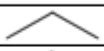
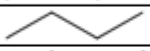
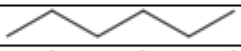
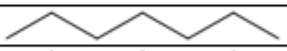
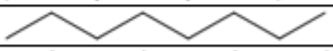
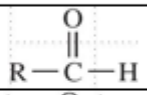
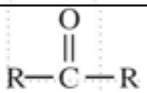
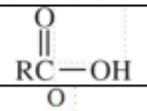
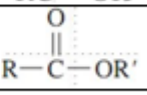
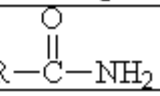
Naming Organic Molecules

Memorize How to Count 1-10

# C	Name	Picture
1	Meth-	CH_4
2	Eth-	
3	Prop-	
4	But-	
5	Pent-	
6	Hex-	
7	Hept-	
8	Oct-	
9	Non-	
10	Dec-	

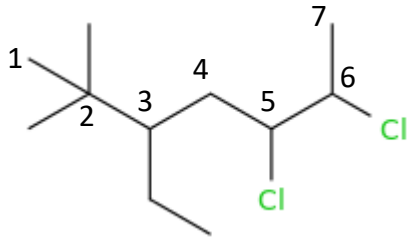
Memorize FG Endings

FG	Name	Structure
Alkane	-ane	C-C
Alkene	-ene	-CH=CH-
Alkyne	-yne	-C≡C-
Alcohol	-ol	R-OH
Ether	"oxy"	R-O-R
Aldehyde	-al	
Ketone	-one	
Carboxylic Acid	-oic acid	
Ester	-oate	
Amine	-amine	$R\text{-}NH_2$
Amide	-amide	

General Rules

1. Find Longest Chain
   a) Must contain FG
   b) If tied choose the most substituted
   c) No SC on SC
2. Identify Side Chains
   1. Carbons
   2. F,Cl,Br,I
   3. Ethers (-OR)
3. Number Longest Chain
   a) FG gets lowest number
   b) SC lowest number
   c) Alphabetical (parent, not #)
4. Multiple SC use di/tri etc.
5. Construct name – arrange all sidechains in alphabetical order

are separated by comma
#/letters are separated by dashes

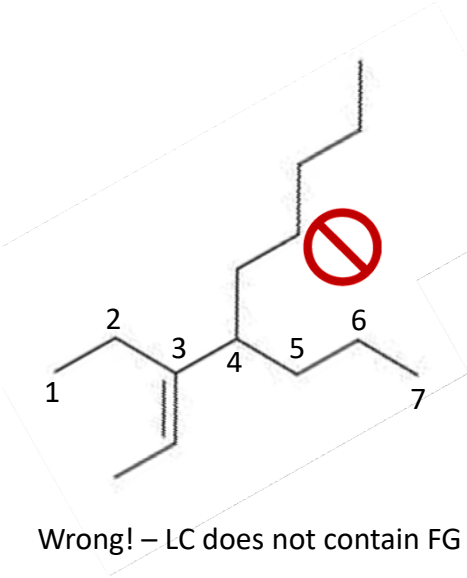


5,6-dichloro-3-ethyl-2,2-dimethylheptane

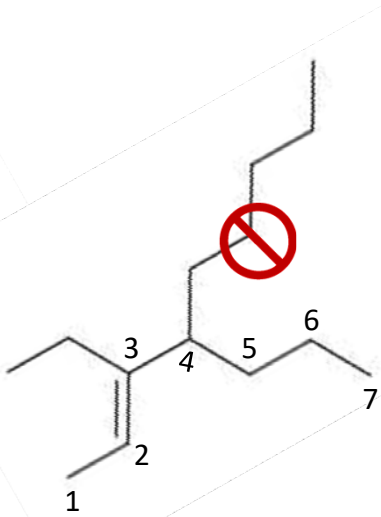
Find The Longest Chain (LC)
"Parent Chain"

Must Contain Functional Group
It can go any direction!

Exceptions – Ethers are Side Chains
Esters – Ketone side is longest

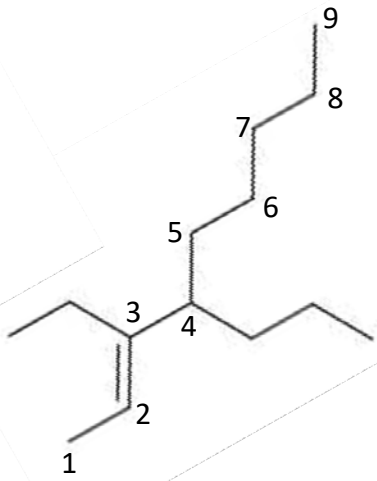


Wrong! – LC does not contain FG

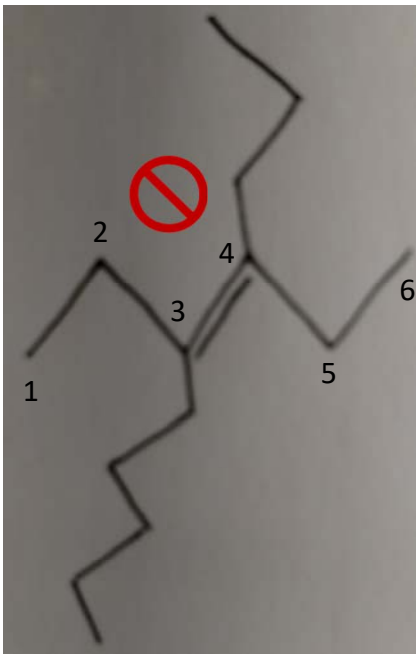


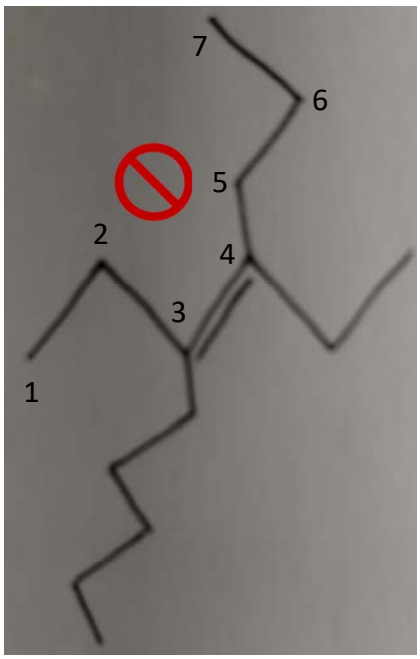
Wrong! – There is a longer chain

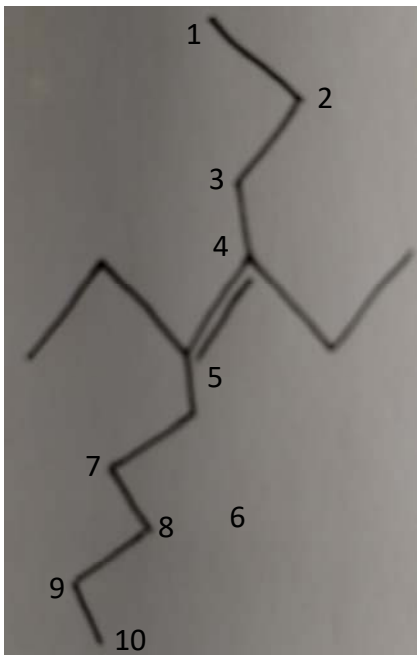
3-ethyl-4-propyl-2-nonene



Correct! – LC and includes FG



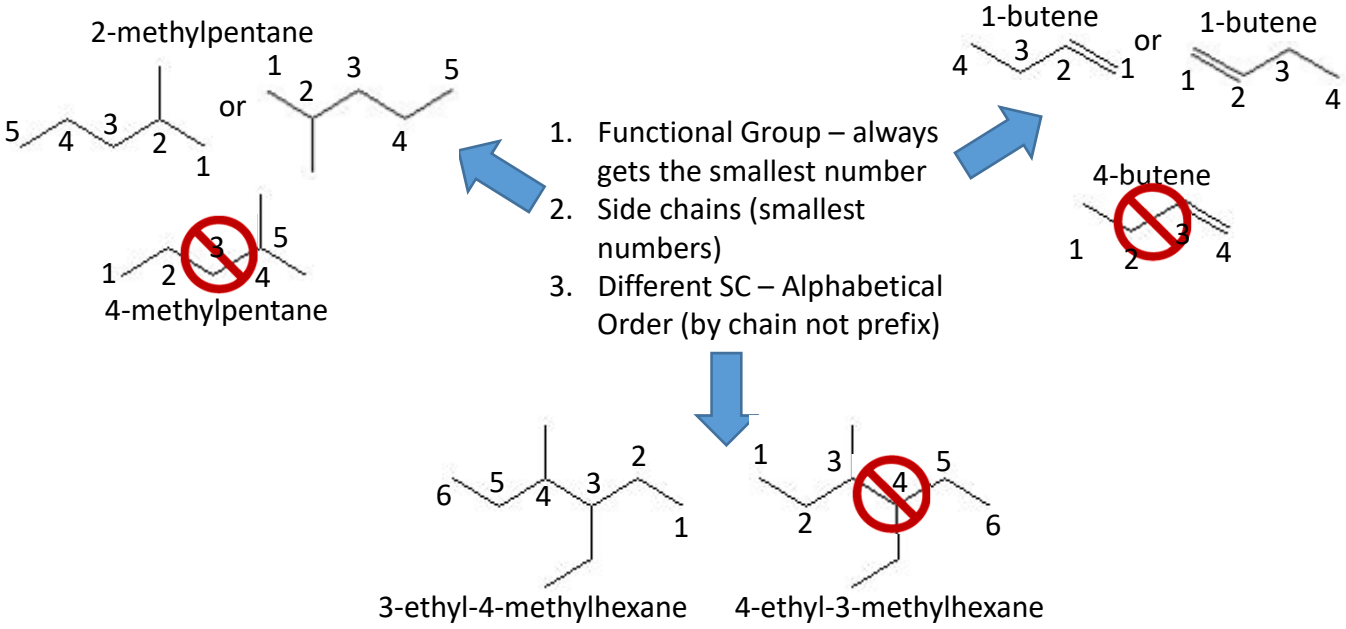




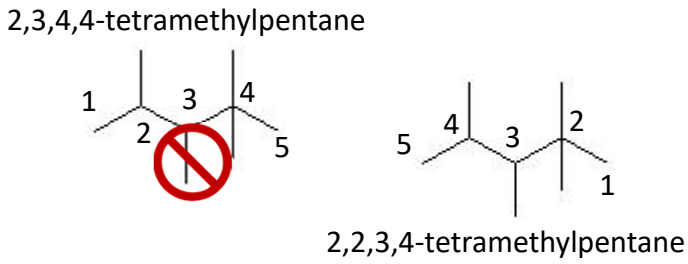
4,5-diethyl-4-decene

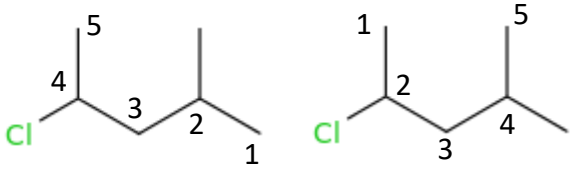
The last picture is correct because the chain is 10 C long and contains the FG

Number the Longest Chain (LC)

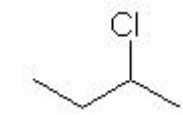


More Examples:

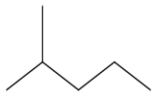




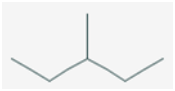
Identify the Shorter Chains (SC) "Side Chains"



2-chlorobutane



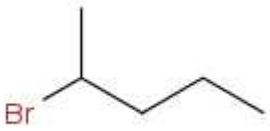
2-methylpentane



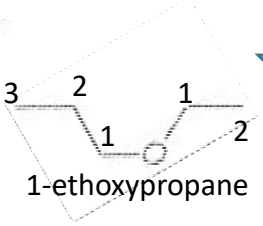
3-methylpentane

1. Carbon Chains
2. Halogens (F,Cl,Br,I)
3. Ethers

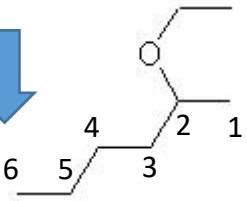
1-methylpentane



2-bromopentane



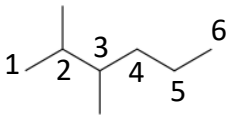
1-ethoxypropane



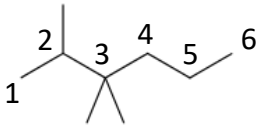
2-ethoxyhexane

Multiple Side Chains

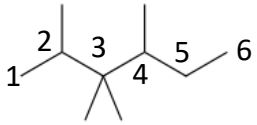
SC	Name
1	-
2	di-
3	tri-
4	tetra-
5	penta-



2,3-dimethylhexane



2,3,3-trimethylhexane



2,3,3,4-tetramethylhexane

Complications (We hope to avoid)

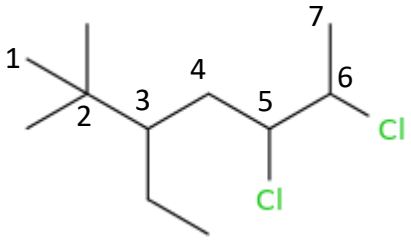
We will try avoid:

1. Side Chains on Side Chains
2. Cyclic Compounds
3. Use of special SC names (Table 19.3)
4. Multiple FG (occasionally)

Putting it all together

Construct name – arrange all sidechains in alphabetical order (ignore di/tri)

are separated by comma
#/letters are separated by dashes



5,6-dichloro-3-ethyl-2,2-dimethylheptane

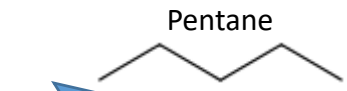
Naming Simple Alkenes and Alkynes

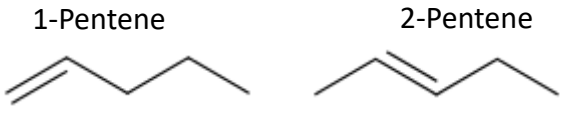
New/Modified Rules

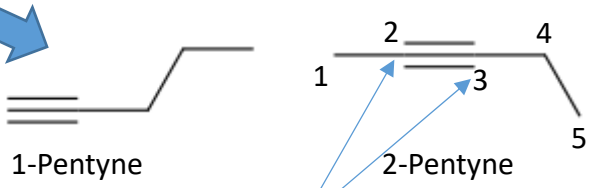
1. FG must be in LC
2. FG always gets smallest number
3. Change ending from –ane to –ene or -yne

FG	Name	Structure
Alkane	-ane	C-C
Alkene	-ene	-CH=CH-
Alkyne	-yne	-C≡C-

*Challenge Question:
Why is there no such thing as 3-pentene or 3-pentyne



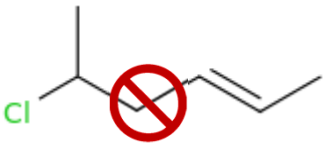




1-Pentyne 2-Pentyne

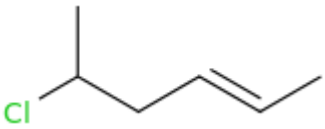
Triple bonds result in a linear geometry.
There is a carbon on either end of the C≡C

More Examples:



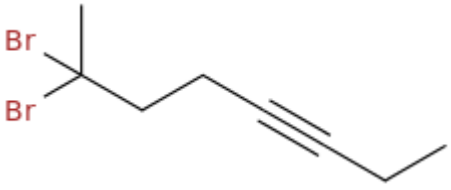
2-chloro-4-hexene

vs



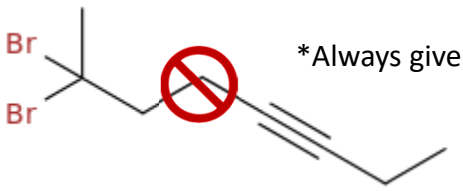
4-chloro-2-hexene

*Always give the FG the lowest number



7,7-dibromo-3-octyne

vs



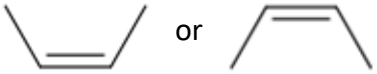
2,2-dibromo-5-octyne

*Always give the FG the lowest number

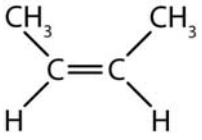
Naming Cis/Trans Isomers

C-C single bonds allow "free rotation" around them.
C=C double bonds are fixed in place resulting in a class of isomers called cis/trans (or geometric isomers).

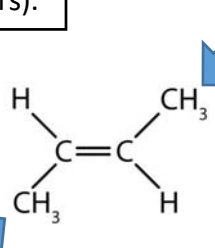
Cis – both groups on top or bottom



or



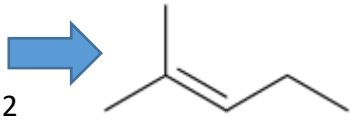
cis-2-butene



trans-2-butene

Trans – groups opposite each other

*Can't make a cis-trans isomer because there are 2 methyl groups on the right side

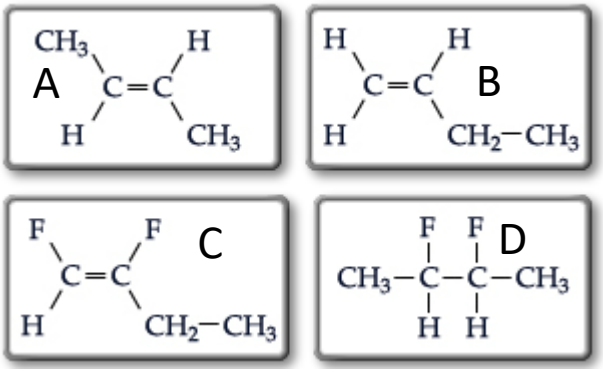


2-methyl-2-pentene

Does a Molecule Have a cis/trans Isomer

Requirements

1. C=C
2. Two different groups on a side



A) trans-2-butane
B) 1-butane, not a cis/trans (2 H on left)
C) cis-1,2-difluoro-1-butene
D) Butane - not a cis/trans (no C=C)

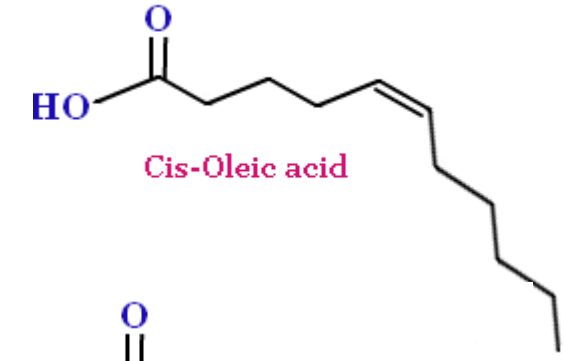
Important in Biochemistry

Preview

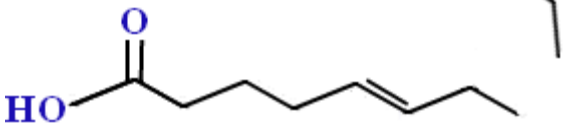
We will see cis/trans isomers again in the Biochemistry chapters

For example we will learn Lipids (Ch. 28) are just large carboxylic acids (Ch. 24).

They can have cis or trans geometry and nutritionally trans-isomers are bad for you.



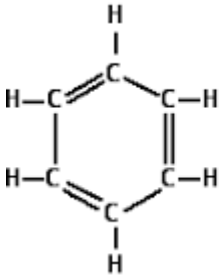
Cis-Oleic acid



trans-Oleic acid

Naming Aromatic Compound

Many different ways to draw aromatics



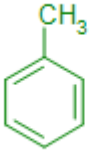
5 sets of rules for naming Aromatic Compounds

1. 6 special groups (memorize)
2. 1 Side Chains (normal rules)
3. 2 Side Chains ("o,m,p")
4. 3+ Side Chains (use #'s)
5. Complicated Side Chains

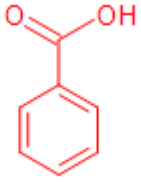
1

6 "Special" groups (memorize)

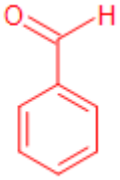
Phenol



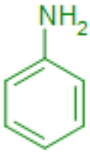
Toluene



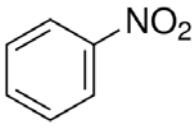
Benzoic Acid



Benzaldehyde



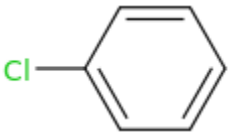
Aniline



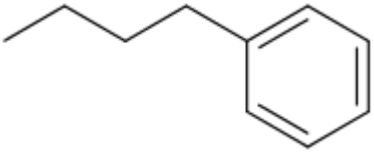
nitrobenzene

2

1 Side Chain (normal rules)



chlorobenzene



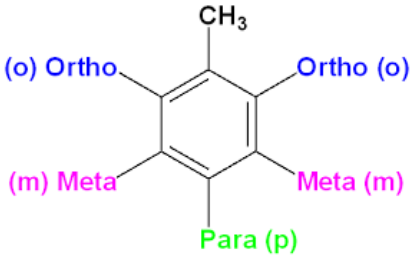
butylbenzene

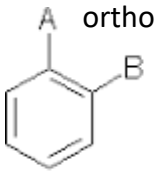
*no # needed because It is redundant

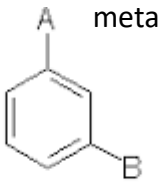
3

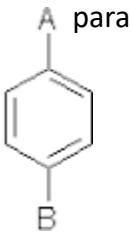
2 Side Chain ("o,m,p")

For aromatics with 2 side chains we use the prefix's
ortho (o) – groups adjacent
meta (m) – groups 1 apart
para (p) – groups 2 apart (opposite sides)

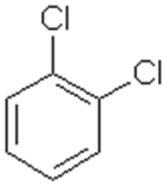




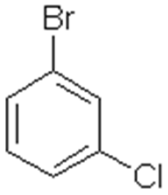




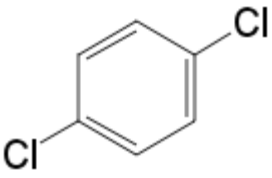
Examples



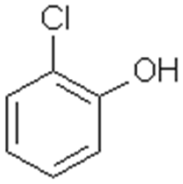
o-dichlorobenzene



m-bromochlorobenzene



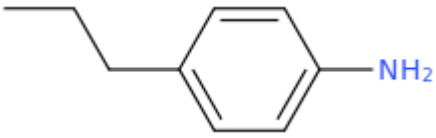
p-dichlorobenzene



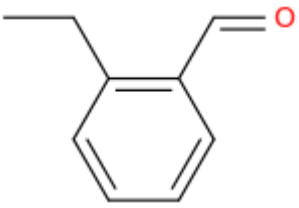
o-chlorophenol

*Don't forget the "special" groups
They take precedence when naming

More Examples

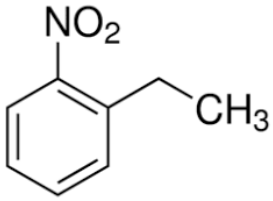


p-propylaniline

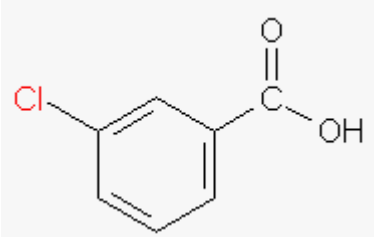


o-ethylbenzaldehyde

p-flurotoluene



o-ethylnitrobenzene



m-chlorobenzoic acid

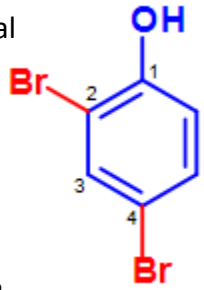
4

3+ Side Chain (use #'s)

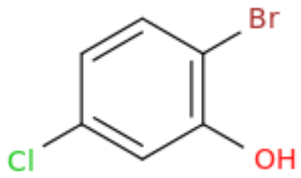
For aromatics with 3+ side chains we numbers like normal

1. The 6 "special" groups are always #1
2. If no special group use lowest set of numbers
3. If there is a tie go alphabetical

2,4-dibromophenol

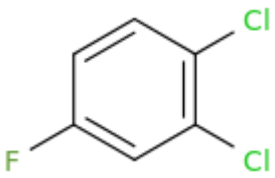


Rule 1



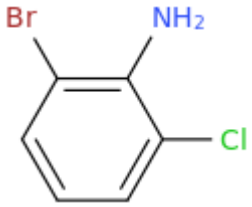
2-bromo-5-chlorophenol

Rule 2



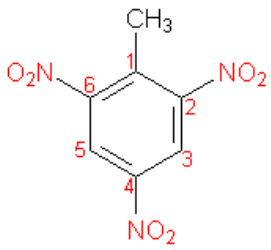
1,2-dichloro-4-fluorobenzene

Rule 3

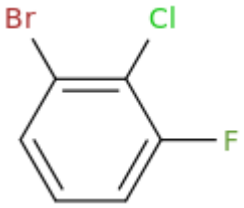


2-bromo-6-chloroaniline

More Examples

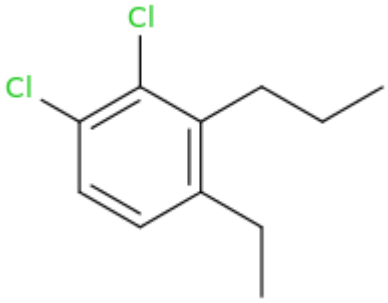


2,4,6-trinitrotoluene "TNT"



1-bromo-2-chloro-3-fluorobenzene

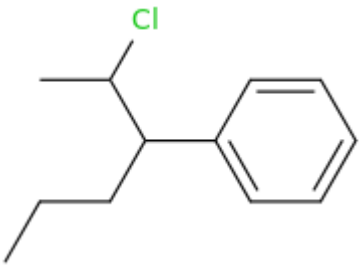
1,2-dichloro-4-ethyl-3-propylbenzene



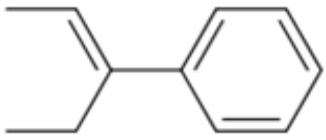
5

Complicated Side Chains

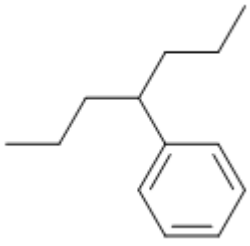
If the Side Chain on a benzene ring is too complex, then you name the molecule as if the Benzene ring were a side chain (called "phenyl").



2-chloro-3-phenylhexane



3-phenyl-2-pentene



4-phenylheptane

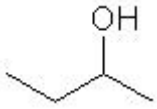
Naming Alcohols and Ethers

Chapter 22

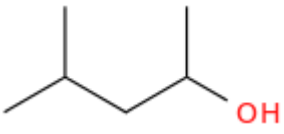
New/Modified Rules

1. FG must be in LC
2. FG <u>always</u> gets smallest number
3. Give the location of FG
4. Change ending from –e to –ol

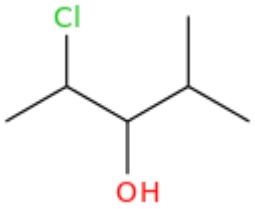
1-butanol



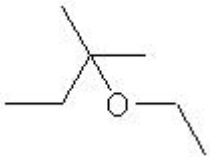
2-butanol



4-mthyl-2-pentanol

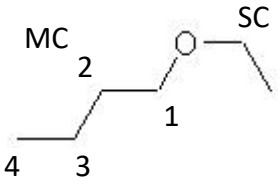


2-chloro-4-methyl-3-pentanol

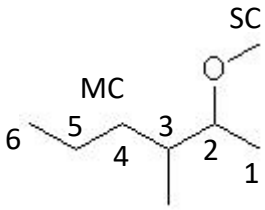


New/Modified Rules

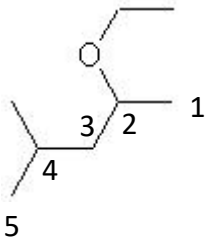
1. Ethers are not named like FG, they are treated as a SC
2. Instead of –yl we use -oxy



1-ethoxybutane



2-methoxy-3-methylhexane

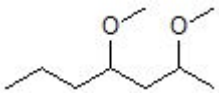


2-ethoxy-4-methylbutane

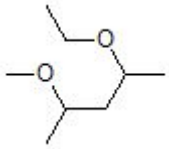
Note:

2-ethoxy
4-methyl

If SC are tied for lowest # then we break the tie alphabetically



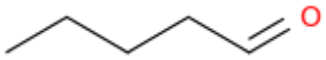
2,4-dimethoxyheptane



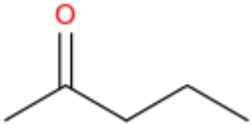
2-ethoxy-4-methoxypentane

Naming Aldehydes and Ketones

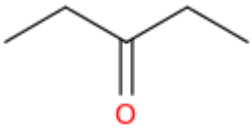
Chapter 23



Pentanal



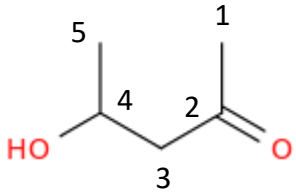
2-Pentanone



3-Pentanone

New/Modified Rules

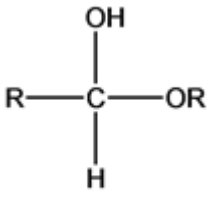
1. Share the same functional group (C=O)
2. FG is given the lowest number possible
3. Aldehydes
   a. no location (must be on end)
   b. Change ending –e to -al
4. Ketone
   a. location required (middle)
   b. Change ending –e to –one
5. Alcohols can be SC (if there is a more important FG in the molecule) The SC is named "hydoxy"



4-hydroxy-2-pentanone

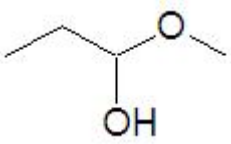
Some Unique Molecules to Recognize (used in reactions and biochemistry)

Acetal – like Aldehydes (always on end)
Ketal – like Ketones (always in the middle)
Hemi – ½ ether, ½ alcohol

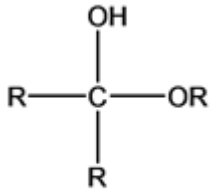


Hemiacetal

1-ether
1-alcohol
1- H
1- R

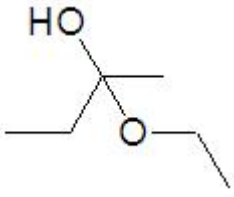


1-methoxy-1-propanol

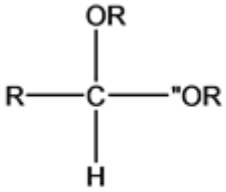


Hemiketal

1-ether
1-alcohol
2- R

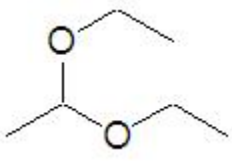


2-ethoxy-2-butanol

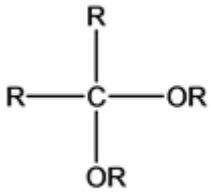


Acetal

2-ether
1 - H
1 - R

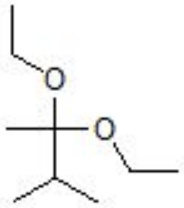


1,1-diethoxyethane



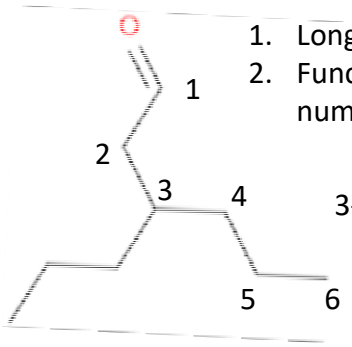
Ketal

2-ether
2- R



2,2-diethoxy-3-methylbutane

Review – it's a good idea to review everything now and then

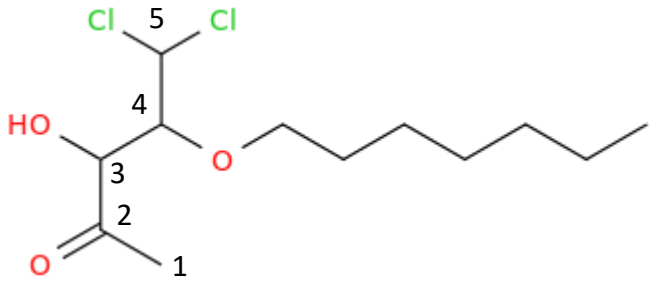


1. Longest chain must contain the FG
2. Functional group must have lowest number

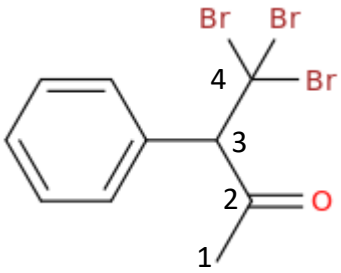
3-propylhexanal

---

1. Longest chain must contain the FG
2. Functional group must have lowest number
3. -OH can be a SC (Hydroxy)
4. The ether is a SC even though the chain is longer (it does not contain the FG)
5. Don't forget your di and tri's

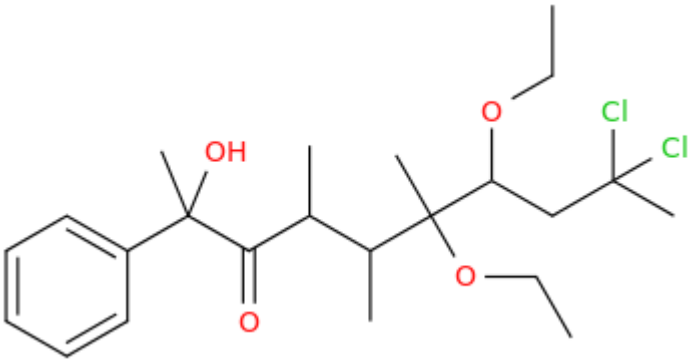


5,5-dichloro-4-heptoxy-3-hydroxy-2-pentanone



1. Longest chain must contain the FG
2. Functional group must have lowest number
3. A benzene ring is called a "phenyl" if it's a SC

3-phenyl-4,4,4-tribromo-2-butanone



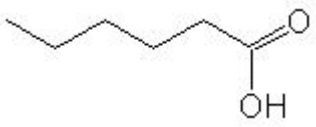
Perhaps a bit over the top, but you should be able to name it!

9,9-dichloro-6,7-diethoxy-2-hydroxy-4,5,6-trimethyl-2-phenyl-3-decanone

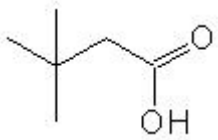
Naming Carboxylic Acids (CA)

New/Modified Rules

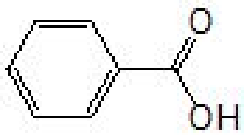
1. The CA FG is always # 1 (no loc)
2. Change ending from e – oic acid



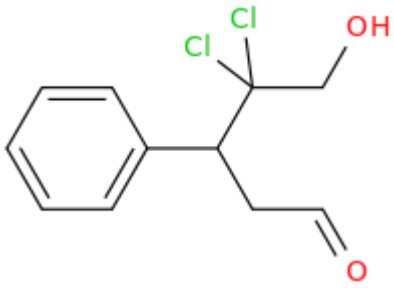
hexanoic acid



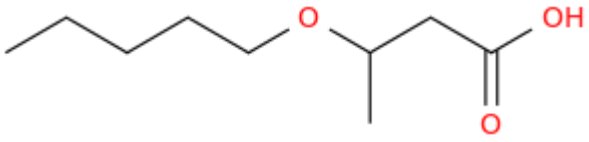
3,3-dimehtylhexanoic acid



benzoic acid



3-phenyl-4,4-dichloro-5-hydroxypentanal

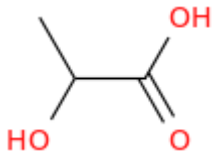


3-pentoxybutanoic acid

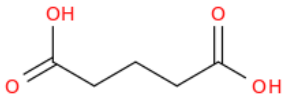
Common CA

(you will see them in the biochemistry chapters)

Lactic Acid
(Glycolysis – Ch. 34)

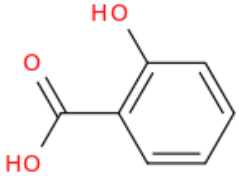


2-hydroxypropanoic acid



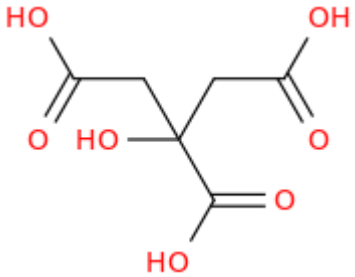
pentanedioic acid

Common name – Glutaric Acid
(formed during Amino Acid Metabolism)



o-hydroxybenzoic acid

Common Name
Salicylic Acid/Asprin



2-hydroxypropane-1,2,3-tricarboxylic acid

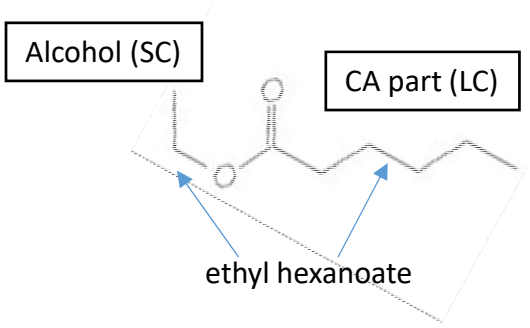
Citric Acid
(aka Citric Acid Cycle)
*no you don't have to name this one

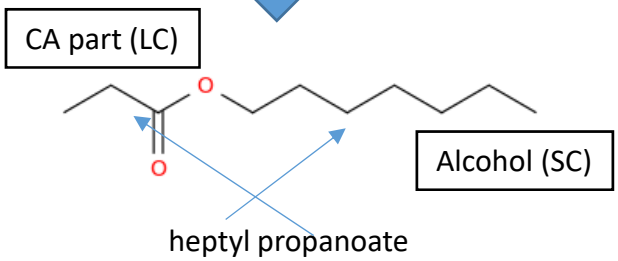
Naming Esters

New/Modified Rules

1. Esters are composed of two parts
   a. CA part – LC
   b. Alcohol part – SC with –yl
2. Ester FG is always #1 (no loc)
3. Leave a space between the Alcohol SC and any other SC's
4. Change ending of LC from –e to –oate

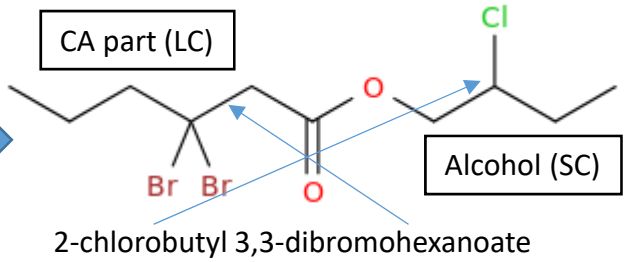
*pay special attention to the carbonyl (C=O) group, that side of the molecule is considered the CA side and is **ALWAYS** the LC (even it its shorter than the alcohol side





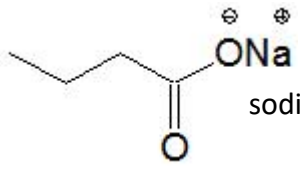
Side Chains

Both the CA and the Alcohol part of an Ester can have side chains, they are named just like normal

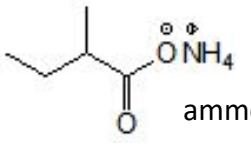


Carboxylic Acid Salts

1. CA Salts are named like Esters (weird huh!)
2. Name the cation then the ester like normal



sodium butanoate



ammonium 2-methylbutanoate

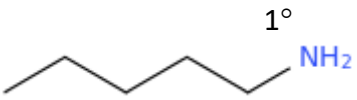
Naming Amines

New/Modified Rules

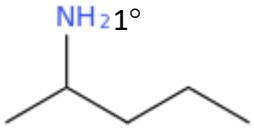
1. Amines are much like alcohols
2. Must give Location (#) of FG
3. The LC is the MC
4. SC attached to the N have a location ion "N"
5. Change ending of LC from –e to –amine

Nomenclature

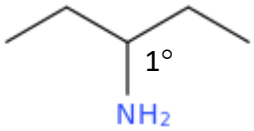
1 bond to C = Primary (1°)
2 bonds to C = Secondary (2°)
3 bonds to C = Tertiary (3°)
4 bonds to C = Quaternary Salt



1-pentanamine



2-pentanamine

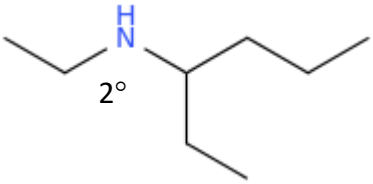


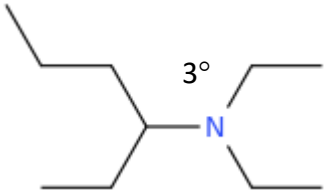
3-pentanamine

Remember the location

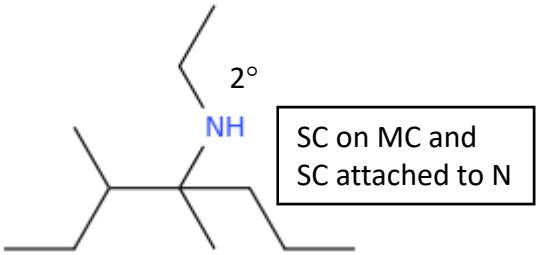
SC attached to N

N-ethyl-1-hexanamine



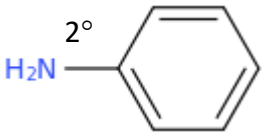


N,N-diethyl-3-hexanamine



SC on MC and SC attached to N

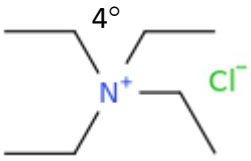
N-ethyl-3,4-dimethyl-4-heptanamine



aniline

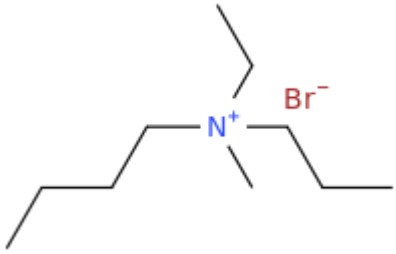
Quaternary Salts

1. Only form when N has 4 bonds and a positive charge.
2. "ammonium ion"



N,N,N,N-tetraethyl ammonium chloride

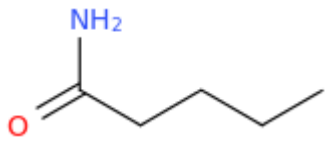
N-butyl-N-ethyl-N-methyl-N-propyl ammonium bromide



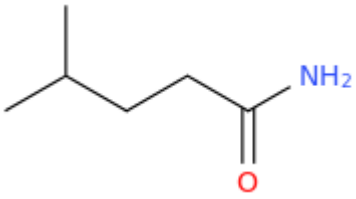
Naming Amides

New/Modified Rules

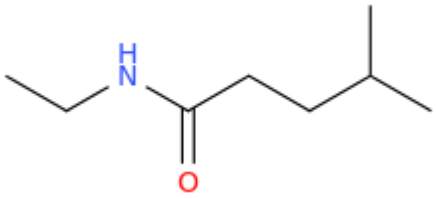
a. Amides are like Esters, composed of two parts
    a. CA part – LC
    b. Amine part – SC with location N and ending –yl
b. Amine FG is always #1 (no loc)
c. Change ending of LC from –e to –amide



pentanamide

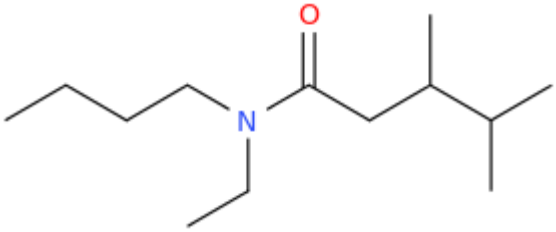


4-methylpentanamide



N-ethyl-4-methylpentanamide

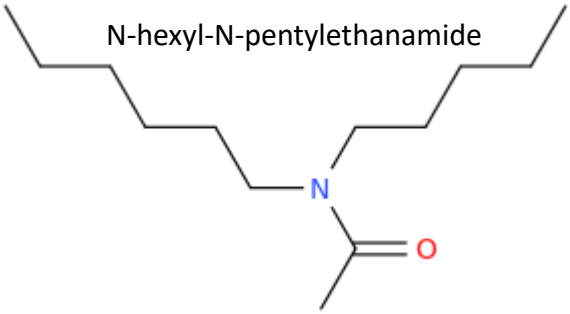
Order SC Alphabetically



N-butyl-N-ethyl-3,4-dimethylpentanamide

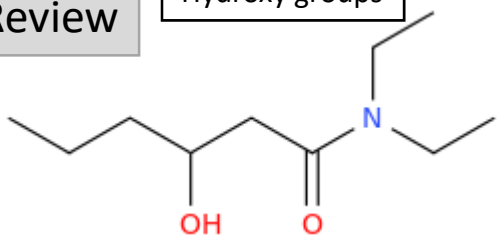
LC has the carbonyl group (C=O)

N-hexyl-N-pentylethanamide



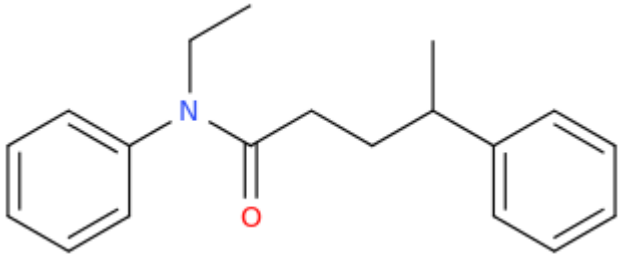
Review

Hydroxy groups

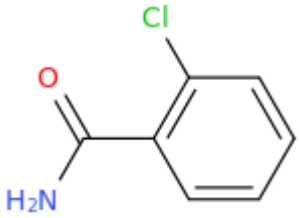


N,N-diethyl-3-hydroxyhexanamide

Don't forget phenyl groups!



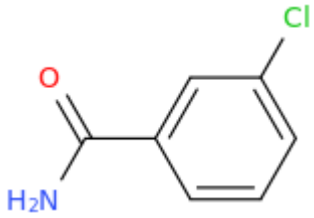
N-phenyl-N-ethyl-4-phenylpentanamide

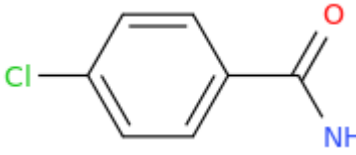


o,m,p

o-chlorobenzamide

m-chlorobenzamide





p-chlorobenzamide