

Chemistry 2500

Chapter 2 Anatomy of an Organic Molecule (sections 2.1-2.5)



- The structure of an organic molecule is the source of its chemical behaviour and physical properties.
- As such, molecules that share structural features also share properties.



• A line structure diagram shows the key features of an organic molecule and emphasizes the particular parts that contribute to its reactivity and physical properties.





- The hydrocarbon portion of most organic compounds does not typically participate in chemical reactions. Rather, the chemical reactions happen primarily through the *functional groups*.
- Functional groups contain reactive bonds and non-bonded electrons.
 - The electronegativity difference between their atoms is an important element of chemical reactivity as is the bonding patterns between their atoms.
- C-H and C-C sigma bonds constitute the hydrocarbon parts of a molecule. These bonds are strong and difficult to break. Hydrocarbon units are therefore generally unreactive and function primarily as a scaffold that holds the functional groups together.

- Molecules and parts of molecules that do not contain rings and have only single bonds connecting the atoms are known as *saturated* molecules. Such structures have the maximum number of hydrogen atoms allowed by the valency of the other atoms in the structure.
- Molecules that have either a ring or double or triple bonds are known as *unsaturated* molecules.





- Most organic molecules contain functional groups groups of one or more atoms whose structure confers a particular pattern of reactivity.
- Functional groups tend to have predictable reactivities due t the pattern of connection among their atoms.
- Functional groups can be identified by two main features:
 - π bonds
 - heteroatoms

π bonds

- There are four type of hydrocarbon functional groups:
 - Alkanes (carbon-carbon single bonds)
 - Alkenes (carbon-carbon double bonds)
 - Alkynes (carbon-carbon triple bonds)
 - Aromatics (ring structures with alternating patterns of single and double bonds)



Heteroatoms

- Recall that a heteroatom is any atom other than carbon or hydrogen.
- Typical heteroatoms have one or more non-bonded pairs of electrons that can participate in reactions.



Heteroatoms

- Most organic molecules contain more than one functional group and exhibit behaviours that can be attributed to all of those groups.
- By understanding *how* reactivity patterns are tied to a molecule's structure, predictions can be made about the kinds of reactions that any organic molecule will undergo.







- The physical properties of a substance are determined by the distribution of electrons about the molecule.
- The distribution of electrons generates *intermolecular forces* between organic molecules.
- Organic molecules that are close to each other exhibit attractive forces toward each other that are collectively strong enough to impart important properties, including its melting point, boiling point, and its solubility.
- Organic molecules interact with each other by means of 4 types of intermolecular forces:
 - Electrostatics
 - dipole-dipole interactions
 - Hydrogen bonding
 - London forces

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Intermolecular Forces

- Intermolecular forces result from charge interactions; opposite charges attract and like charges repel.
- The distribution of electrons in a molecule produces areas of high electron density (- charge areas) and areas of low electron density (+ charge areas).
- An electrostatic potential map uses a colour spectrum to represent the likelihood of finding electrons at any point around a molecule.





electron-rich



- The positive regions of one molecule are attracted to the negative regions of neighbouring molecules, and vice versa.
- The strength of such attractions depends on the number and size of the charges involved.
- Larger charges or more interactions bind molecules together tightly, whereas small charges or fewer interactions lead to weaker intermolecular forces.



Electrostatic Interactions

- *Electrostatic* interactions take place between functional groups that have full formal charges.
- These interactions represent the strongest type of intermolecular forces between molecules and result in ionic structures.





Dipole-Dipole Interactions

- *Dipole-dipole* interactions result from attractive forces between the negative end of the permanent dipole in a molecule and the positive end of a permanent dipole in a neighbouring molecule.
- Dipoles are possible whenever there is a significant electronegativity difference between atoms in a functional group.



Oxygen is more electronegative, so electrons in the carbon-oxygen bond spend more time around oxygen which becomes slightly negative.

Carbon is less electronegative, so electrons in the carbon-oxygen bond spend less time around carbon which becomes slightly positive.

Dipole-Dipole Interactions



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Hydrogen Bonding

- *Hydrogen bonding* is a special kind of dipole-dipole interaction that is possible for groups with very electronegative atoms bonded to hydrogen atoms.
- This interaction is very important in the case of –OH and –NH groups.



London Forces (Dispersion Forces)

- *London forces* are attractive interactions that exist between all molecules in close proximity. They are the result of small temporary dipoles induces in each molecule by the other.
- London forces are generally the weakest of the intermolecular forces. The strength of these interactions usually depends on the amount of surface area contact between the groups involved.











- The structure of an organic molecule determines what intermolecular forces the molecule is capable of, and so a molecule's structure controls its physical properties.
- A critical examination of structure can lead to predictions of molecular properties and behaviour.
- The greater the intermolecular forces, the more difficult it is to separate molecules from each other, and therefore more energy is required to do so.
- The melting point or boiling point of a substance provides a measure of the amount of energy required to separate molecules.



• When London forces are dominant, large surface areas and many contact points will typically increase the melting/boiling point.





• The greater the polarity of the functional group, the stronger the dipoledipole interactions which will generally increase the melting/boiling point. Hydrogen bonding in particular provides very strong intermolecular interactions.

Boiling point (°C)



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• Electrostatics, the strongest intermolecular force, has a large influence on melting/boiling point values.

	Melting point (°C)	Boiling point (°C)		
о Н	-125	21		
OH	-114	78		
ОН	16.2	117		
O ↓ O Na	>300	N/A		



- The solubility of a molecule is governed by the type and strength of the intermolecular forces between molecules of a *solvent* and molecules of a *solvent* and molecules of a *solute*, the material that is dissolved.
- Organic solvents can be classified into three families according to the type of intermolecular forces they can create:
 - Polar protic solvents (hydrogen bond donors)
 - Polar aprotic solvents (strong dipoles, most act as hydrogen bond acceptors)
 - Non-polar solvents (mostly London forces)
- The general rule of thumb is that 'likes dissolve likes'. That is, polar solvents tend to dissolve polar molecules, and non-polar solvents will dissolve non-polar molecules.

Common organic solvents:

Polar protic solvents

н^{́О}́Н H^OCH₃ methanol water

H^OCH₂CH₃ ethanol

Polar aprotic solvents

⊂_N_CH₃

H₃C⁻CH₃

acetone

DMF (dimethylformamide)

ĊHa

DMSO (dimethylsulfoxide)

Polar solvents

H₃C^IO^{CH₂CH₃}

CHCl₃

THF

ethyl acetate

benzene

chloroform

Non-polar solvents

.0.

ether



- Water, being highly polar, presents a special situation for organic compounds.
- Although some organic compounds are soluble in water, the vast majority are not.
- Non-polar molecules such as hydrocarbons do not dissolve in water. These molecules are referred to as *hydrophobic* (water fearing).
- Water solubility increases as the number of polar groups on a molecule increases. These molecules are said to be *hydrophilic* (water loving).

- The degree to which an organic compound dissolves in water is governed by the relative proportion of its hydrophobic and hydrophilic regions.



- Branching creates less surface area thus allowing water to hydrogen bond with itself. Therefore, branched organic molecules are more soluble than their equivalent linear counterparts.
- Charged molecules can interact with water by electrostatics and often show significant water solubility.



The Functional Groups









Organic Nomenclature



Systematic IUPAC Nomenclature – Compound names have four fields.



•The first field includes the names and positions of substituents.

- •The second field contains the compound root word (longest carbon chain).
- •The third field indicated the saturation index (single or multiple bonds).
- •The fourth field defines the principal functional group (drop the terminal 'e' from the saturation index and add the appropriate suffix).

Compound Root – Second Field



the compound root name is based on the number of carbon atoms in the longest continuous chain or ring.

n	C_nH_{2n+2}	alkane
1	CH ₄	meth-ane
2	CH ₃ CH ₃	eth-ane
3	CH ₃ CH ₂ CH ₃	prop-ane
4	CH ₃ (CH ₂) ₂ CH ₃	but-ane
5	CH ₃ (CH ₂) ₃ CH ₃	pent-ane
6	CH ₃ (CH ₂) ₄ CH ₃	hex-ane
7	$CH_3(CH_2)_5CH_3$	hept-ane
8	CH ₃ (CH ₂) ₆ CH ₃	oct-ane
9	CH ₃ (CH ₂) ₇ CH ₃	non-ane
10	CH ₃ (CH ₂) ₈ CH ₃	dec-ane

For cyclic molecules, the prefix ' cyclo' is added before the compound root prefix.



Saturation Index – Third Field

The presence of multiple bonds is indicated by "ene" (carbon-carbon double bonds) and/or "yne" (carbon-carbon triple bonds) in the third field of the name •hexane



•1-hexene (or hex-1-ene)

•1-hexyne (or hex-1-yne)

When a *principal* functional group is not present, number the chain to give the multiple bond the lowest number. If there are multiple multiple bonds, add the prefix di, tri, tetra, etc to indicate the number of double or triples bonds in the molecule and give a number to indicate its position.

•1,3-hexadiene (or hexa-1,3-diene)

•1,5-hexadiene (or hexa-1,5-diene)

•1-hexen-3-yne (or hex-1-en-3-yne)

•1-hexen-5-yne (or hex-1-en-5-yne)

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- •1-hexen-3-yne (or hex-1-en-3-yne)
- •1-hexen-5-yne (or hex-1-en-5-yne)

Substituents – First Field

Substituents are structural elements (often functional groups) that are not part of the longest chain, but attached to it. Substituents appear first in a name and are numbered with respect to their position. Substituents take last priority when numbering the main chain. Substituents are listed *alphabetically* and their location indicated by a number. Multiples of the same substituent are numbered *and* indicated by a prefix (di, tri, tetra, penta, etc).

•5-chloro-1-hexene (or 5-chlorohex-1-ene)

•4,5-dichloro-5-fluoro-1-hexene (or 4,5-dichloro-5-fluorohex-1-ene)



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2 4 3 5 ;cl:

•4,5-dichloro-5-fluoro-1-hexene (or 4,5-dichloro-5-fluorohex-1-ene)



Principal Functional Groups – Fourth Field

A Principal Functional Group will always take priority when numbering the main chain (followed by multiple bonds followed by substituents). The following table lists the Principal Functional Groups that you are responsible for in Chem 2500. They are listed in order of highest priority down to lowest priority.

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 certain functional groups are never considered as a principal functional group and are always treated as a substituent. These include the halogens, ethers, and nitro groups.

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Principal Functional Groups – Fourth Field

There can only be one Principal Functional Group in a molecule. The functional group with the highest priority according to the previous table is named as the principal functional group and all others are named as substituents.



•5-chloro-1-hexen-3-ol (or 5-chlorohex-1-en-3-ol)

•2-chloro-5-hexen-1-ol (or 2-chlorohex-5-en-1-ol)

•2-chloro-4-hydroxy-5-hexenal (or 2-chloro-4-hydroxyhex-5-enal)

Note that no number is necessary for principal functional groups that must be terminal because they include the first carbon atom of the main chain.

Principal Functional Groups – Fourth Field

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Nomenclature Formatting

• any stereochemistry (cis/trans, R/S) is placed in front of the name.

e.g. trans-3,4-dibromopent-3-en-2-one

- numbers and letters are separated by hyphens.
- numbers are separated by comas.

e.g. 2-chloro-3-isopropylhex-5-enal

- substituents are listed alphabetically.
- prefixes such as di-, or tri- are not used alphabetically and neither do italicized letters such as *s*-butyl or *t*-butyl.
 - e.g. 4,4-dichloro is 'c' alphabetically

2,2,6-tribromo is 'b' alphabetically

3-*tert*-butyl is 'b' alphabetically

isopropyl is 'i' alphabetically

The priority to determining the numbering of your chain or ring is always as follows:

1. Principal Functional group

- 2. Saturation
- 3. Substituents (lowest series of numbers)
- 4. Alphabetical



Organic Nomenclature Summary:

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

– Find the principal functional group.



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* to the front of the name if necessary.

trans-3,4-dibromo-5-methoxy-3-penten-2-one



Substituent List

Below is a list of all substituents that you are responsible for in Chem 2500.



	Name		Name		Name
-CH ₃	methyl	-OCH ₃	methoxy	-F	fluoro
-CH ₂ CH ₃	ethyl	-OCH ₂ CH ₃	ethoxy	-Cl	chloro
-CH ₂ CH ₂ CH ₃	propyl	-OCH ₂ CH ₂ CH ₃	propoxy	-Br	bromo
-CH ₂ CH ₂ CH ₂ CH ₃	butyl	-OCH ₂ CH ₂ CH ₂ CH ₃	butoxy	-I	iodo
etc.		etc.			
				-NH ₂	amino
-CH(CH ₃) ₂	isopropyl	-OCH(CH ₃) ₂	isopropoxy	-NO ₂	nitro
-CH ₂ CH(CH ₃) ₂	isobutyl	-OCH ₂ CH(CH ₃) ₂	isobutoxy	-CN	cyano
- CH(CH ₃)CH ₂ CH ₃	<i>s</i> -butyl	- OCH(CH ₃)CH ₂ CH ₃	s-butoxy		
-C(CH ₃) ₃	<i>t</i> -butyl	-OC(CH ₃) ₃	<i>t</i> -butoxy	-OH	hydroxy
-C ₆ H ₅	phenyl	-OC ₆ H ₅	phenoxy	=0	охо
-CH ₂ C ₆ H ₅	benzyl	-OCH ₂ C ₆ H ₅	benzoxy	-SH	mercapto

Naming Carbon-Based Substituents







Notice that the only difference between n-propyl and isopropyl is the *point of attachment*.





Again, notice that the only difference is the *point of attachment*.





Other names you need to know...



Molecules with this substructure are treated as a class – arenes.



*these are not IUPAC names but common names that you should know.

Aryl based Substituents





Name the following molecules







Name the following molecules









Name the following molecules







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