Reference Sheet 2: Naming Compounds

IUPAC System of Naming

Typical Naming Directions:

- 1. Find the parent chain (longest consecutive chain of carbons)
 - If there's more than one potential parent chain, use the chain with the most substituents on it.
 - Have a ring of carbons (cyclic parent chain)? Add the prefix "cyclo" to the beginning of the parent name.

TABLE 4.1 PARENT NAMES FOR ALKANES					
NUMBER OF CARBON ATOMS	PARENT	NAME OF ALKANE	NUMBER OF CARBON ATOMS	PARENT	NAME OF ALKANE
1	meth	methane	11	undec	undecane
2	eth	ethane	12	dodec	dodecane
3	prop	propane	13	tridec	tridecane
4	but	butane	14	tetradec	tetradecane
5	pent	pentane	15	pentadec	pentadecane
6	hex	hexane	20	eicos	eicosane
7	hept	heptane	30	triacont	triacontane
8	oct	octane	40	tetracont	tetracontane
9	non	nonane	50	pentacont	pentacontane
10	dec	decane	100	hect	hectane

Saturated Hydrocarbons- No pi bonds; IUPAC suffix of parent chain: -ane

- 2. Identify substituents (IUPAC suffix of substituent(s): -yl)
 - Count the number of carbons in each side group and name accordingly using the suffix for substituents above.

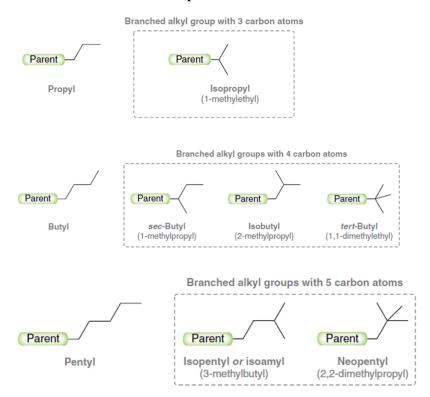
TABLE 4.2 NAMES OF ALKYL GROUPS				
NUMBER OF CARBON ATOMS IN SUBSTITUENT	TERMINOLOGY			
1	Methyl			
2	Ethyl			
3	Propyl			
4	Butyl			
5	Pentyl			
6	Hexyl			
7	Heptyl			
8	Octyl			
9	Nonyl			
10	Decyl			

Note: Depending upon the number of carbons present, a ring could be a parent chain or a substituent. However, a parent chain may not include both some carbons in a ring as well as other carbons that are not part of a ring. *Make sure to NOT include the parent chain carbons as part of your substituent carbons in naming!!!

~ Have substituents with complex branches:

- 1. Count longest carbon chain **WITHIN** the substituent, starting with the carbon that's directly attached to the main (parent) chain.
- 2. Name the substituent
- 3. Name and number the substituent's side group

Common Substituents Examples:



3. In assembling the full name of the compound, number the parent chain and assign a locant (number; as well as a prefix if necessary) to each substituent.

NOTE: GUIDELINES OF NUMBERING PARENT CHAIN:

- Have one substituent present: number parent chain where substituent has the smallest number possible.
- Have multiple substituents present: number parent chain where the first substituent has the smallest number possible.
- If the first substituent numbering on either side of the parent chain is a tie (for example, if numbering from either direction of the parent chain produces a tie concerning the substituent's numbering), if a second locant is present, then that should have the smallest number possible.
- Have no ties regarding substituents: assign smallest number alphabetically.

[NOTE: These bullet points apply to cycloalkanes as well].

4. List these numbered substituents before the name of the parent chain in alphabetical order.

Notably, if multiple substituents are the same on a parent chain, use a prefix (i.e.- di, tri, tetra, penta, (etc)).

^*It is crucial to keep in mind that these prefixes aren't a part of determining the alphabetical order in which the substituents are listed in the name. There are only a few prefixes that should be considered when ordering the substituents alphabetically: "iso," "neo," and "cyclo."

<u>IUPAC Naming Bicyclic Compounds (Compounds with two fused rings):</u> Include prefix "bicyclo"; if it's a saturated bicyclic compound, suffix: -ane

Directions:

1. In numbering the bicyclo parent chain, start at a bridgehead carbon and number the longest carbon chain connecting to the other bridgehead first. Then, number into the second longest loop before numbering the shortest loop of carbons connecting the bridgeheads

NOTE: Don't violate the rule above when performing "2."!!!!

2. Give substituents the smallest numbers possible.

Note directions of typical naming here too!!

#Example of bicyclic compounds and their names:

Bicyclo[3.1.1]heptane

Bicyclo[2.2.1]heptane

IUPAC Using cis and trans prefixes when naming Disubstituted Cycloalkanes/Rings and Structures with C=C Double Bonds:

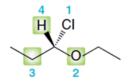
Use prefixes-

- 1. cis- when there's two identical substituents on the same side of a ring or on the same side of a C=C double bond
- 2. trans- when the two identical substituents are on opposite sides of a ring or on the same side of a C=C double bond

^{*}This is used to distinguish between stereoisomers!!!

<u>Determining R/S Configuration (AKA The Cahn, Ingold, and Prelog System)</u> Directions:

1. Prioritize the four groups attached to the chirality center using atomic numbers; the higher the atomic number is, the higher the priority.

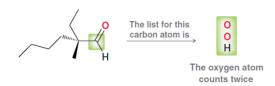


Note this regarding prioritizing:

- If two or more groups bonded to the chiral center have the same element directly bonded to the chiral center, then look to the second layer of atoms in determining priority (if they're the same as well, continue extending outward until one group has a higher priority than the other). Keep in mind that the priority at a chiral carbon is based on atomic number!!!
- NOTE THAT CHIRALITY CENTERS HAVE DIFFERENT GROUPS &/OR ATOMS ATTACHED TO A CARBON!!!!

Example:

Also remember that in prioritizing groups, double bonds count as two single bonds.



2. Arrange the molecule in space so the smallest priority group faces away from you (it's beneficial to use the model kit here). \bigcirc

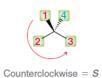
[THIS STEP IS OPTIONAL; IF IT MAKES IT EASIER FOR YOU, USE IT, AND UTILIZE THE BOLDED SECTION OF 4. in terms of determining R/S configurations (clockwise/counterclockwise)]



3. Count the group priorities from 1-3 and see if the order progresses in a clockwise or counterclockwise direction.

Clockwise: R and Counterclockwise: S

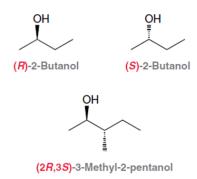
Example:



Note: If the priority group is facing toward you: Clockwise: R & Counterclockwise: S

*If the priority group is facing away from you (you haven't done "2."): Clockwise: S & Counterclockwise R

IUPAC Naming Regarding R/S Configuration Examples:



<u>IUPAC Naming Alkyl Halides (Compounds where a carbon group (alkyl) is bonded to a halide (F, Cl, Br, or I):</u>

#Note the steps in naming a molecule above. Treat the halide atom as a substituent (see substituent names below)

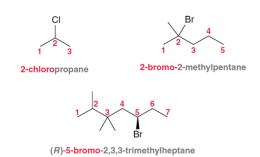
F- floro

Cl- chloro

Br- bromo

I- iodo

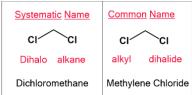
Examples:



<u>COMMON NAMES OF ALKYL HALIDES (NOT IUPAC SYSTEM): The alkyl group is named as</u> the substituent and the halide is treated as the parent name.

Examples:





IUPAC Naming Alkenes (compounds with C=C double bonds) Directions:

1. Identify the parent chain (this <u>should</u> include the C=C double bond). Also, the parent name should end in "-ene" rather than "-ane". THE LARGEST PARENT CHAIN CONTAINING THE DOUBLE BOND SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!



- 2. Identify & name the substituents
- 3. Assign a locant (and prefix if needed) to each substituent. Notably, the C=C double bond should have the smallest number possible. Start numbering the parent chain from the side closest to the double bond. Remember that there's one locant for the pi bond, not two. The locant of the double bond is the carbon with the smaller number.

Example:



*(The carbon circled is the locant for the double bond)

- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The C=C double bond locant is placed either just before the parent name or just before the -ene suffix.

Example:



IUPAC Alkene cis/trans and *E/Z* notation Naming:

Note: cis & trans modifiers are strictly utilized to describe double bonds with identical groups on each carbon. (i.e. Hydrogens are the identical groups in the double bond of the compound below):



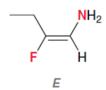
Note: *E/Z* notation is used for molecules with different groups attached to the C=C double bond. Cis and trans terms cannot be used to distinguish between the compounds below, because while these compounds are stereoisomers, they don't have identical groups positioned in either a cis or trans configuration. Rather, they must be distinguished with an *E* or *Z* designation.

Directions in Assigning *E* **or** *Z***:**

1. Prioritize two groups attached to each individual carbon of the C=C double bond based on atomic number, as shown here:

#If the top priority groups are on the SAME SIDE of the C=C double bond- Z

#If the top priority groups are on the OPPOSITE SIDE of the C=C double bond- E



WANT TO REMEMBER THIS: Note =>

Same starts with S; S & Z are Consonants

Opposite starts with O; O & E are Vowels

IUPAC Naming Alkynes (carbon compounds with a triple bond) Directions:

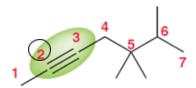
1. Identify the parent chain (INCLUDES THE C≡C TRIPLE BOND). Also, the parent name should end in the suffix, "-yne". THE LARGEST PARENT CHAIN CONTAINING THE TRIPLE BOND SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!

Example:



- 2. Identify & name the substituents
- 3. Assign a locant (and prefix if needed) to each substituent. Notably, the C≡C triple bond should have the smallest number possible. Remember that there's one locant for the triple bond, not two. The locant of the triple bond is the carbon with the smaller number.

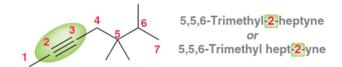
Example:



*(The circled carbon is the locant for the triple bond)

- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The C≡C triple bond locant is placed either just before the parent name or just before the -yne suffix.

Example:



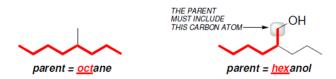
COMMON NAMES OF ALKYNES (NOT IUPAC SYSTEM): The carbon group(s) are named as the substituent and the triple bond is treated as the parent name (in this case, the parent name is acetylene).



IUPAC Naming Alcohols (carbon compounds with an OH (hydroxyl) group) Directions:

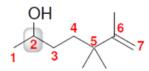
 Identify the parent chain (INCLUDES THE OH GROUP). Also, the parent chain should end in "-ol". THE LARGEST PARENT CHAIN CONTAINING THE CARBON WITH AN OH GROUP SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!

Example:



- 2. Identify & name the substituents
- 3. Assign a locant (and prefix if needed) to each substituent. Notably, the carbon containing the OH group should have the smallest number possible. Remember that the carbon that the OH group is attached to the smallest number possible has a higher priority over C=C double bonds (this concerns the numbering of the carbon chain and the locants of the OH group versus C=C double bonds).

Example:



*(The carbon circled has the OH group have a smaller locant compared to the C=C double bond's locant). Notice how both the alcohol and the C=C double bond are **BOTH** included in the parent chain!!!

- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The OH group locant is placed either just before the parent name or just before the -ol suffix.

#If necessary, R/S configurations are ALWAYS shown at the beginning of the name:

Example:

(R)-2-chloro-3-phenyl-1-propanol

<u>For Cyclic Alcohols, the OH group is ALWAYS on the first carbon, so usually the locant is unnecessary.</u>

Examples:

<u>COMMON NAMES OF ALCOHOLS (NOT IUPAC SYSTEM): The carbon group(s) are named as the substituent and the OH group is treated as the parent name.</u>

Examples:

Note: When an OH group is attached to a benzene ring, the parent name is "-phenol".

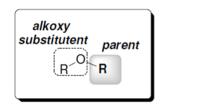
#Treat the OH group as the top priority group, and make sure the substituents on the benzene ring have the smallest numbers possible!!!

4-chloro-2-nitrophenol

IUPAC Naming Ethers (carbon compounds with an OR (R- some carbon group or alkyl group Directions:

- 1. Make the larger of the -R groups the parent chain
- 2. Name the smaller of the -R groups as an alkoxy substituent

Example:



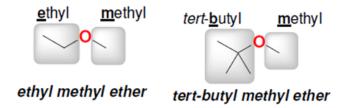
EXAMPLE ethoxy pentane

<u>COMMON NAMES OF ETHERS (NOT IUPAC SYSTEM): The carbon group(s) are named as the substituent and the oxygen (O) is treated as the parent name (in this case, it's "ether").</u>

Directions:

- 1. Name each -R group
- 2. Arrange them alphabetically
- 3. End with the word, "ether"

Examples:



Note Regarding Cyclic Ethers: Size of ring determines parent name of the molecule =>

 $\stackrel{\mathsf{O}}{\sim}$

l

 \bigcirc

pyran ring system

oxirane ring system oxetane ring system furan ring system

rıng systei

Also Note: Epoxides (also known as oxiranes) can have up to 4 -R group substituents =>



a substituted oxirane (an epoxide)



ethylene oxide (the simplest epoxide)

IUPAC Naming Epoxides (Oxiranes):

1. The oxygen is treated as a side group, and 2 numbers are given as its locants!!!!

Example:



3-ethyl-2-methyl-2,3-epoxypentane

OR

2. "Oxirane" is used as the parent name.

Example:



1,1-diethyl-2,2-dimethyloxirane

#Use Naming IUPAC directions noted above!

IUPAC Naming Thiols (carbon compounds with an SH group) Directions:

1. Identify the parent chain (INCLUDES THE SH GROUP). Also, the parent chain should end in "-thiol". THE LARGEST PARENT CHAIN CONTAINING THE CARBON WITH AN SH

GROUP SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!

- 2. Identify & name the substituents
- 3. Assign a locant (and prefix if needed) to each substituent. Notably, the carbon containing the SH group should have the smallest number possible.
- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The SH group locant is placed either just before the parent name or just before the -thiol suffix.

Example:

#Note the difference: the "e" of butane is **NOT** dropped in the name of the thiol!!!!

Consider this: Thiols are also known as mercaptans!

The -SH group can also be named as a part of the side group rather than as a part of a parent chain (in the example below, one sees that OH group takes priority over the SH group)!!!

3-mercapto-3-methyl-1-butanol

IUPAC Naming Sulfides (carbon compounds with an SR (R- some carbon group or alkyl group) Directions:

- 1. Make the larger of the -R groups the parent chain
- 2. Name the smaller of the -R groups as an alkylthio substituent

Example:

4,4-dichloro-1-(methylthio)cyclohexane

<u>COMMON NAMES OF SULFIDES (NOT IUPAC SYSTEM): The carbon group(s) are named as the substituent and the sulfur (S) is treated as the parent name (in this case, it's "sulfide").</u>

Directions:

- 1. Name each -R group
- 2. Arrange them alphabetically
- 3. End with the word, "sulfide"

Example:



diethyl sulfide

Note: Sulfides can be oxidized (keep in mind the names!!!)

#Treat naming as Common Naming: Use common naming directions above!!!

Example:

methyl phenyl sulfoxide

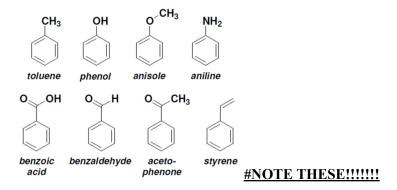
Nomenclature of Benzene Derivatives:

Parent name of monosubstituted derivatives: -benzene

Examples:



Many benzene derivatives have common names; for some compounds, the <u>COMMON NAME</u> becomes the <u>PARENT NAME!!!</u>



*If the substituent is LARGER than the ring, the substituent becomes the parent chain, and the benzene ring becomes a "phenyl" substituent!!!

Example:

<u>Xylene- Common Name for Dimethyl Benzene Derivatives</u>

Examples:

Ortho-substituents are on two adjacent carbons (at locants 1 & 2).

Meta-substituents are at locants 1 & 3.

Para- substituents are on opposite sides of the ring (at locants 1 & 4).

Directions:

1. Identify the parent chain (longest consecutive chain of carbons; usually, it's the aromatic ring); often a common name can be the parent chain!!!

- 2. Identify and name substituents
- 3. Number the parent chain & assign a locant (& a prefix if needed) to each substituent (<u>NOTE: A substituent that's part of the parent name MUST be assigned locant NUMBER 1!!!)</u>
- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).

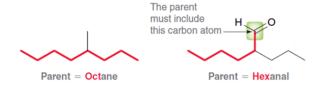
IUPAC Naming Aldehydes (carbon compounds with a carbonyl: O=CRH) Directions:

1. Identify the parent chain (INCLUDES THE CARBONYL GROUP). Also, the parent chain should replace the e with an "-al".

Example:

THE LARGEST PARENT CHAIN CONTAINING THE CARBON WITH A CARBONYL GROUP SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!

Example:



- 2. Identify & name the substituents (side groups)
- 3. Assign a locant or number (and prefix if needed) to each substituent.

#Notably, numbering the carbonyl group of the aldehyde takes priority over other groups!!!!



4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).

IUPAC Naming Ketones (carbon compounds with a carbonyl: O=CRR) Directions:

1. Identify the parent chain (INCLUDES THE CARBONYL GROUP). Also, the parent chain should replace the e with an "-one".

Example:



- 2. Identify & name the substituents (side groups)
- 3. Assign a locant or number (and prefix if needed) to each substituent.
- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The locant (showing where the C=O is located) is placed either just before the parent name or just before the -one suffix.

Example:



IUPAC Naming Carboxylic Acids (carbon compounds with a carboxyl: O=CROH) Directions:

1. Identify the parent chain (INCLUDES THE CARBOXYL GROUP). Also, the parent chain should replace the e with an "-oic acid".

Example:

butanoic acid

THE LARGEST PARENT CHAIN CONTAINING THE CARBON WITH A CARBOXYL GROUP SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!

- 2. Identify & name the substituents (side groups)
- 3. Assign a locant or number (and prefix if needed) to each substituent.

#Notably, numbering the carboxyl group of the carboxylic acid takes priority over other groups!!!!

4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).

NOTE: When the carboxylic acid group is attached to a ring, it's named as an alkane carboxylic acid. Example:

cyclohexane carboxylic acid

COMMON NAMES OF CARBOXYLIC ACIDS (NOT IUPAC SYSTEM):

Examples:

IUPAC Naming Dicarboxylic Acids (carbon compounds with 2 carboxyl groups: O=CROH)

Directions: #Basically the same way how one would go about naming a typical carboxylic acid, with exception to the suffix in the parent name: "-dioic acid"

Example:

COMMON NAMES OF DICARBOXYLIC ACIDS (NOT IUPAC SYSTEM):

Examples:

CARBOXYLIC ACID DERIVATIVES EXAMPLES:

Nitrile has the same oxidation state, it's also an acid derivative (though it doesn't have a carbonyl group).

Naming Carboxylic Acid Derivatives:

IUPAC ☐ From Carboxylic Acid to Acid Halide- replace "-ic acid" with "-yl halide"

Examples:

From Carboxylic Acid (with a ring attached) to Acid Halide- replace "-carboxylic acid" with "-carbonyl halide"

Example:

From Carboxylic Acid to Anhydride- replace "acid" with "anhydride"

Examples:

Naming Asymmetrical Anhydrides- List the acids alphabetically & replace the word "acid" with "anhydride".

Example:

acetic benzoic anhydride

From Carboxylic Acid to Ester- naming the alkyl group attached to the oxygen followed by replacing "-ic acid" with "-ate".

Examples:

From Carboxylic Acid (with a ring attached) to Ester- naming the alkyl group attached to the oxygen followed by replacing "carboxylic acid" with "carboxylate".

Example:

methyl cyclohexanecarboxylate

From Carboxylic Acid to Amide- naming the alkyl group attached to the oxygen followed by replacing "-ic acid" or "-oic acid" with "amide".

From Carboxylic Acid (with a ring attached) to Amide-replacing "carboxylic acid" with "carboxamide".

Example:

cyclohexanecarboxamide

NOTE: If the nitrogen atom of the amide group bears alkyl substituents, their names are placed at the beginning of the name with "N" as their locant.

Examples:

$$H_3C$$
 H_3C
 H_3C
 H_3C
 CH_3
 CH_3

From Carboxylic Acid to Nitrile- replace "-ic acid" or "-oic acid" with "-onitrile".

Examples:

$$H_3C$$
 \longrightarrow H_3C $-C \equiv N$ \longrightarrow OH \longrightarrow \longrightarrow OH \longrightarrow \longrightarrow OH \longrightarrow \longrightarrow OH \longrightarrow \longrightarrow \longrightarrow \longrightarrow OH \longrightarrow \longrightarrow \longrightarrow \longrightarrow \longrightarrow \longrightarrow \longrightarrow \longrightarrow

IUPAC Naming Primary Amines (NH2R) Directions:

Simple Primary Amines: Name the alkyl group in "yl" followed by the word "amine".

Examples:

Complex Primary Amines:

- 1. Identify the parent chain (INCLUDES THE NH2 GROUP). Also, the parent chain should end in "-amine". THE LARGEST PARENT CHAIN CONTAINING THE CARBON WITH AN NH2 GROUP SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE COMPOUND!!!
- 2. Identify & name the substituents
- 3. Assign a locant (and prefix if needed) to each substituent. Notably, the carbon containing the NH2 group should have the smallest number possible.
- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The NH2 group locant is placed either just before the parent name or just before the -amine suffix.

Example:

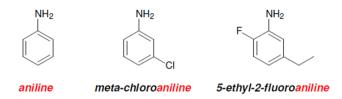
(2R,3R)-4,6-dimethyl-2-heptanamine

Amines as a Side Group: Use the term "amino".

Examples:

Note: If the amine is DIRECTLY attached to an aromatic ring, the parent chain MAY be called "aniline". #(Depends on the compound).

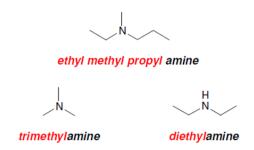
Examples:



IUPAC Naming Secondary Amines (NHR2) Directions:

Simple Secondary Amines: Name the alkyl groups ending in "yl", followed by the word "amine".

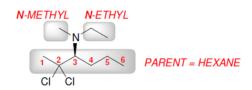
Examples:



Complex Secondary Amines:

- Identify the parent chain (INCLUDES THE NHR2 GROUP). Also, the parent chain should end
 in "-amine". THE LARGEST PARENT CHAIN CONTAINING THE CARBON WITH AN
 NHR2 GROUP SHOULD BE THE MAIN PARENT CHAIN WHEN NAMING THE
 COMPOUND!!!
- 2. Identify & name the substituents
- 3. Assign a locant (and prefix if needed) to each substituent. Notably, the carbon containing the NHR2 group should have the smallest number possible.
- 4. List the numbered substituents before the parent name in alphabetical order (ignore prefixes except the exceptions mentioned above).
- The NHR2 group locant is placed either just before the parent name or just before the -amine suffix. *(NOTE: Smaller groups attached to the amine should be named as alkyl groups with the N-locant).

Example:



(3S)-2,2-dichloro-N-ethyl-N-methyl-3-hexanamine