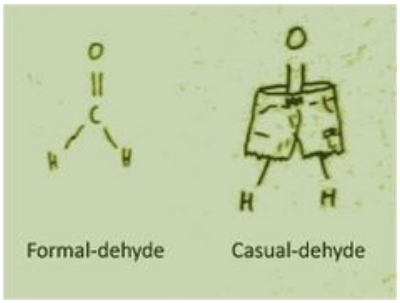
Naming Organic Molecules



Three Categories:

1. Naming Hydrocarbons

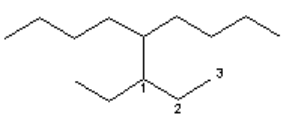
2. Cyclic Hydrocarbons

3. Functional Groups

Complex Branches

To complicate the naming of organic molecules, the branches on the parent chain can have branches themselves. The branched branch is numbered (starting at the carbon attached to the main chain as number 1) and the position of the branches on the branch indicated using this numbering scheme. The complex substituent is then placed in parentheses to remove any confusion over numbering.

Example 1.)

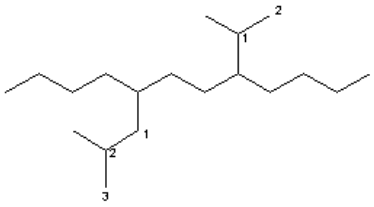


The compound is named: 5-(1-ethylpropyl)nonane

Note :

- that putting the branched branch in parentheses clearly designates the '1' as referring to the position of the ethyl group on the propyl branch (numbered in the above diagram).
- that the carbon of the propyl branch that is attached to the main chain is designated '1'.

Example 2.)



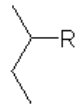
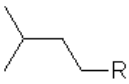
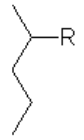
This compound is named: 5-(1-methylethyl)-8-(2-methylpropyl)dodecane

Note :

- that the methylethyl proceeds methylpropyl alphabetically.
- that when there is no preference in numbering right-to-left or left-to-right on the parent chain, the convention is to give the substituent that comes first alphabetically the lower number.

Complex Branches

There are a number of common names used for smaller complex substituents. This has arisen from past attempts to provide a systematic method for naming complex organic molecules. These common names identify the branched branches and attachment points of the branch(es) within this complex substituent. (NOTE: in the following examples the parent chain of the entire molecule is referred to as "R", a common shorthand in organic chemistry).

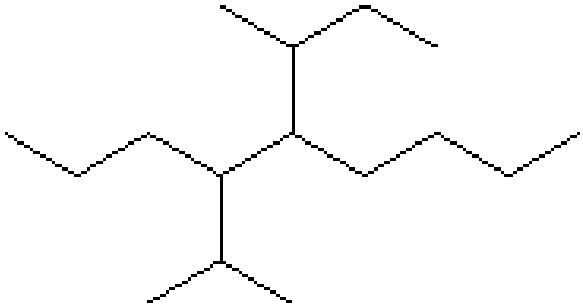
Number of C Atoms	Line Drawing	Name
3		isopropyl
4		isobutyl
4		*sec*-butyl
4		*tert*-butyl
5		isopentyl
5		*sec*-pentyl

Notes on the use of these names:

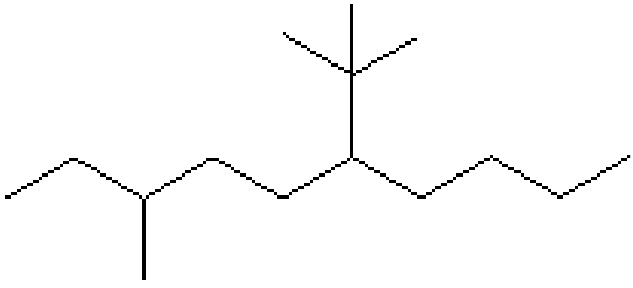
- iso is considered to be a part of the name of the alkyl group and so the letter " i " is used to place the groups in alphabetical order.
- the other prefixes, which are hyphenated, are not considered to be a part of the group's name when placing the groups in alphabetical order. E.g. *sec*-butyl is placed in order by the letter "b" (not "s").

Try it on your own

Example 1

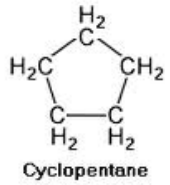


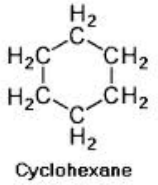
Example 2



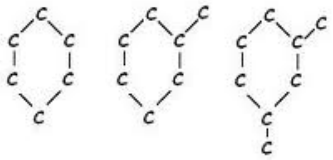
2. A **cyclic hydrocarbon** is a compound that contains a hydrocarbon ring and has cyclo in its name

Cycloalkanes: ring contains only single bonds

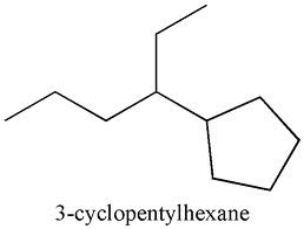




Condensed structural formula



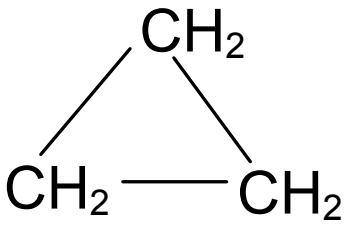
Skeletal structure



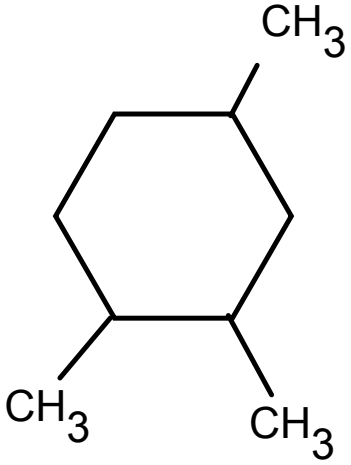
Line structure

**Numbering of ring must start at a substituent branch. If there are multiple branches, number in a way that gives the lowest branch numbers. if there is only 1 branch-no numbering is needed. Otherwise, naming is very similar to hydrocarbon alkanes

Example 1



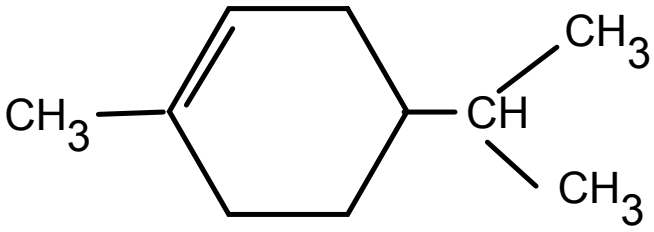
Example 2



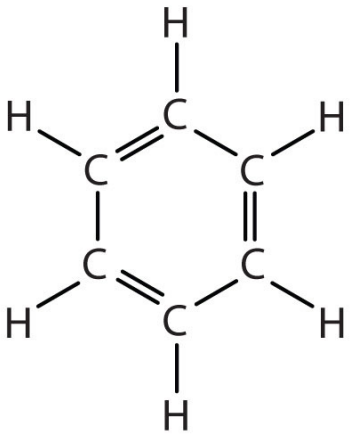
Cycloalkenes: ring contains 1 or more double bonds

**similar to cycloalkanes, however, ending must be changed to "ene"

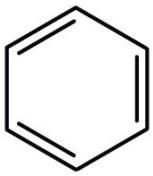
Example 1



Example 2



or

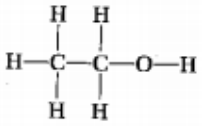
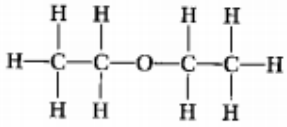
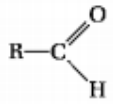
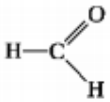
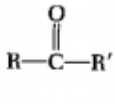
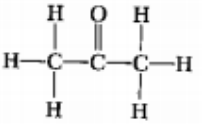
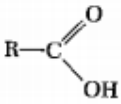
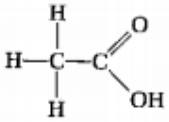
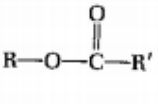
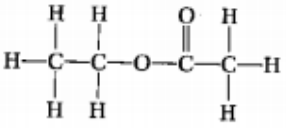
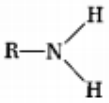
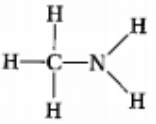


2. Function Groups are specific groups of atoms within molecules that are responsible for the characteristics of that molecule

Some common functional groups are listed in the table below

Table 23-4

COMMON FUNCTIONAL GROUPS FOUND IN ORGANIC COMPOUNDS

GENERAL STRUCTURE	GROUP NAME	EXAMPLE	
R—O—H	alcohol		ethanol
R—O—R′*	ether		ethoxyethane
	aldehyde		methanal
	ketone		propanone
	acid		ethanoic acid
	ester		ethyl acetate
	amine		methylamine

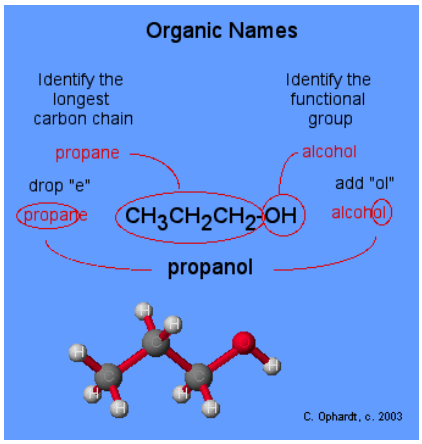
*R and R′ symbolize the general hydrocarbon group of the molecule. They may be the same group or different groups.

1. Alcohols:

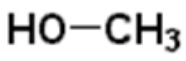
- Contains 1 or more -OH (hydroxyl) groups that replace an H atom on the hydrocarbon chain
- This group makes the compound polar.
- Alcohols are miscible with water and are good fuels (flammable).

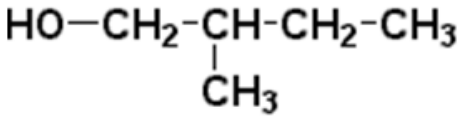
Naming:

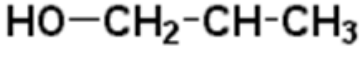
1. Find the parent chain. Name according to hydrocarbon naming rules.
2. Replace the final "e" with the ending "-ol"
3. A number with a hyphen indicates which C atom the -OH group is found on
4. If more than one-OH group is present, use prefixes before the -ol

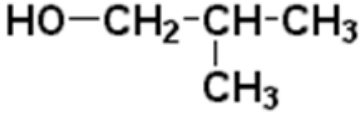


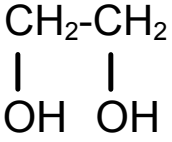
Examples





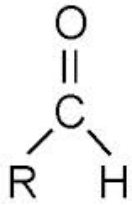






2. Aldehyde

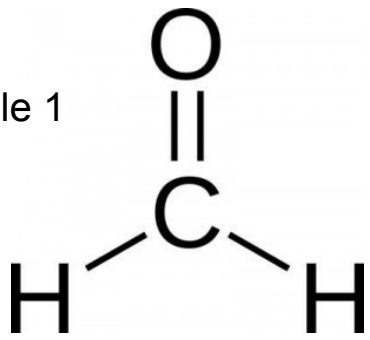
- Contain a carbonyl functional group bonded to a hydrocarbon chain and a hydrogen atom
- can have pleasant odor (ie. oil of cinnamon)



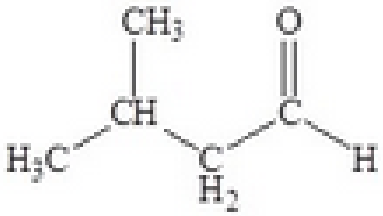
Naming:

1. Find the parent chain. Name according to hydrocarbon naming rules.
2. Replace the final "e" with the ending "-al"
3. No numbering is needed because carbonyl group is always at end of chain

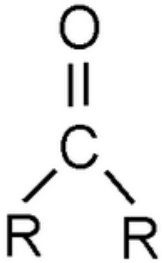
Example 1



Example 2



3. Ketone

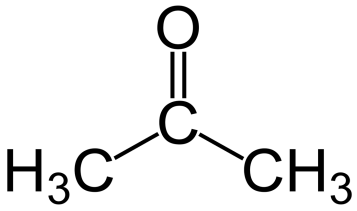


- Contain a carbonyl group bonded to two other hydrocarbon chains
- similar properties to aldehydes

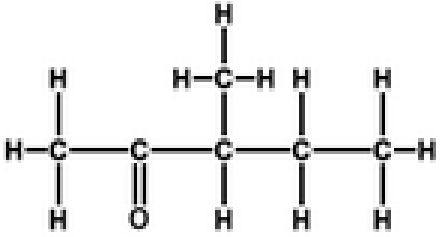
Naming:

1. Find the parent chain. Name according to hydrocarbon naming rules.
2. Replace the final "e" with the ending "-one"

Example 1



Example 2



Functional Groups greatly increase the number of isomers of a molecule

4. Carboxylic Acids:

- Contain one or more carboxyl groups -COOH
- polar and reactive
- Give the molecule weak acidic properties

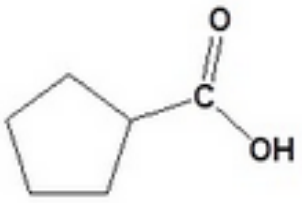
Naming:

1. Find the parent chain. Name according to hydrocarbon naming rules.
2. Replace the final "e" with the ending "-anoic acid"

Example 1

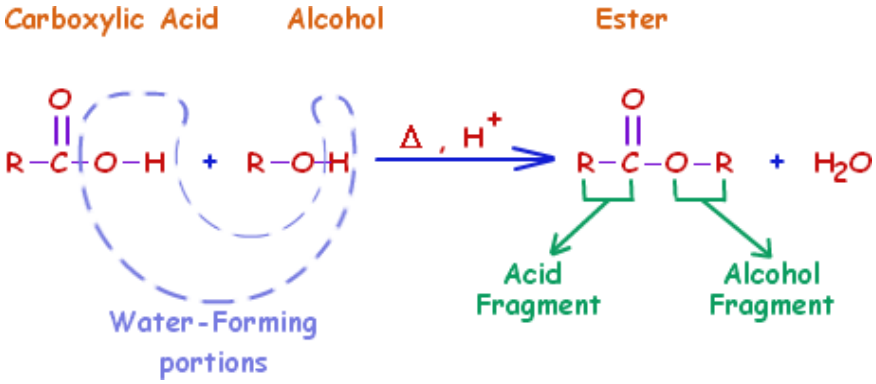
$CH_3\,CH_2\,COOH$

Example 2



5. Ester

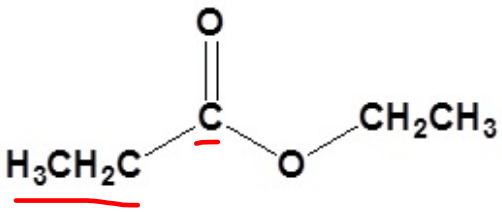
- are produced from a reaction between an acid and an alcohol (esterification)
- dehydration reaction
- possess distinct aromas and flavors



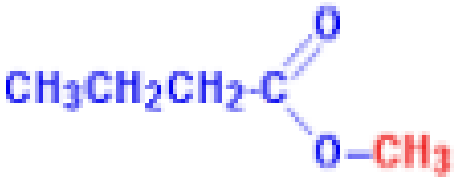
Naming:

1. Identify the alcohol and carboxylic acid
2. Change the ending of the alcohol to "yl" (treat it like a branch but don't assign a number)
3. Name the parent strand of the carboxylic acid but remove the "e" and change the ending to "oate"

Example 1



Example 2



A compound can contain multiple (and different) functional groups

6. Alkyl Halides:

- Contain one or more halogen groups (group 17)
- higher boiling points and more reactive than basic alkane chains

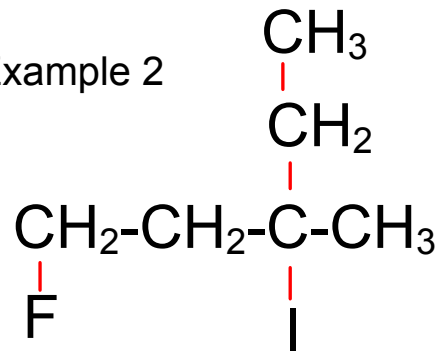
Naming:

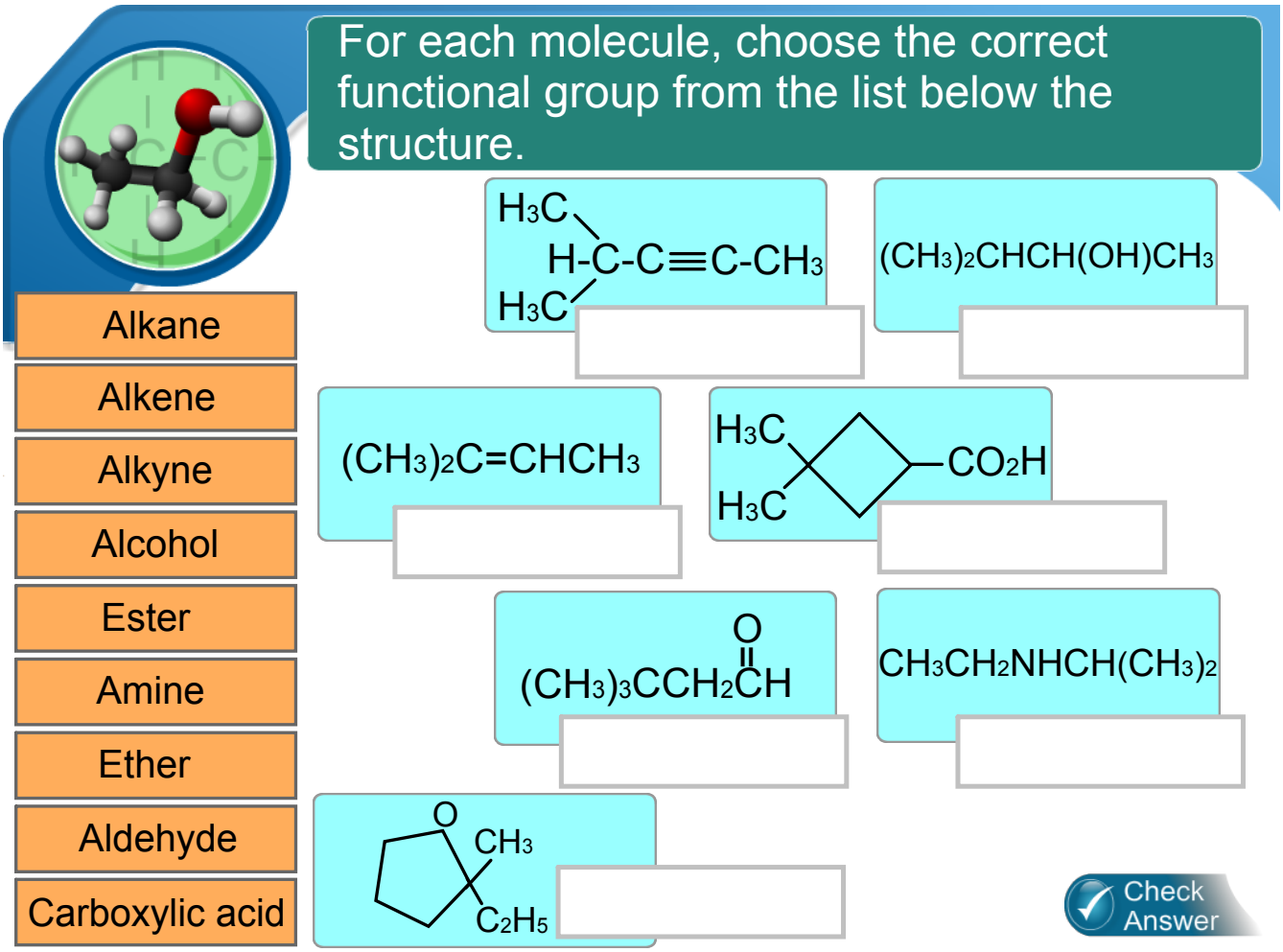
1. Find the parent chain. Name according to hydrocarbon naming rules.
2. If the halide group is anywhere but the 1st C atom, a number with a hyphen indicates which C atom the halide group is found on
3. Name the compound as if the halide is a simple branch

Example 1

$CH_3\,CHFCH_2\,CH_3$

Example 2



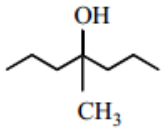

For each molecule, choose the correct functional group from the list below the structure.
Alkane
Alkene
Alkyne
Alcohol
Ester
Amine
Ether
Aldehyde
Carboxylic acid
H3C
H-C-C≡C-CH3
H3C
(CH3)2CHCH(OH)CH3
(CH3)2C=CHCH3
H3C
H3C
CO2H
O
(CH3)3CCH2CH
CH3CH2NHCH(CH3)2
O
CH3
C2H5
Check Answer

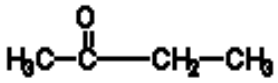
3.3 Assignment

1. Place the following substances in order of increasing boiling point.

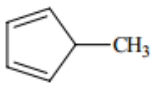
2-cloropentane 1-bromohexane butane
2-iodopentane 3-methylpentane

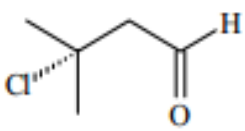
2. Write the correct IUPAC name for the compounds below

a) 

b) 

c) 

d) 

e) 

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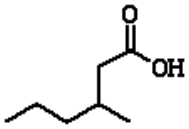
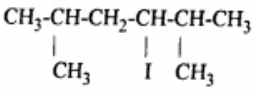
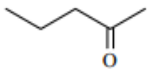
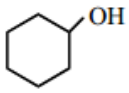
g) 

h) 

i) 

j) 

3.3 Assignment Cont...

3. Draw the correct structure for the following names

a) 2-chloro-1-propanol

b) 1,3-dibromo-4-chlorocyclohexane

c) 1-chloro-2,2-dimethylpropane

d) cyclohexanone

e) 3,3 dimethylbutanoic acid

f) 2-ethyl-4-methylpentanal

g) ethyl haxanoate