



CHEMISTRY 2500

Topic #2: Isomers and Naming Organic Molecules

Spring 2020

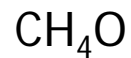
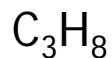
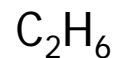
Dr. Susan Findlay



Isomers

- What happens when an organic molecule is simply described by its molecular formula?
 - In a few cases, the molecular formula gives enough information.

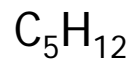
Draw:





Isomers

- Usually, molecular formula is not enough. Draw:
 C_4H_{10}



For practice, draw each of the molecules' structural formula then convert it to line-bond notation.



Isomers

- Molecules which have the same molecular formula but different connectivity are referred to as **constitutional isomers**. Constitutional isomers often behave differently due to their different shapes. In some cases, they even have different functional groups!
- Draw all of the constitutional isomers for C_3H_8O , and identify the functional group in each molecule.

For practice, draw each of the molecules' structural formula then convert it to line-bond notation.



Isomers

- Now we will add just one carbon atom... Draw all of the constitutional isomers for C_4H_8O .

If you Google this question, you'll find websites telling you there are 1, 5 or 15 structures. They're wrong. Be very careful asking the Internet for homework help... Please don't actually do this before class; you'll spoil the learning experience.



Isomers



Nomenclature (Naming Organic Molecules)

- When you have to draw a lot of isomers, one way to be sure that no two are the same is to name them all. If the names are different, the isomers are different. If the names are the same, you drew the same thing twice.
- Nomenclature also makes it easier for us to talk about organic chemistry in situations where we can't just draw the molecules.
- Nomenclature is described in detail in Ogilvie chapter 2. You are responsible for this information.

Organic Nomenclature

- Given the large number of organic compounds – many of which differ from each other only slightly, it is necessary to have a systematic method for naming organic compounds. IUPAC (International Union of Pure and Applied Chemistry) has devised such a system.
- Each name contains exactly enough information for us to draw exactly one organic compound.

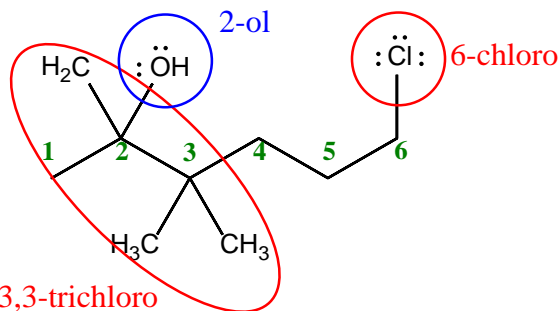
e.g.

6-chloro-2,3,3-trimethylhexan-2-ol

substituents

main chain/ring

principal functional group



Prefixes tell us how many of a particular substituent or functional group are present. Numbers tell us which carbon atom of the main chain/ring they're attached to. Punctuation counts!



Organic Nomenclature

- When drawing an organic molecule, we start with the main chain/ring. This is the chain/ring of carbon atoms that contains the principal functional group and all double/triple bonds (*if possible*). The following prefixes are used to indicate the length of the main chain/ring:

# C	Prefix
1	meth
2	eth
3	prop
4	but
5	pent

# C	Prefix
6	hex
7	hept
8	oct
9	non
10	dec

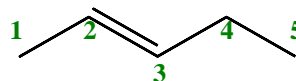
Thus, a linear alkane with 6 carbon atoms is hexane.

- If there is a main **ring** instead of a main chain, the prefix **cyclo** is added before the #carbons prefix.

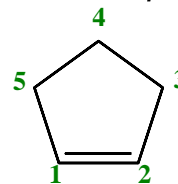
Thus, **cyclohexane** is an alkane with a **ring** of 6 carbon atoms.⁹

Organic Nomenclature

- Once we know the length of the main chain/ring, we need to know its saturation. Does it contain any C=C or C≡C bonds?
 - If not, the main chain/ring will end in **-ane** (*as in the examples on the previous page*).
 - If it contains a C=C bond, the main chain/ring will end in **-ene**.
 - If it contains a C≡C bond, the main chain/ring will end in **-yne**.
 - The main chain/ring is numbered starting at the end which gives the lower number to the principal functional group. The location of the first atom in each C=C or C≡C bond is indicated by a number.
- Thus, 2-pentene is a 5-carbon chain with a double bond between carbons 2 and 3:



- Cyclopentene is a 5-carbon ring with a C=C bond. No number is necessary because the double bond must, by definition, be between carbons 1 and 2:





Organic Nomenclature

- The principal functional group in an organic molecule is indicated by a suffix. If a molecule has two functional groups, the suffix corresponds to the higher priority functional group:

Functional Group	Suffix
Carboxylic acid	-oic acid
Sulfonic acid	-sulfonic acid
Ester*	-oate
Acid Chloride	-oyl chloride
Amide*	-amide
Nitrile	-nitrile
Aldehyde	-al
Ketone	-one
Alcohol (including phenol)	-ol
Thiol	-thiol
Amine	-amine

Note that ethers are not on this table because there is no suffix for ethers. Alkenes and alkynes are considered 'less important' than all functional groups in this table.

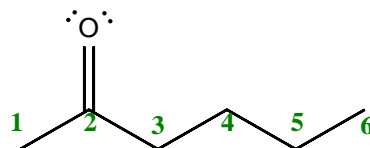
*Esters and amides have two 'halves' to be named.

For details on naming esters and/or amides, consult Sorrell p.702.

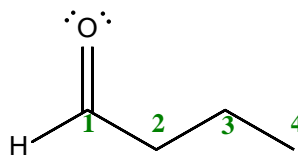
Organic Nomenclature

- As noted previously, the main chain/ring is numbered starting at the end which gives the lower number to the principal functional group. Where there would be any question, the location of the functional group is indicated by a number.

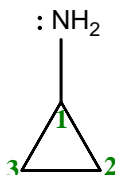
- Thus, 2-hexanone has a ketone at carbon 2:



- Butanal does not need a number because, by definition, the aldehyde is at carbon 1:

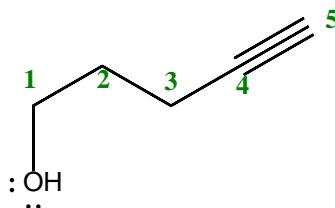


- Cyclopropanamine does not need a number because, by definition, the amine is at carbon 1:

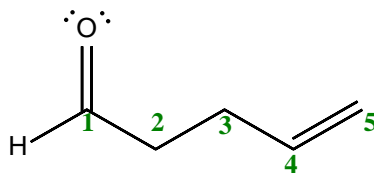


Organic Nomenclature

- If there is both a C=C or C≡C bond and another functional group, the functional group suffix goes at the end of the alkene/alkyne name with the location number immediately in front of it.
 - Thus, 4-pentyn-1-ol is a 5-carbon chain with an alcohol at carbon 1 and a triple bond between carbons 4 and 5:

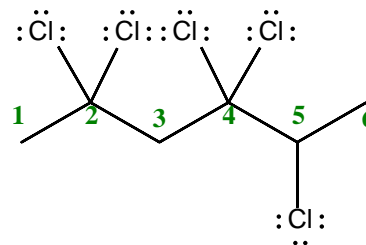


- 4-Pentenal is a 5-carbon chain with an aldehyde at carbon 1 (by definition) and a double bond between carbons 4 and 5:



Organic Nomenclature

- All of the examples thus far have been completely linear or a single ring. The final step in naming an organic compound is to list the substituents in alphabetical order at the front of the name. A number* is used to indicate the location of each substituent, and a prefix (di, tri, tetra, etc.) is used to group together multiple substituents of the same type.
- **If** there is no functional group or multiple bond, the main chain is numbered from the end giving the lower number to the first substituent. If it's the same number either way, the number of the second substituent is used as the tie-breaker (and so on until a difference is found).
- Thus, we have 2,2,4,4,5-pentachlorohexane not 2,3,3,5,5-pentachlorohexane:



*The nitrogen atom of an amine is "numbered" *N*. e.g. *N*-methylethanamine

Organic Nomenclature

- Substituents (including functional groups which were lower priority than the principal functional group):

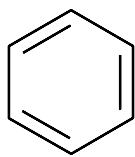
	Name
-CH ₃	methyl
-CH ₂ CH ₃	ethyl
-CH ₂ CH ₂ CH ₃	propyl
-CH ₂ CH ₂ CH ₂ CH ₃	butyl
etc.	
-CH(CH ₃) ₂	isopropyl
-CH ₂ CH(CH ₃) ₂	isobutyl
-CH(CH ₃)CH ₂ CH ₃	<i>s</i> -butyl
-C(CH ₃) ₃	<i>t</i> -butyl
-C ₆ H ₅	phenyl
-CH ₂ C ₆ H ₅	benzyl

	Name
-OCH ₃	methoxy
-OCH ₂ CH ₃	ethoxy
-OCH ₂ CH ₂ CH ₃	propoxy
-OCH ₂ CH ₂ CH ₂ CH ₃	butoxy
etc.	
-OCH(CH ₃) ₂	isopropoxy
-OCH ₂ CH(CH ₃) ₂	isobutoxy
-OCH(CH ₃)CH ₂ CH ₃	<i>s</i> -butoxy
-OC(CH ₃) ₃	<i>t</i> -butoxy
-OC ₆ H ₅	phenoxy
-OCH ₂ C ₆ H ₅	benzoyl

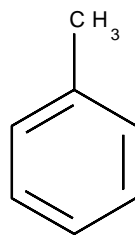
	Name
-F	fluoro
-Cl	chloro
-Br	bromo
-I	iodo
-NH ₂	amino
-NO ₂	nitro
-CN	cyano
-OH	hydroxy
=O	oxo
-SH	mercapto

Organic Nomenclature

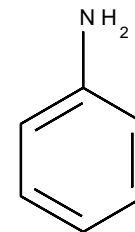
- Other names you should know:



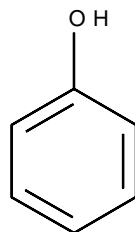
benzene



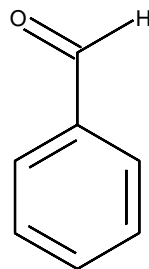
toluene*



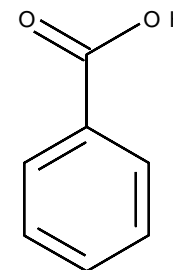
aniline*



phenol



benzaldehyde

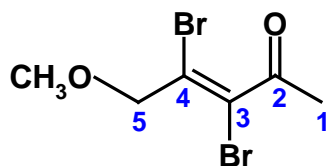
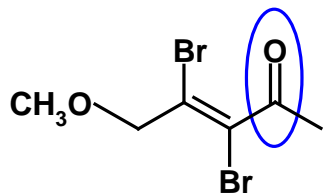


benzoic acid

* = not official IUPAC name but a very common name that you're likely to encounter

Organic Nomenclature

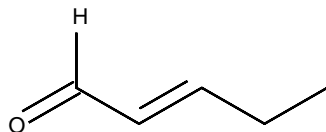
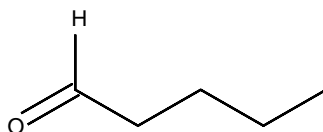
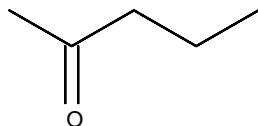
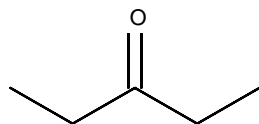
- In summary, to name an organic molecule, work back-to-front:



- Find the principal functional group.
- Find the longest chain (*or ring*) including the principal functional group and all double/triple bonds.
- Number the chain starting at whichever end gives the principal functional group the lower number. (*For a ring, start numbering at the principal functional group.*)
- Name the principal functional group, numbering if necessary. **-2-one**
- Name the main chain (*or ring*), numbering the C=C or C≡C bonds if necessary. If this gives a name in which the next letter after the 'e' of 'ane', 'ene' or 'yne' is a vowel, drop the 'e'. **-3-penten-2-one**
- Name and number the substituents on the main chain. If a substituent appears more than once, use a prefix to indicate how many there are and include a number for **each** appearance. List the substituents in alphabetical order (*not counting prefixes*) followed by the main chain (*or ring*) name. **3,4-dibromo-5-methoxy-3-penten-2-one**
- Finally, add *cis-* or *trans-* (or *E-* or *Z-* or *R-* or *S-*) to the front of the name if necessary. ***trans*-3,4-dibromo-5-methoxy-3-penten-2-one**

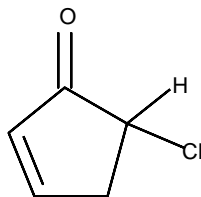
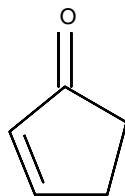
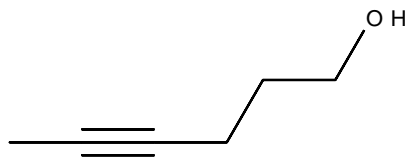
Organic Nomenclature

- And now for some practice... Name the following:

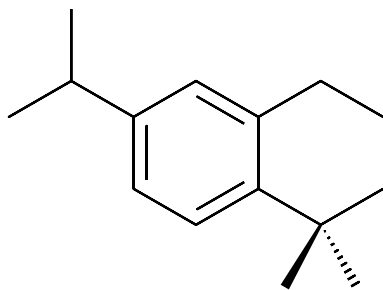
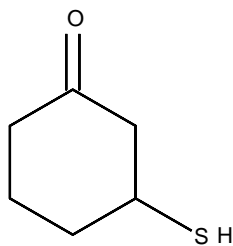
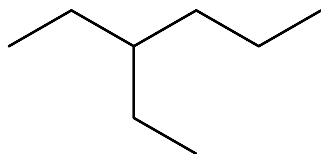


If you're not yet comfortable with line-bond structures, redraw each of these molecules as the structural formula first.

Organic Nomenclature

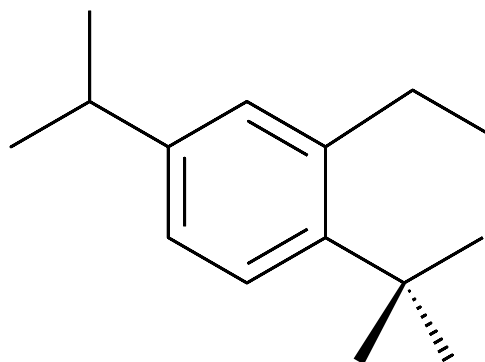


Organic Nomenclature



Classification of Carbon Atoms

- Carbon atoms are often classified according to how many other carbon atoms they are bonded to. In the last example on the previous page, there are examples of **primary**, **secondary**, **tertiary** and **quaternary** carbon atoms:

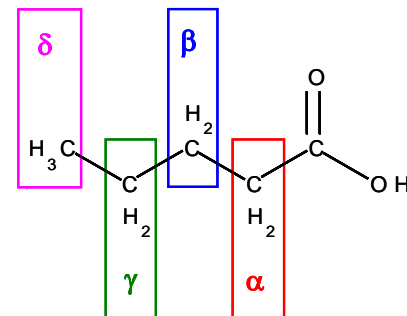


- These classifications only apply to saturated carbons (no multiple bonds). The carbon atoms that form the benzene ring are described as **aryl** to indicate that they are part of an aromatic ring. Other carbon atoms from double bonds are classified as **alkenyl** while those from triple bonds are classified as **alkynyl**. We will use this terminology throughout the course.

Classification of Carbon Atoms

- Occasionally, we also need to refer to carbon atoms (or other groups) in terms of distance from each other. For this purpose, Greek letters are used.
 - α refers to the atom attached to a group
 - β is the next atom
 - γ is the one after that
 - δ is the one after that
 - ϵ is the one after that
 - etc.

- In one example, the “group” of interest is a carboxylic acid, and the Greek letters refer to the carbon atoms:



- In another example, the “group” of interest is a carbocation, and the Greek letters refer to the hydrogen atoms:

