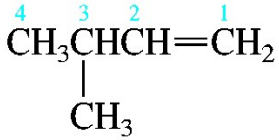
Nomenclature of ALKENES

- Suffix : -ene
- The longest continuous includes the double bond.
- Indicate the position of the double bond, lower number

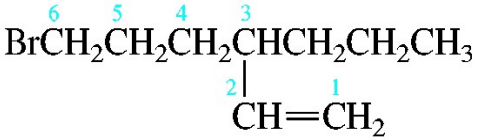
1-Butene
(not 1,2-butene)



2-Hexene
(not 4-hexene)



3-Methyl-1-butene
(not 2-methyl-3-butene)

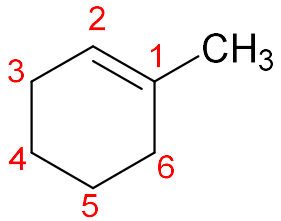


6-Bromo-3-propyl-1-hexene
(longest chain that contains double bond is six carbons)

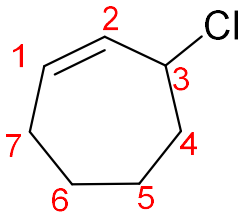
Cycloalkenes

- Prefix –cyclo
- Number the cycloalkane so that the double bond is between C-1 and C-2.

Cyclopentene



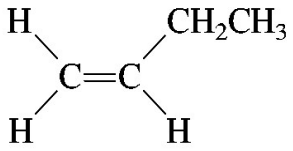
1-Methylcyclohexene



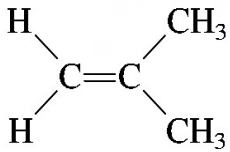
3-Chlorocycloheptene
not (1-chloro-2-cycloheptene)

ISOMERISM IN ALKENES

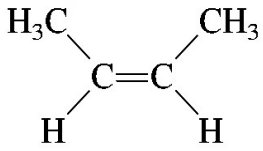
Alkenes show cis-trans isomerism.



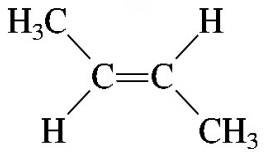
1-Butene



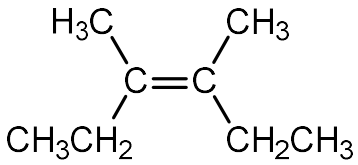
2-Methylpropene



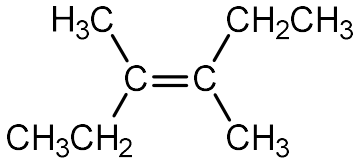
cis-2-Butene



trans-2-Butene

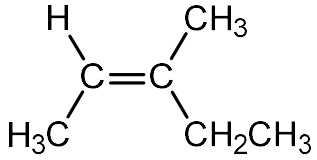


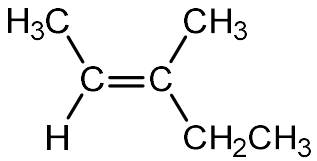
cis-3,4-dimethyl-3-hexene



trans-3,4-dimethyl-3-hexene

- *cis*-isomer: identical groups on the same side of the double bond
- *trans*-isomer: identical groups on opposite sides of the double bond.





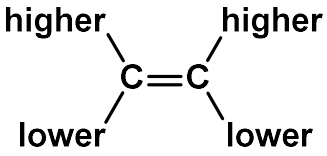
Cis or trans ?

Such isomers named based on an atomic number criterion for ranking substituents on the doubly bonded carbons. The system is called the *E/Z* nomenclature.

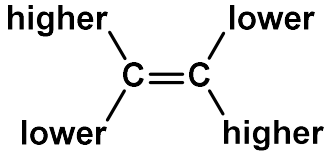
E/Z nomenclature

Cahn-Ingold-Prelog rules for assigning priority

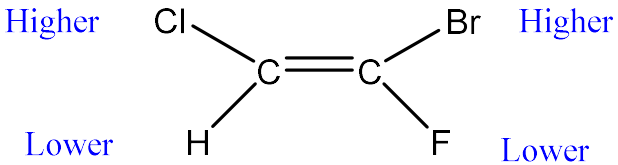
1. Look at atoms directly attached to the double bond. Higher atomic number = higher priority
2. If no difference exist at the first attachment atom, keep going down the line until the first difference reached.
3. Multiple bonded atoms are equivalent to the same number of single bonded atoms.



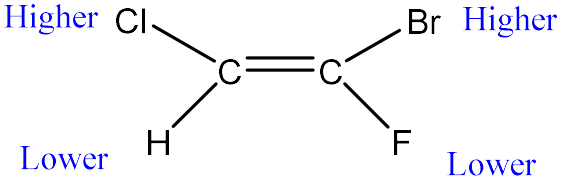
Z (zusammen)



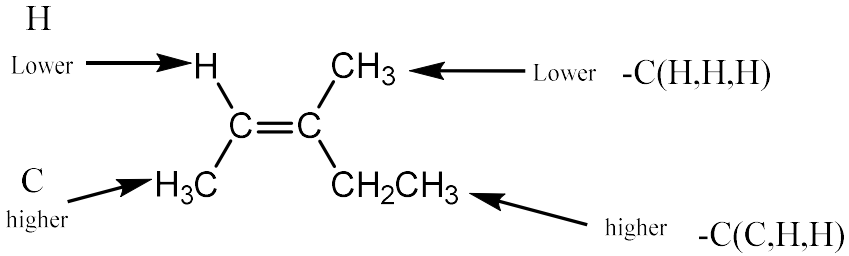
E (entgegen)



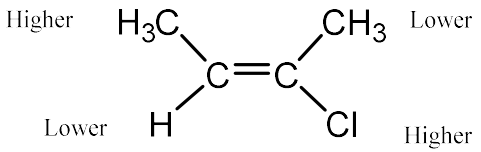
Z configuration



E configuration

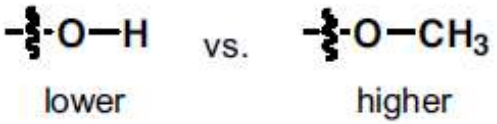


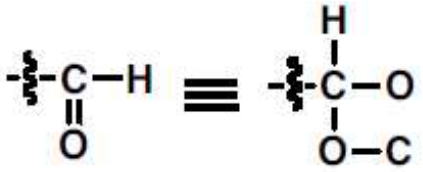
(Z)- 3-methyl-2-pentene

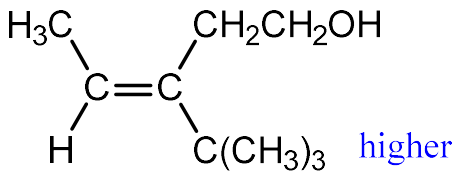


(E)- 2-chloro-2-butene

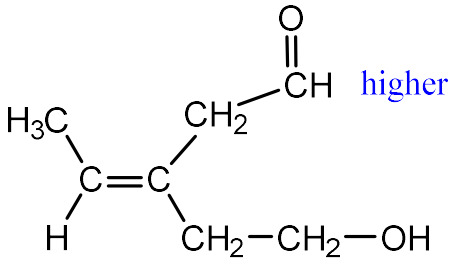
Multiple bonded atoms are equivalent to the same number of single bonded atoms.







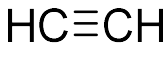
(*E*)-



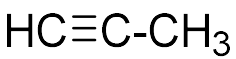
(*Z*)-

Nomenclature of ALKYNES

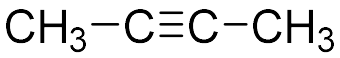
- -yne suffix (with number)



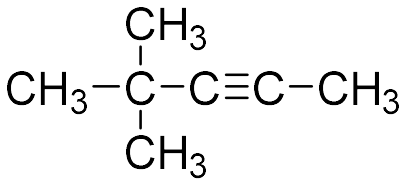
Ethyne



Propyne



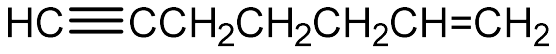
2-Butyne



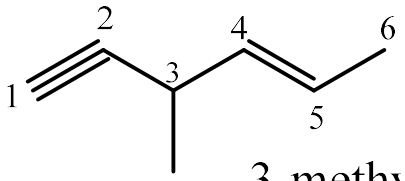
4,4-Dimethyl-2-pentyne

Enynes: containing both double and triple bond.

- suffix is -en-yne.
- numbering is from the end closer to a multiple bond.
- When there is equal chance in numbering, double bond receives lower number than triple bond.



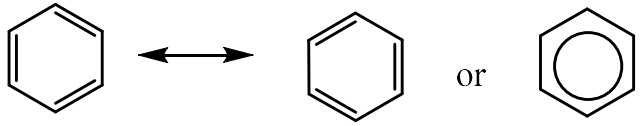
1-Hepten-6-yne



3-methyl-4-hexene-1-yne

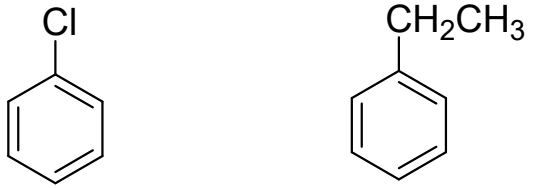
Nomenclature of Aromatic Hydrocarbons

Aromatic hydrocarbon includes benzene and its derivative.



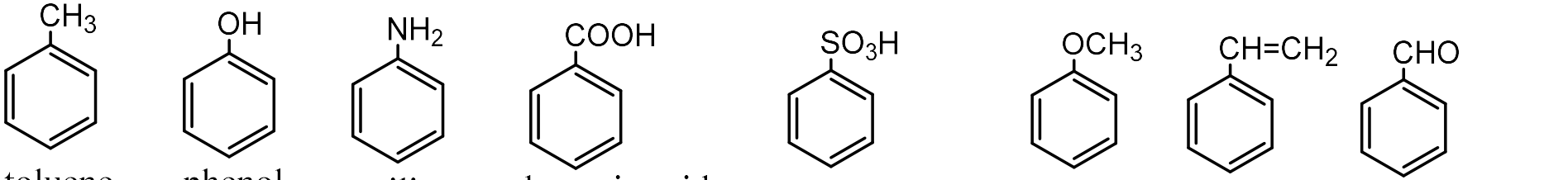
Benzene

Monosubstituted benzenes are named as "substituent benzene"



Chlorobenzene Ethylbenzene

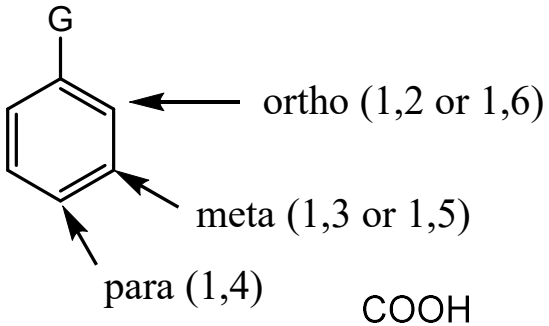
Common names of special monosubstituted benzenes that are also used in IUPAC system

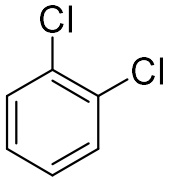


toluene phenol aniline benzoic acid benzenesulphonic acid anisol styrene benzaldehyde

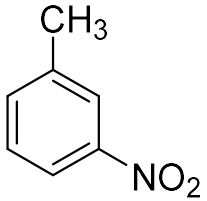
Disubstituted benzene

- Ortho-Meta-Para Designation
- Numbering approach

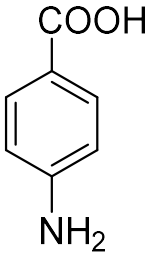




ortho-dichorobenzene
(1.2-dichlorobenzene)



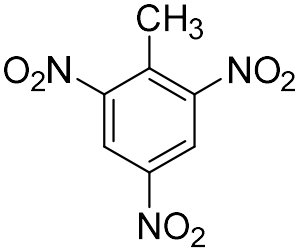
meta-nitrotoluene
(3-nitrotoluene)



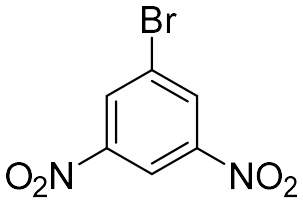
para-aminobenzoic acid
(4-aminobenzoic acid)

Polysubstituted benzene

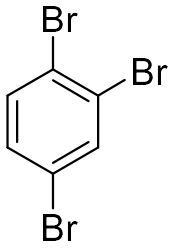
The benzene ring is numbered so as to give the lowest possible number to the substituent.



2,4,6-trinitrotoluene
(TNT)



3,5-dinitrobromobenzene

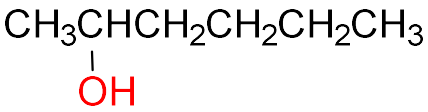


1,2,4-tribromobenzene

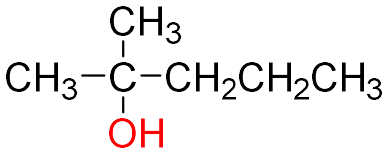
Nomenclature of ALCOHOL

- -ol suffix with number designation
- OH group takes priority (even over -ene or -yne)
- the direction of numbering gives it the lowest possible number

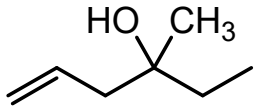
Ethanol



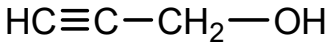
2-Hexanol



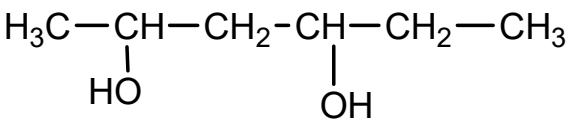
2-Methyl-2-pentanol



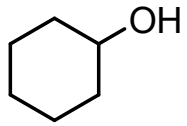
3-methyl-5-hexen-3-ol



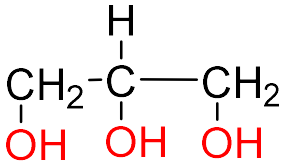
2-propynol



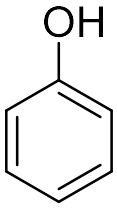
2,4-hexanediol
(Hexane-2,4-diol)



cyclohexanol



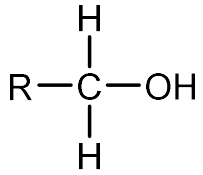
Propane-1,2,3-triol
(Glycerin)



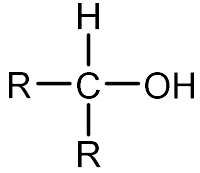
Phenol

CLASSES OF ALCOHOLS

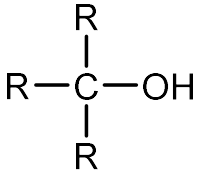
Alcohols are classified as primary, secondary, or tertiary according to the degree of substitution of the carbon that bears the functional group.



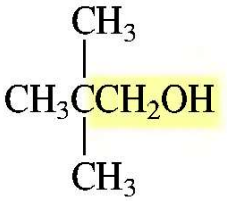
Primary alcohol(1°)



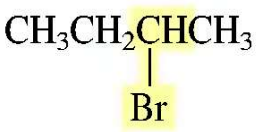
Secondary alcohol(2°)



Tertiary alcohol(3°)

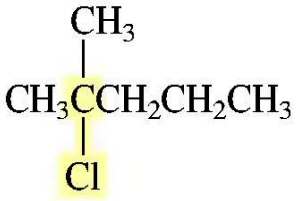


2,2-Dimethyl-1-propanol
(a primary alcohol)



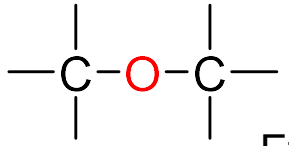
2-Bromobutane
(a secondary alkyl halide)

1-Methylcyclohexanol
(a tertiary alcohol)



2-Chloro-2-methylpentane
(a tertiary alkyl halide)

Nomenclature of Ethers and Epoxides



Ether

R–O–R'

$H_3C–O–CH_3$

$H_3C–O–CH_2CH_3$

Naming: List the two alkyl groups in the general structure ROR' in alphabetical order as separate words, and then adding the word ether at the end.

$CH_3–O–CH_3$

Dimethyl ether

(Methoxymethane)

$CH_3CH_2–O–CH_2CH_3$

Diethyl ether

(Ethoxyethane)

$CH_3CH_2–O–CH_3$

Ethyl methyl ether

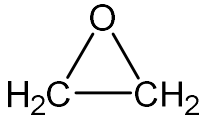
(Methoxyethane)

$CH_3CH_2–O–CH_2CH_2CH_2Cl$

3-Chloropropyl ethyl ether

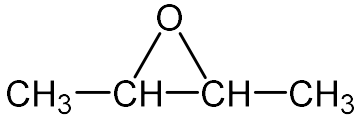
(1-Chloro-3-ethoxypropane)

Epoxide (Oxiranes) are cyclic ethers with three membered ring containing one oxygen



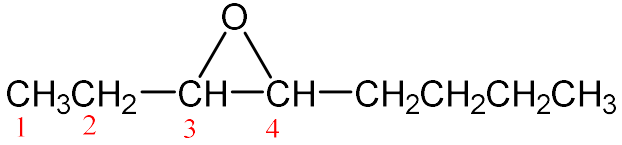
Ethylene oxide

(Oxirane)



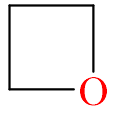
2-butene oxide

(2,3-dimethyloxirane)

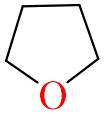


3,4-epoxyoctane

Cyclic Ethers

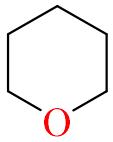


Oxetane



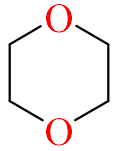
Oxolane

(Tetrahydrofuran)



Oxane

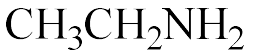
(Tetrahydropyran)



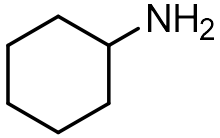
1,4-dioxane

Nomenclature of Amines $R-NH_2$

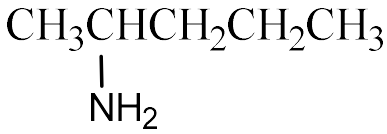
- Name either as *alkylamines* or as *alkanamines*
- When named as alkylamines, the ending -amine is added to the name of the alkyl group that bears the nitrogen.
- When named as alkanamines, the alkyl group is named as an alkane and the -e ending replaced by -amine.



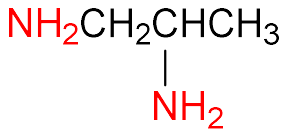
Ethylamine
(Ethanamine)



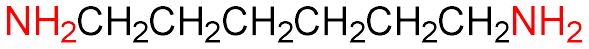
cyclohexanamine



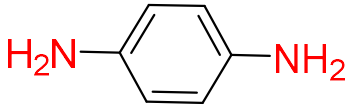
1-Methylbutylamine
(2-pentanamine)



1,2-Propanediamine



1,6-Hexanediamine



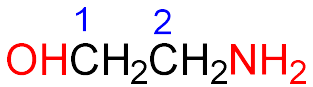
1,4-Benzenediamine

When two or more functional groups found in a molecule, the parent hydrocarbon is determined by priority order:

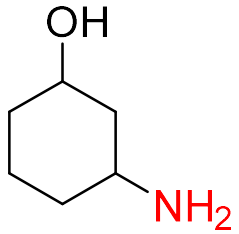
Priority order from highest to lowest:

Carboxylic acid acid > ester > amide > nitrile > aldehyde > ketone > alcohol > amine > alkene > alkyne

The amine group is named as a substituent when the amine group takes low priority

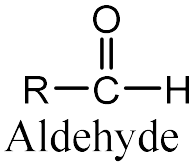


2-Aminoethanol

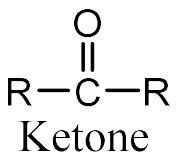


3-aminocyclohexanol

Nomenclature of Aldehydes and Ketones



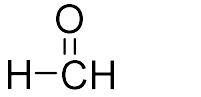
Aldehyde



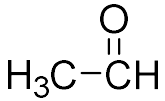
Ketone

Aldehyde

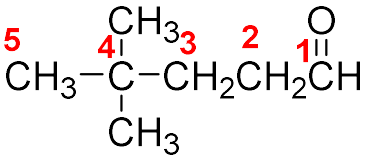
- The *-e* ending of the corresponding alkane name is replaced by *–al*
- The aldehyde group takes C-1 (not necessary to indicate the position of the aldehyde).



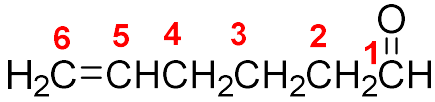
Methanal
(Formaldehyde)



Ethanal
(Acetaldehyde)

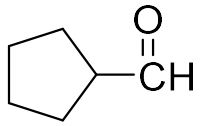


4,4-Dimethylpentanal

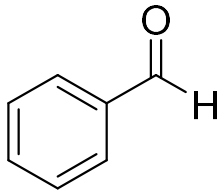


5-Hexenal

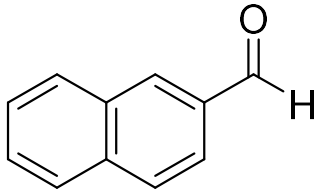
When a formyl group (-CH=O) is attached to a ring, the ring name is followed by the suffix -carbaldehyde.



Cyclopentanecarbaldehyde



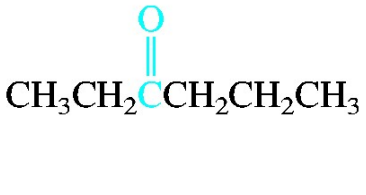
Benzenecarbaldehyde
(Benzaldehyde)



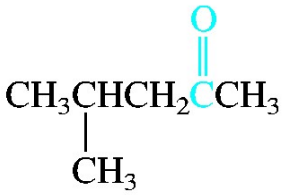
2-Naphthalenecarbaldehyde

Ketone

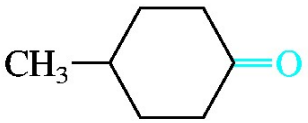
- *-one* suffix
- The carbonyl carbon of a cyclic ketone is C-1 and the number does not appear in the name.



3-Hexanone



4-Methyl-2-pentanone

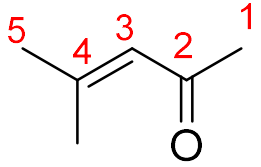


4-Methylcyclohexanone

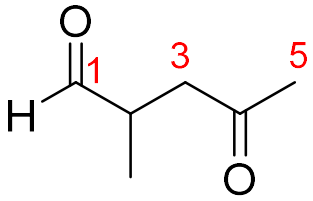
Priority order :

Carboxylic acid acid > ester > amide > nitrile > aldehyde > ketone > alcohol > amine > alkene > alkyne

The carbonyl oxygen of the ketone is considered an oxo-substituent in the presence of higher priority functional group.

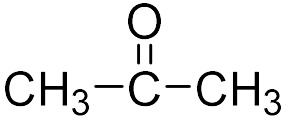


4-Methyl-3-penten-2-one

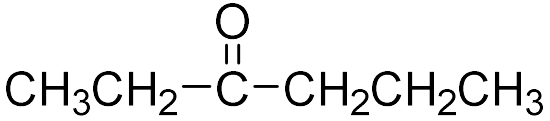


2-Methyl-4-oxopentanal

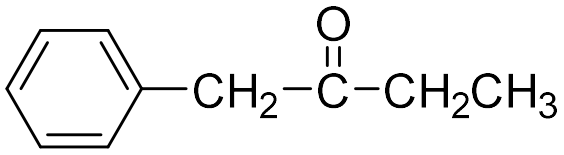
Ketones also named by functional class nomenclature.



Dimethyl ketone
(Acetone)

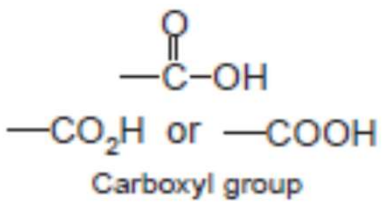


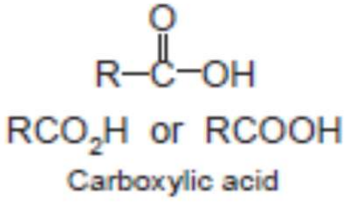
Ethyl propyl ketone



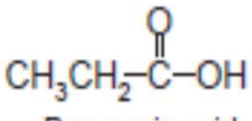
Benzyl ethyl ketone

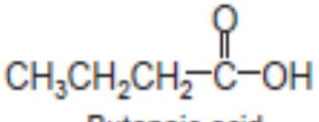
Nomenclature of Carboxylic Acids and their Derivatives

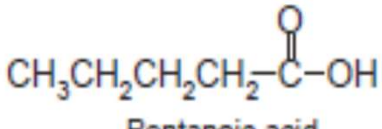


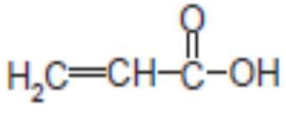


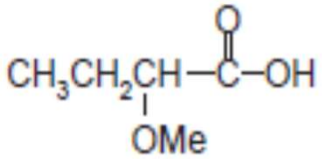
-oic acid suffix

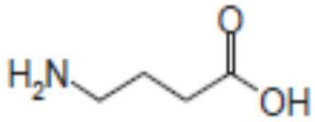




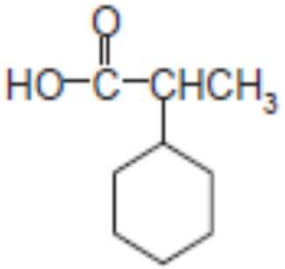


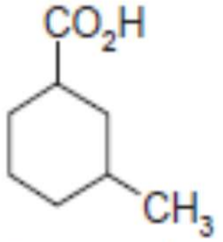


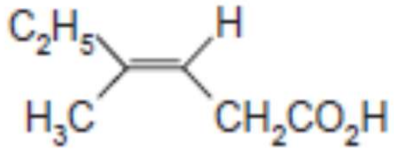




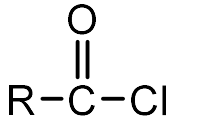
Cycloalkanes with carboxyl substituents are named as cycloalkanecarboxylic acids. Unsaturated acids are named using the name of the alkene with *-e* replaced with *-oic acid*.

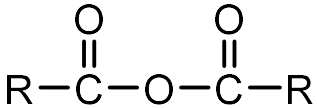


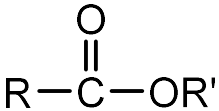


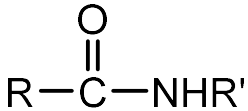


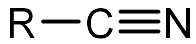
Carboxylic Acids Derivatives


Acid chloride
RCOCl

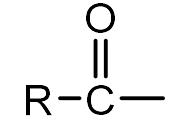

Acid anhydride
$(RCO)_2O$

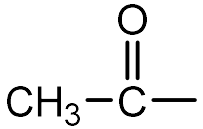

Ester
RCO_2R'

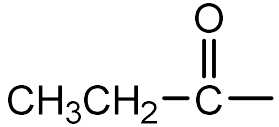

Amide
$RCONH_2$

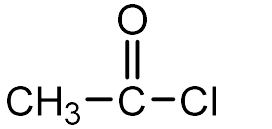

Nitrile

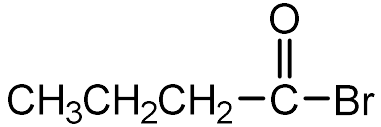
- Acyl groups are named by replacing the -ic acid ending of the corresponding carboxylic acid by -yl.
- Acyl halides are named by placing the name of the appropriate halide after that of the acyl group.

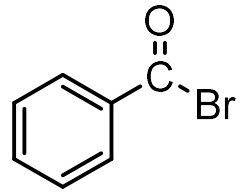

Acyl group


acetyl


propanoyl

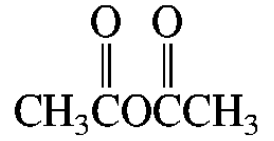

Acetylchloride

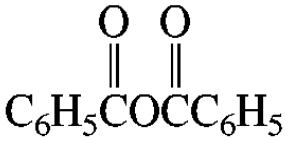

Butanoylbromide

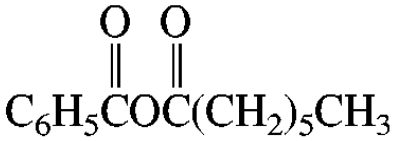

Benzoylbromide

acid anhydrides

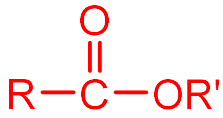
replace acid by anhydride.


Acetic anhydride

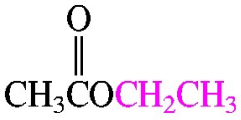

Benzoic anhydride


Benzoic heptanoic anhydride

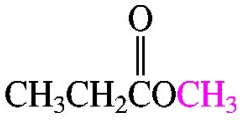
Esters



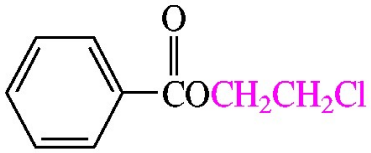
-named as alkyl alkanoate. R' cited first followed by the acyl portion.
The acyl portion is named by substituting the suffix –ate for the –ic acid ending of the corresponding acid.



Ethyl acetate



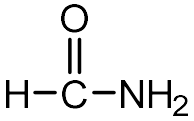
Methyl propanoate



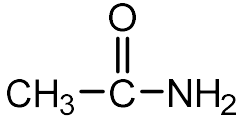
2-Chloroethyl benzoate

Amides

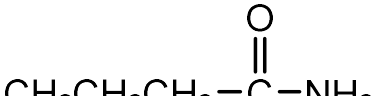
-replacing the suffix –oic acid or -ic acid by -amide



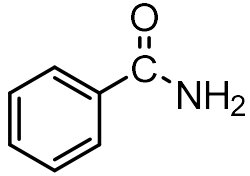
Formamide



Acetamide



Butanamide

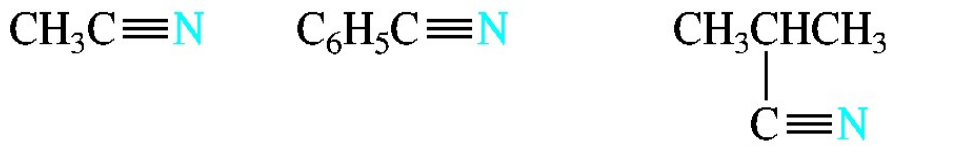


Benzamide

Nitriles $R-C\equiv N$

-add the suffix -nitrile to the name of the parent hydrocarbon chain that includes the carbon of the cyano group.

-by replacing the -ic acid or -oic acid ending of the corresponding carboxylic acid with *-onitrile*.



Ethanenitrile (acetonitrile) | Benzonitrile | 2-Methylpropanenitrile (isopropyl cyanide)