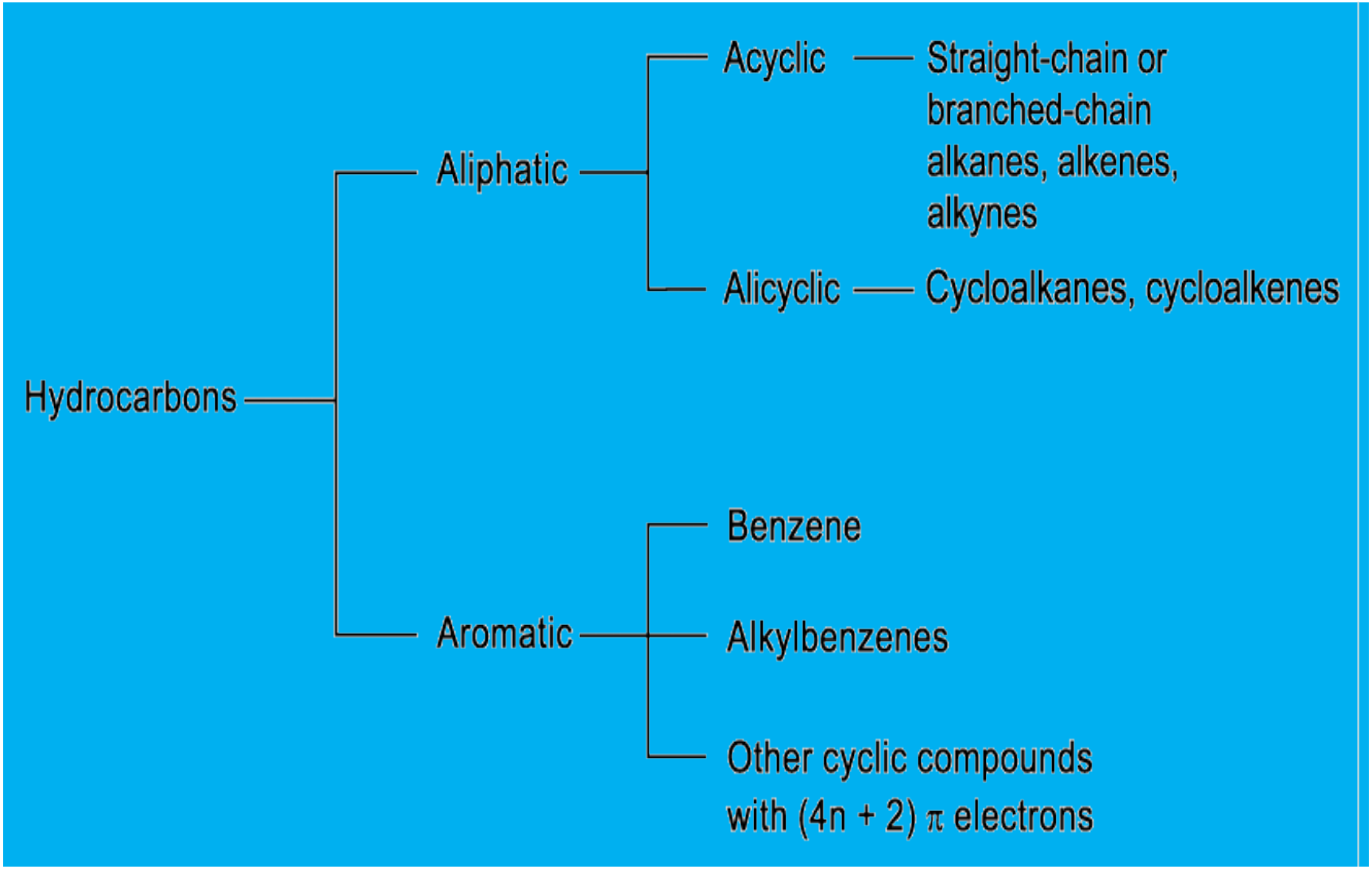
Unit 2- Nomenclature


Hydrocarbons
Aliphatic
Acyclic
Straight-chain or branched-chain alkanes, alkenes, alkynes
Alicyclic
Cycloalkanes, cycloalkenes
Aromatic
Benzene
Alkylbenzenes
Other cyclic compounds with (4n + 2) π electrons

Alkane

- Alkane is saturated hydrocarbon.
- When hydrocarbons contain only single bonds, they are called **alkanes**.
- Alkanes are named using a prefix for the number of carbon atoms they contain, followed by the suffix –ane.

Number of carbon atoms	**Prefix**	**Compound name**
1	Meth-	Methane
2	Eth-	Ethane
3	Prop-	Propane
4	But-	Butane
5	Pent-	Pentane
6	Hex-	Hexane
7	Hept-	Heptane
8	Oct-	Octane
9	Non-	Nonane
10	Dec-	Decane

Common names for alkyl substituents

Structural formula	Name
CH_3-	methyl
CH_3**C**H_2-	ethyl
CH_3CH_2**C**H_2-	propyl
$(CH_3)_2$**C**H-	isopropyl
$CH_3CH_2CH_2$**C**H_2-	butyl
CH_3**C**HCH_2CH_3	sec-butyl or s-butyl
$(CH_3)_2CH$**C**H_2-	isobutyl
$(CH_3)_3$C-	tert-butyl or t-butyl

Rules for naming of alkanes

1. Identify the longest carbon chain. This chain is called the parent chain.
2. Identify all of the substituents (groups appending from the parent chain).
3. Number the carbons of the parent chain from the end that gives the substituents the lowest numbers.If two or more side chains are in equivalent positions, assign the lowest number to the one which will come first in the name.
4. If the same substituent occurs more than once, the location of each point on which the substituent occurs is given. In addition, the number of times the substituent group occurs is indicated by a prefix (di, tri, tetra, etc.).

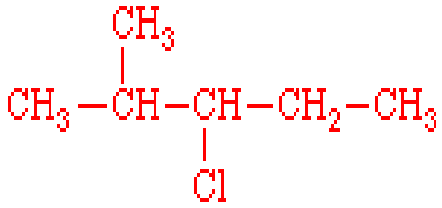
5. If there are two or more different substituent's they are listed in alphabetical order using the base name (ignore the prefixes).

- The only prefix which **is** used when putting the substituents in alphabetical order is **iso** as in isopropyl or isobutyl.
- The prefixes sec- and tert- are not used in determining alphabetical order except when compared with each other.

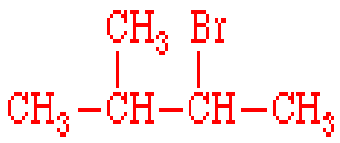
6. A cyclic (ring) hydrocarbon is designated by the prefix **cyclo-** which appears directly in front of the base name.

7. The name of the compound is written out with the substituent's in alphabetical order followed by the base name (derived from the number of carbons in the parent chain).

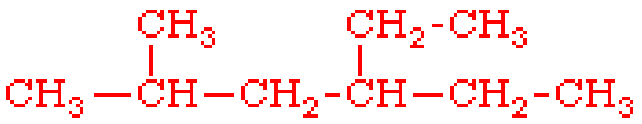
Here are some examples:



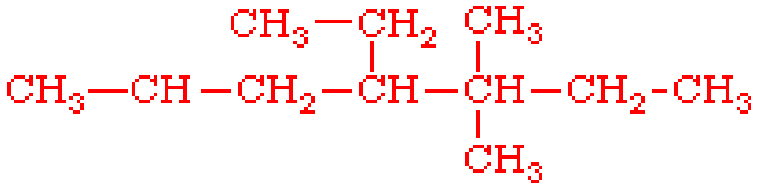
3-chloro-2-methylpentane



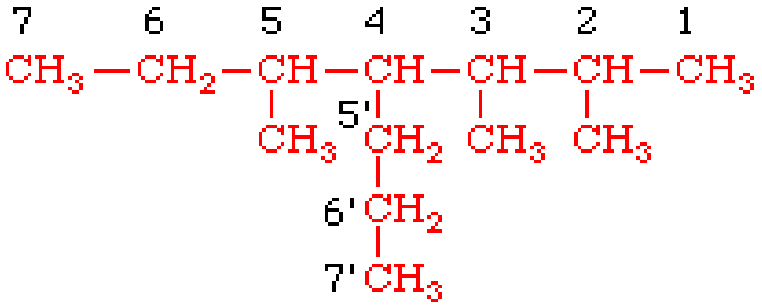
2-bromo-3-methylbutane



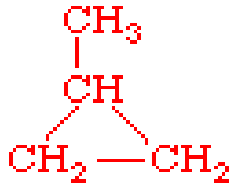
4-ethyl-2-methylhexane



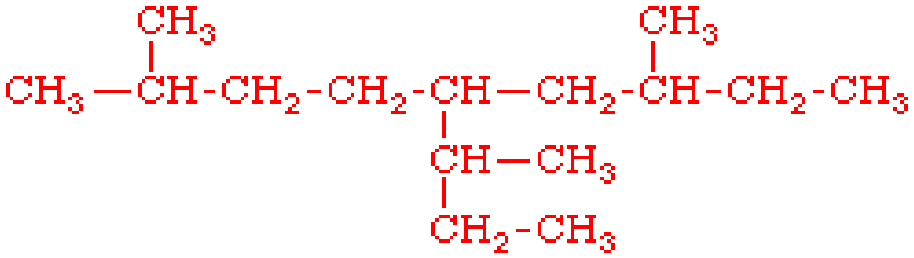
4-ethyl-3,3-dimethylheptane



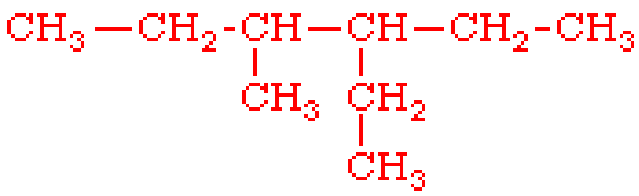
2,3,5-trimethyl-4-propylheptane
(NOT: 2,3-dimethyl-4-sec-butylheptane)



methylcyclopropane



5-sec-butyl-2,7-dimethylnonane



3-ethyl-4-methylhexane

Alkenes and Alkynes

- Alkenes and Alkynes - unsaturated hydrocarbon
- Double bonds in hydrocarbons are indicated by replacing the suffix **-ane** with **-ene**.
- Triple bonds are named in a similar way using the suffix **-yne**.

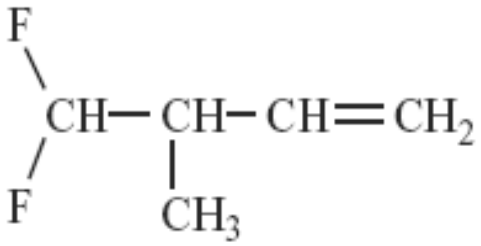
Rules for naming of alkenes and alkynes

1. The parent chain is numbered so that the multiple bonds have the lowest numbers (double and triple bonds have priority over alkyl and halo substituents).

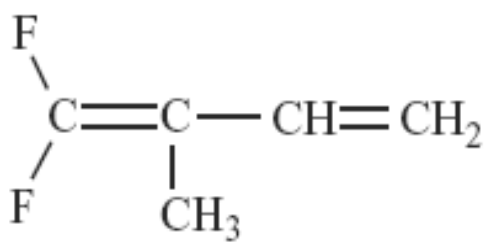
Assigning Priority

- Alkenes and alkynes are considered to have equal priority
- In a molecule with **both** a double and a triple bond, whichever is closer to the end of the chain determines the direction of numbering.
- In the case where each would have the same position number, the double bond takes the lower number.
- In the name, “ene” comes before “yne” because of alphabetization.

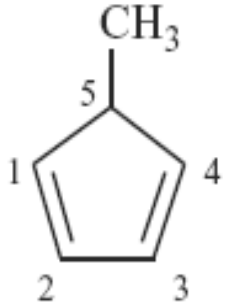
Multiple Double/Triple Bonds



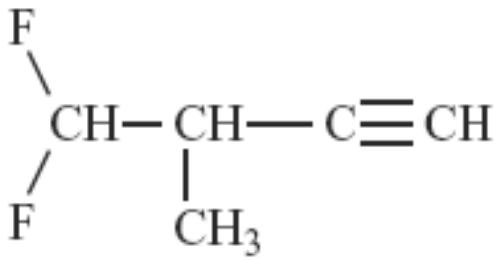
4,4-difluoro-3-methylbut-1-ene



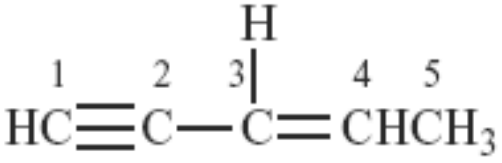
1,1-difluoro-2-methyl-buta-1,3-diene



5-methylcyclopenta-1,3-diene

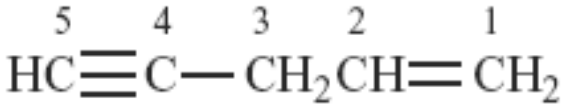


4,4-difluoro-3-methylbut-1-yne



pent-3-en-1-yne

("yne" closer to end of chain)

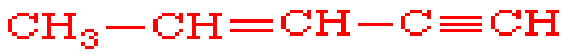


pent-1-en-4-yne

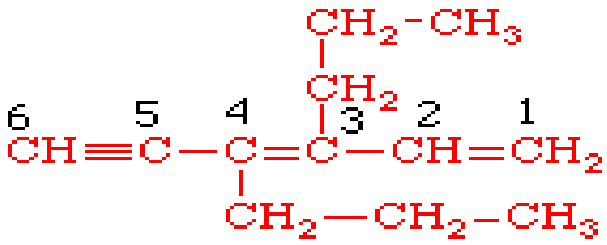
("ene" and "yne" have equal priority unless they have the same position number, when "ene" takes the lower number)



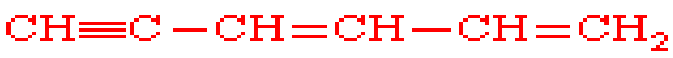
1,4-hexadiene



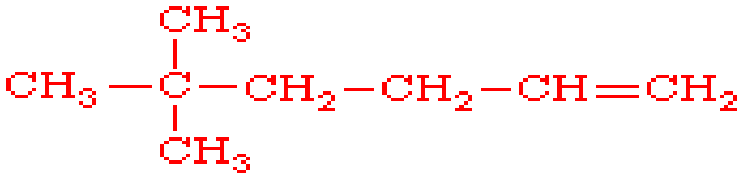
3-penten-1-yne



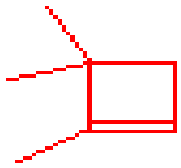
3,4-dipropyl-1,3-hexadien-5-yne



1,3-hexadien-5-yne



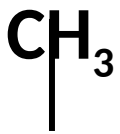
5,5-dimethyl-1-hexene



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

Write the IUPAC name for each of the following unsaturated compounds:

A. $CH_3CH_2C \equiv CCH_3$



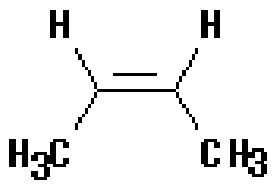
B. $CH_3C{=}CHCH_3$

C.

Cis and Trans Isomers

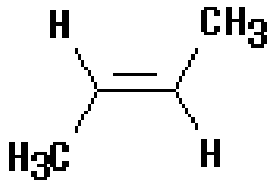
- **Double bond is fixed**
- **Cis/trans Isomers are possible**
- E -*entgegen*, opposite sides

- Z - *zusammen*, together on the same side



cis-2-butene

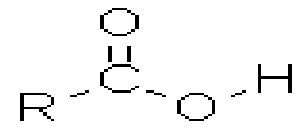
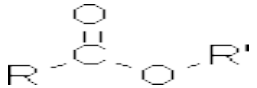
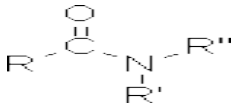
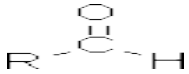
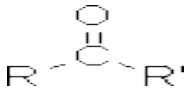
(Z)-2-butene



trans-2-butene

(E)-2-butene

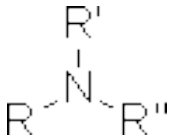
Functional Groups

Functional Group	Formula
• Carboxylic Acids	
• Acid Anhydrides	
• Esters	
• Acyl Halides	
• Amides	
• Nitriles	
• Aldehydes	
• Ketones	
• Alcohols	

- **Thiols**



- **Amines**



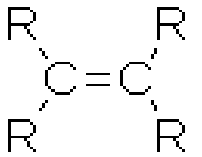
- **Ethers**



- **Sulfides**



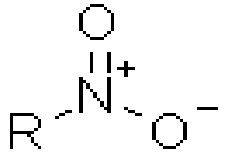
- **Alkenes**



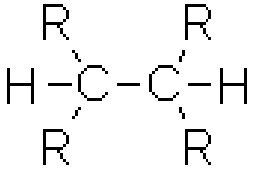
- **Alkynes**



- **Alkyl Halides**



- **Nitro**



- **Alkanes**

Naming Priority

Highest ranking

Lowest ranking

1. Acids
2. Esters
3. Aldehydes
4. Ketones
5. Alcohols
6. Amines
7. Alkenes
8. Alkynes
9. Alkanes
10. Ethers
11. Halides

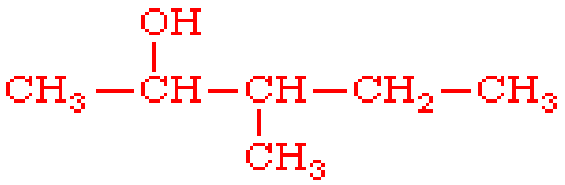
Alcohols

- Alcohols contain an OH group connected to saturated C (sp^3).
- They are important solvents and synthesis intermediates.
- Methanol, CH_3OH, called methyl alcohol, is a common solvent, a fuel additive, produced in large quantities.

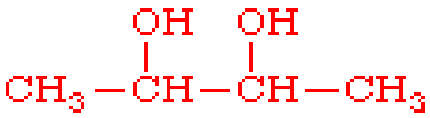
Classification of alcohol

- **Primary**: the carbon with –OH is bonded to only one other carbon.
- **Secondary**: the carbon with –OH is bonded to only two other carbons.
- **Tertiary**: the carbon with –OH is bonded to only three other carbons.

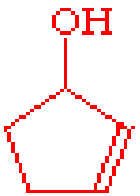
- Alcohols are named by replacing the suffix **-ane** with **-anol**.
- The hydroxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.



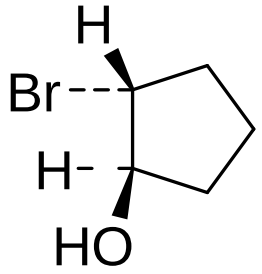
3-methyl-2-pentanol



2,3-butanediol



2-cyclopenten-1-ol



?

Unsaturated Alcohols

- Hydroxyl group takes precedence. Assign that carbon the lowest number.
- Use alkene or alkyne name.

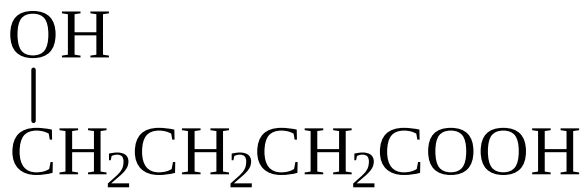


4-penten-2-ol (old)

pent-4-ene-2-ol
(1997 revision of IUPAC rules)

Hydroxy Substituent

- When -OH is part of a higher priority class of compound, it is named as hydroxy.
- Example:

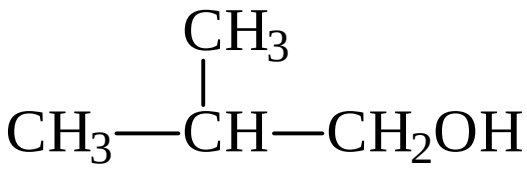


4-hydroxybutanoic acid

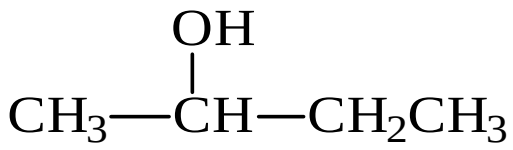
Common Names

- Alcohol can be named as alkyl alcohol.
- Useful only for small alkyl groups.

Examples:



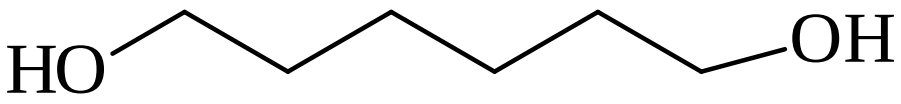
isobutyl alcohol



sec-butyl alcohol

Naming Diols

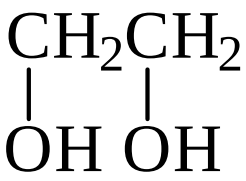
- Two numbers are needed to locate the two -OH groups.
- Use -diol as suffix instead of -ol.



1,6-hexanediol

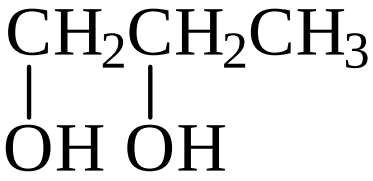
Glycols

- 1, 2 diols (vicinal diols) are called glycols.
- Common names for glycols use the name of the alkene from which they were made.



1,2-ethanediol

ethylene glycol



1,2-propanediol

propylene glycol

Aldehydes

- Aldehydes are named by replacing the suffix **-ane** with **–anal**

In naming:

- The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.



propanal



3-methylbutanal



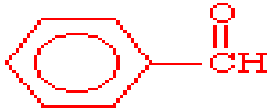
3-methyl-3-butenal



methanal
(common name: formaldehyde)



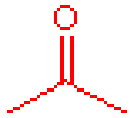
ethanal
(common name: acetaldehyde)



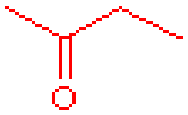
Benzaldehyde

Ketone

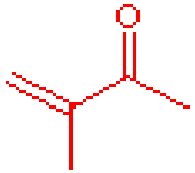
- Ketones are named by replacing the suffix **-ane** with **-anone**.
- The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.



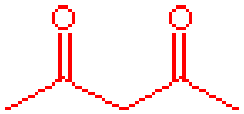
propanone
(common name: acetone)



2-butanone



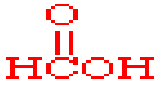
3-methyl-3-buten-2-one



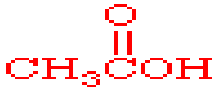
2,4-pentanedione

Carboxylic Acids

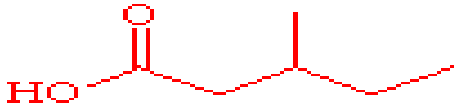
- Carboxylic acids are named by counting the number of carbons in the longest continuous chain including the carboxyl group and by replacing the suffix **-ane** of the corresponding alkane with **-anoic acid**
- The carboxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
- If the carboxyl group is attached to a ring the parent ring is named and the suffix -carboxylic acid is added.
- When both double bonds and carboxyl groups are present, the -en suffix follows the parent chain directly and the -oic acid suffix follows the -en suffix (notice that the e is left off, **-en** instead of -ene).



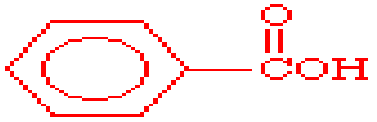
methanoic acid
(common name: formic acid)



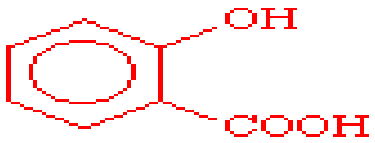
ethanoic acid
(common name: acetic acid)



3-methylpentanoic acid



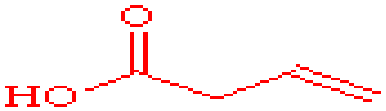
benzoic acid



salicylic acid
(common name)



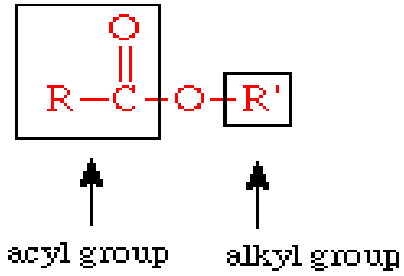
ethanedioic acid
(common name: oxalic acid)



3-butenoic acid

Esters

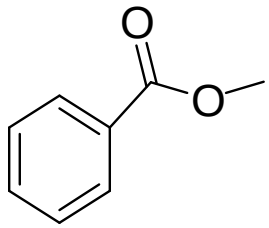
- Esters are formed through reactions between an acid and an alcohol with the elimination of water.
- Systematic names of esters are based on the name of the corresponding carboxylic acid. Remember esters look like this:



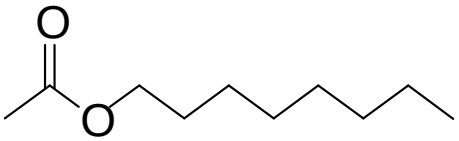
- The alkyl group is named like a substituent using the **-yl** ending. This is followed by a space.
- The acyl portion of the name (what is left over) is named by replacing the **-ic acid** suffix of the corresponding carboxylic acid with **-ate**.

Example

$CH_3COOCH_2CH_3$ –methyl propanoate



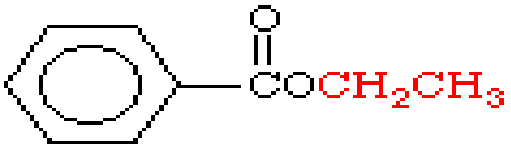
Methyl benzoate



Octyl ethanoate



methyl propanoate



ethyl benzoate

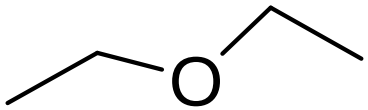


tert-butyl acetate

Ether

- Ethers are characterized by two alkyl groups being bonded to a central oxygen atom (i.e. R-O-R).
- The alkyl groups need not be the same, and may contain other function groups.
- Unfortunately there are several ways to name ethers.
- An older, but still common method for simple ethers, is to name it as an alkyl alkyl ether (note the spaces between the words).
- If the two alkyl groups are the same it is named as a dialkyl ether.
- The most common way of naming ethers is as an alkoxy substituent on a parent chain (or ring).

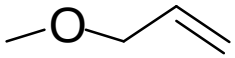
Example



Diethyl ether



Ethyl methyl ether



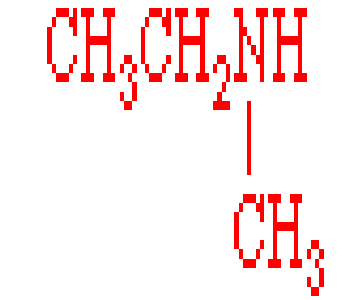
3-methoxy -1-propene

Amines

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

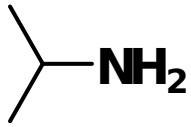


dimethylamine

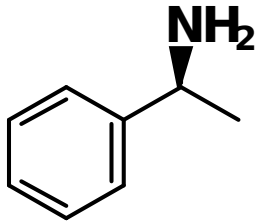


ethylmethylamine

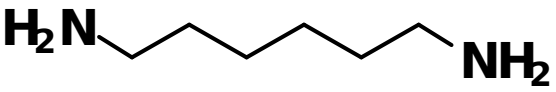
- Aliphatic amines: replace the suffix -e of the parent alkane by -amine.



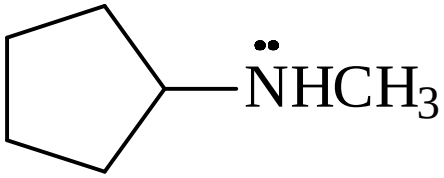
2-Propanamine



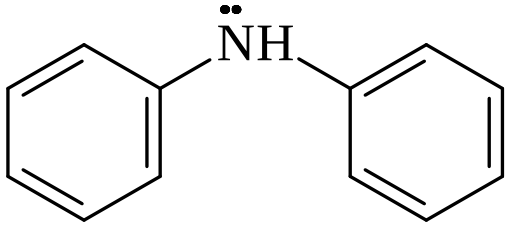
(S)-1-Phenyl-ethanamine



1,6-Hexanediamine

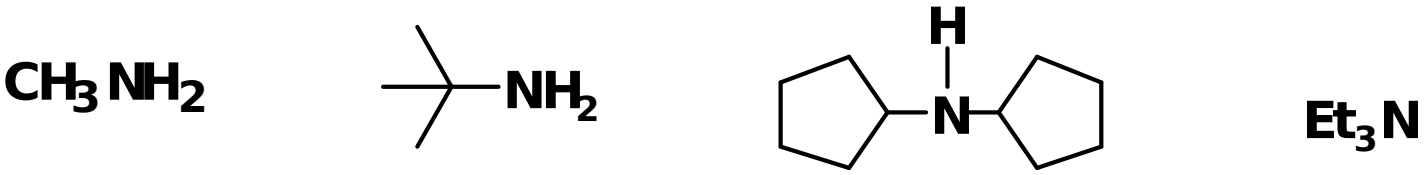


cyclopentylmethylamine



Diphenylamine

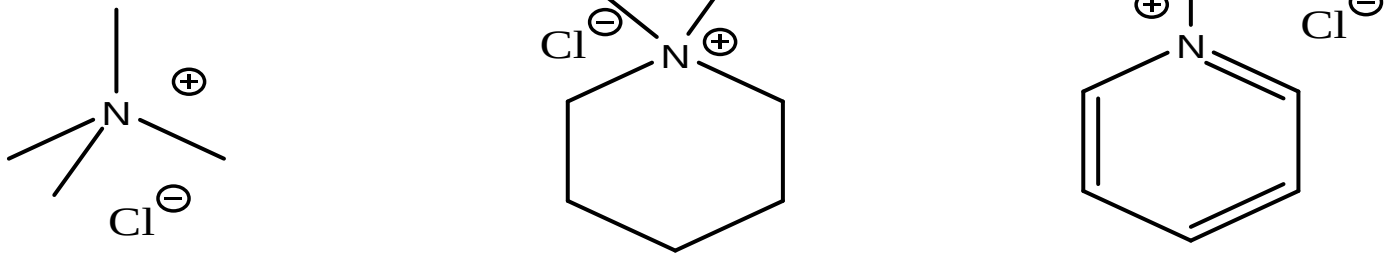
- Common names for most aliphatic amines are derived by listing the alkyl groups bonded to nitrogen in one word ending with the suffix-amine.



Methylamine **_tert_-Butylamine** **Dicyclopentylamine** **Triethylamine**

- When four groups are bonded to nitrogen, the compound is named as a salt of the corresponding amine.

1-ethyl-1-methylpiperidinium chloride

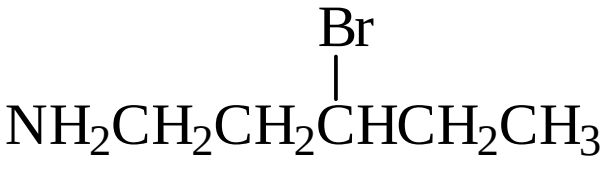


tetramethylammonium chloride

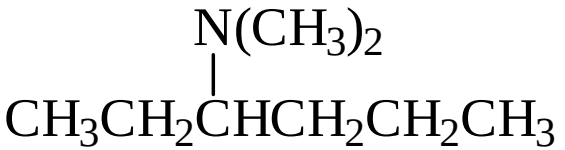
1-ethylpyridinium chlride

IUPAC Names

- Name is based on longest carbon chain.
- -*e* of alkane is replaced with -*amine*.
- Substituents on nitrogen have *N*- prefix

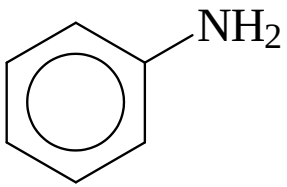


3-bromo-1-pentanamine

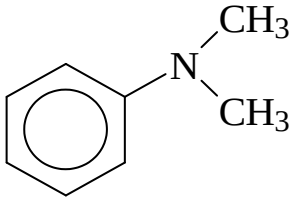


N,*N*-dimethyl-3-hexanamine

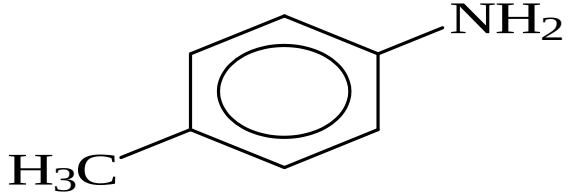
- Amino group is bonded to a benzene ring. Parent compound is called aniline.



aniline



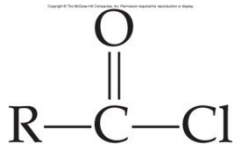
N,*N*-dimethylaniline



4-methylaniline or *p*-toluidine

Acid Chlorides

- Acid chlorides are derivatives of carboxylic acids having the general formula:



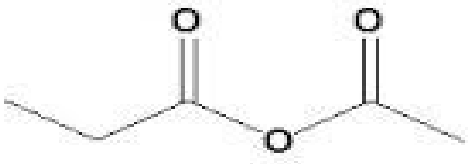
- Are named: by replacing the –oic acid ending of the IUPAC name with –oyl chloride

ethanoyl chloride
(acetyl chloride)

Acid Anhydrides

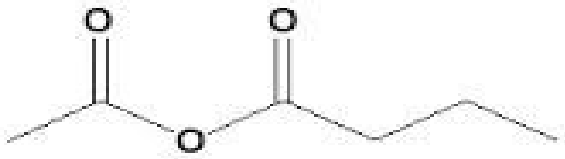
- Acid anhydrides have the formula:
- The molecule is 2 carboxylic acid molecules with a water molecule removed
  - *Anhydride* means without water
- Symmetrical anhydrides are those with *both* acyl groups the same
- Symmetrical anhydrides are named by replacing the -acid ending of the acid with –anhydride
- Unsymmetrical acid anhydrides are named by first naming each component carboxylic acid alphabetically arranged (without the word acid) followed by spaces and then the word anhydride.

ethanoic anhydride
acetic anhydride



Ethanoic propanoic anhydride

(Acetic propionic anhydride)



Butanoic ethanoic anhydride

(Acetic butyic anhydride)