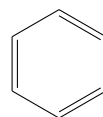


## Chapter 2 - Families of Carbon Compounds

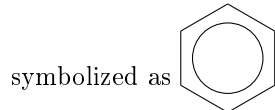
### 2.1 - Hydrocarbons: Representative Alkanes, Alkenes, Alkynes, and Aromatic Compounds

- **Hydrocarbons** are compounds that contain only hydrogen and carbon
- **Alkanes** are hydrocarbons that are entirely composed of single bonds, C—C, between carbon atoms (members of this family have suffixes of -ane)
- **Alkenes** contain at least one C=C bond (members of this family have suffixes of -ene)
- **Alkynes** contain at least one C≡C bond (members of this family have suffixes of -yne)
- **Aromatic compounds** contain a special type of ring, the most common being a benzene ring
- Compounds with only single bonds are known as **saturated compounds** because they contain a maximum number of hydrogen
- Compounds with multiple bonds are known as **unsaturated compounds** because they contain fewer than the maximum possible number of hydrogen atoms

- A benzene ring using the so-called **Kekulé structure** is indicated as



- The Kekulé structure is not accurate because of the resonance nature of benzene. A correct hybrid is



- As a result, all of the carbon-carbon bonds are 1.5 bonds, have a bond length in between that of a single and double bond, and have a bond angle of 120°
- The six electrons associated with the *p* orbitals that have overlapping lobes above and below the ring are said to be **delocalized** about the six carbon atoms in benzene

### 2.2 - Polar Covalent Bonds

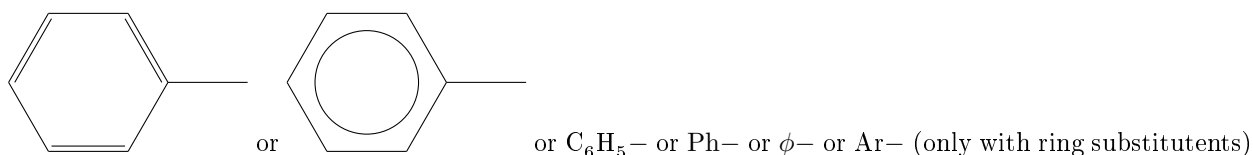
- A complete transfer of electrons, unlike the shared nature of a covalent bond, produces an **ionic bond**
- If an electronegativity difference exists between two bonded atoms, and they are not large enough to produce an ionic bond, the electrons are not shared equally and produce a **polar covalent bond**
- **Electronegativity** is simply the ability of an atom to attract electrons that it is sharing in a covalent bond
- If there is a partial charge ( $\delta +$  or  $\delta -$ ) on an atom, the molecule ends up having a **dipole moment** and is said to be a **dipole**
- The direction of polarity of a polar bond can be symbolized by  $\text{---}\rightarrow$  with the cross being the positive end and the arrow head being the partially negative end
- The definition of the dipole moment is  $\mu = e \times d$ , where  $\mu$  is the dipole moment,  $e$  is the electric charge, and  $d$  is distance
- One **debye** is a convenient dipole moment unit with an equivalent value of  $1 \times 10^{-18} \text{ esu cm}$
- **Functional groups** are defined groups of atoms in a molecule that give rise to the function of the molecule, and, many times, polar covalent bonds composed these groups
- Atoms that form covalent bonds and have unshared electron pairs, such as oxygen, nitrogen, and sulfur, are known as **heteroatoms**
- A **map of electrostatic potential (MEP)** can help visualize the distribution of charge in a molecule with negative regions colored red and positive regions colored blue

### 2.3 - Polar and Nonpolar Molecules

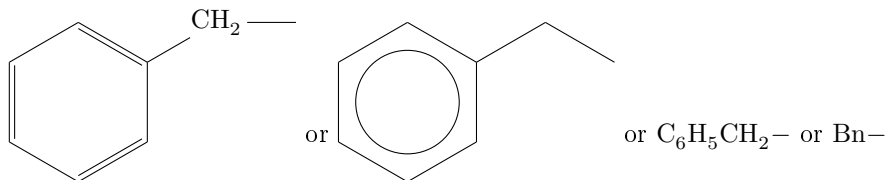
- A molecule with a dipole moment is known as a **polar molecule**
- Of course, a molecule can have polar covalent bonds and still be nonpolar due to symmetry in its molecular geometry

### 2.4 - Functional Groups

- **Alkyl groups** are the functional groups that we identify for purposes of naming compounds if a hydrogen atom is removed from the alkane (eg: For ethane,  $\text{CH}_3\text{CH}_3$ , the alkyl group is ethyl,  $\text{CH}_3\text{CH}_2-$ , with an abbreviation of Et-)
- For propane,  $\text{CH}_3\text{CH}_2\text{CH}_3$ , there is a propyl group of  $\text{CH}_3\text{CH}_2\text{CH}_2-$  if a hydrogen is taken off of the end of the chain, but a hydrogen atom can be taken off from the middle to make an isopropyl group
- When a benzene ring is attached to some other group of atoms it is called a **phenyl group** and can be represented by one of the following ways:



- The combination of a phenyl group and a **methylene group** ( $-\text{CH}_2-$ ) is called a **benzyl group**, which can be written in the following ways:



### 2.5 - Alkyl Halides or Haloalkanes (RX)

- Alkyl halides, or **haloalkanes**, are compounds in which a halogen atom replaces a hydrogen atom of an alkane
- If the carbon atom that bears the halogen is attached to only one other carbon, the carbon atom is said to be a **primary carbon atom** with the alkyl halide being classified as a **primary alkyl halide** ( $1^\circ$ )
- If the carbon that bears the halogen is attached to two other carbon atoms, it is the **secondary carbon** of a **secondary alkyl halide** ( $2^\circ$ )
- If the carbon that bears the halogen is attached to three other carbon atoms, then it is the **tertiary carbon** of a **tertiary alkyl halide** ( $3^\circ$ )

### 2.6 - Alcohols

- An **alcohol** has the functional group known as a hydroxyl group,  $-\text{OH}$ , that attaches to an  $sp^3$ -hybridized carbon atom
- In an analogous method described previously with the alkyl halides, alcohols can be classified into a primary alcohol, secondary alcohol, or tertiary alcohol

### 2.7 - Ethers

- **Ethers** have the general formula of  $\text{R}-\text{O}-\text{R}'$  where the two groups are composed of different alkyl (or phenyl) groups
- The bond angle at the oxygen atom of an ether is only slightly larger than that of  $\text{H}_2\text{O}$

## 2.8 - Amines

- **Amines** have the functional group of  $\text{-NH}_2$ ,  $\text{-NH}$ , or  $\text{-N}$  depending on the type of amine
- The classification of primary, secondary, or tertiary amine is different from alcohols and alkyl halides and, instead, refers to the number of organic groups that are attached to the nitrogen atom
- If there is only one organic group, the amine is primary and has a general functional group of  $\text{-NH}_2$
- If there are two organic groups attached to the nitrogen atom, the amine is secondary and has a general functional group of  $\text{-NH}$
- If there are three organic groups attached to the nitrogen atom, the amine is tertiary and has a general functional group of simply  $\text{-N}$
- Amines, like ammonia, have a trigonal pyramidal shape with a bond angle of  $108.7^\circ$

## 2.9 - Aldehydes and Ketones

- An **aldehyde** can be classified as  $\text{R}-\overset{\text{O}}{\underset{\text{H}}{\text{C}}}$  while a **ketone** can be classified as  $\text{R}-\overset{\text{O}}{\underset{\text{R}'}{\text{C}}}$
- Both aldehydes and ketones have the **carbonyl group**, which is the carbon atom double-bonded to the oxygen ( $\text{C=O}$ )
- The carbonyl group of an aldehyde is bonded to one hydrogen atom and one carbon atom except for formaldehyde, which is the only aldehyde bearing two hydrogen atoms (so, R equals H)
- The carbonyl group of a ketone is bonded to two carbon atoms
- The bond angles of the carbonyl group in aldehydes and ketones are close to that of a normal trigonal planar geometry with two  $121^\circ$  angles for the  $\text{R}-\overset{\text{O}}{\underset{\text{H}}{\text{C}}}$  angles and one  $118^\circ$  for the  $\text{R}-\text{C}-\text{H}$  or  $\text{R}-\text{C}-\text{R}'$  bond

## 2.10 - Carboxylic Acids, Esters, and Amides

- **Carboxylic acids** have a carboxyl group, which is represented as  $\text{-COOH}$ , since it comes from the carbonyl group and a hydroxyl group
- Carboxylic acids thus are classified as  $\text{RCOOH}$
- **Esters** have the general formula of  $\text{RCOOR}'$  with a carbonyl group bonded to an alkoxyl group ( $\text{-OR}$ )
- Esters can be produced from the reaction of a carboxylic acid and an alcohol through the acid-catalyzed loss of a molecule of water with the OH taken from the carboxylic acid and the other H taken from the alcohol

Example:  $\text{CH}_3\text{COOH} + \text{HOCH}_2\text{CH}_3 \longrightarrow \text{CH}_3\text{COOCH}_2\text{CH}_3 + \text{H}_2\text{O}$

- **Amides** have a carbonyl (look for that  $\text{C=O}$ ) group bonded to a nitrogen atom bearing hydrogen and/or alkyl groups and therefore have the possible general formulas of  $\text{RCONH}_2$ ,  $\text{RCONHR}'$ , and  $\text{RCONR}'\text{R}''$

## 2.11 - Nitriles

- A **nitrile** has a cyanide group attached to the carbon to make a general formula of  $\text{R-CN}$  with linear  $sp$ -hybridization
- With nitriles, the carbon atom of the  $\text{-C}\equiv\text{N}$  group is carbon number 1
- Acetonitrile is the common name for  $\text{CH}_3\text{CN}$ , and acrylonitrile is the common name for  $\text{CH}_2=\text{CHCN}$
- Nitriles are normally named by adding the suffix *-nitrile* to the name of the corresponding hydrocarbon
- Cyclic nitriles are named by adding the suffix *-carbonitrile* to the name of the ring system to which the  $\text{-C}\equiv\text{N}$  group is attached.
- Benzonitrile is the common name for  $\text{C}_6\text{H}_5\text{CN}$

## 2.12 - Summary of Important Families of Organic Compounds

Alkane	Alkene	Alkyne	Aromatic	Haloalkane	Alcohol	Ether
$\text{C}-\text{H}$ and $\text{C}-\text{C}$ bonds	$\text{C}=\text{C}$	$\text{C}\equiv\text{C}$	Aromatic ring	$\text{C}-\ddot{\text{X}}:$	$\text{C}-\ddot{\text{O}}\text{H}$	$\text{C}-\ddot{\text{O}}-\text{C}$
$\text{RH}$	$\text{RCH}=\text{CH}_2$ $\text{RCH}=\text{CHR}$ $\text{R}_2\text{C}=\text{CHR}$ $\text{R}_2\text{C}=\text{CR}_2$	$\text{RC}\equiv\text{CH}$ $\text{RC}\equiv\text{CR}$	$\text{ArH}$	$\text{RX}$	$\text{ROH}$	$\text{ROR}$

Amine	Aldehyde	Ketone	Carboxylic Acid	Ester	Amide	Nitrile
$\text{C}-\text{N}:$	$\text{C}(=\text{O})\text{H}$	$\text{C}(=\text{O})\text{C}$	$\text{C}(=\text{O})\text{OH}$	$\text{C}(=\text{O})\text{O}-\text{C}$	$\text{C}(=\text{O})\text{N}$	$\text{C}\equiv\text{N}:$
$\text{RNH}_2$ $\text{R}_2\text{NH}$ $\text{R}_3\text{N}$	$\text{RCHO}$	$\text{RCOR}'$	$\text{RCOOH}$	$\text{RCOR}'$	$\text{RCNH}_2$ $\text{RCNHR}'$ $\text{RCNRR}'\text{R}''$	$\text{RCN}$

## 2.13 - Physical Properties of Molecular Structure

- The **melting point** of a substance is the temperature at which an equilibrium exists between the well-ordered crystalline state and the more random liquid state
- The **ion-ion forces** of an ionic compound are the strong electrostatic lattice forces that act between the positive and negative ions in the solid state (therefore, ionic substances have higher melting points)
- The **boiling points** of ionic compounds are also higher than covalent compounds and oftentimes decompose before they are able to boil<sup>1</sup>
- Intermolecular forces (IMFs) that are dispersion forces are also referred to as **van der Waals forces**
- **Dipole-Dipole Forces** are due to a permanent dipole moment resulting from a nonuniform distribution of bonding electrons in polar molecules
- **Hydrogen bonding** is a very strong dipole-dipole force between hydrogen atoms bonded to oxygen, nitrogen, or fluorine and nonbonding electron pairs on other such electronegative atoms
- Since H-bonding is a strong IMF, it raises the boiling point of water, which is why it's a liquid at STP
- The compactness and rigidity of individual molecules can affect melting point
- Molecules that are symmetrical have abnormally high melting points
- **(London) Dispersion forces** can be thought of as an instantaneous dipole moment that can induce other dipole moments in neighboring molecules
- The more polarizable a molecule is, the larger dispersion forces it has since it can have a larger instantaneous dipole moment
- Large atoms are easily polarizable and small atoms are not. Also, atoms with unshared electron pairs are more polarizable than atoms with only bonding pairs
- Molecules that are longer, flatter (think long chains), or cylindrical have more surface area and thus have larger dispersion forces

<sup>1</sup>Be careful when distinguishing boiling point and solubility. For instance, consider ethanol and decanol. The solubility (in water) of ethanol will be higher due to a more polar structure. However, decanol will have a higher boiling point due to a larger overall structure causing much more London Dispersion forces.

- The **boiling point** of a liquid is the temperature at which the vapor pressure of the liquid equals the pressure of the atmosphere above it
- If pressure is reduced then boiling point is subsequently reduced
- Heavier molecules boil at higher boiling points because it takes more kinetic energy to get them to the speed at which they separate from one another to form a gas
- The **solubility** of a solid substance is how well it dissolves in a liquid
- Water dissolves solute particles by **hydrating** or **solvating** the ions due to its high polarity (large **ion-dipole forces**<sup>2</sup>)
- **Hydrophobic** means incompatible with water while **hydrophilic** means compatible with water (“like-dissolves-like”)
- The **hydrophobic effect** is when a hydrocarbon chain, for instance, with a large hydrophobic portion does not dissolve in a polar solvent even though it has a hydrophilic functional group like  $\text{—OH}$
- The reason for the hydrophobic effect is that there is an **unfavorable entropy change** because water must become more ordered around the hydrocarbon chain in order to solvate it, and this goes against the favorable entropy flow of the universe
- With soaps and detergents there is a long hydrophobic chain with a strong hydrophilic group at the end of the chain. The long chain embeds itself in the oily layer of what we wash while the hydrophilic ion portion attract the polar water molecules
- A substance is considered soluble in water if at least  $3\text{ g}$  of the organic compound dissolves in  $100\text{ mL}$  of water
- Compounds with one to three carbon atoms are water soluble if the compound has only one hydrophilic group. Compounds with four to five carbons are borderline, and compounds with six or more carbons are insoluble

## 2.14 - Summary of Attractive Forces

- Here are the IMFs in order of increasing strength: London Dispersion, Dipole-Dipole, Hydrogen Bonding, Ion-Dipole, Covalent Bonds

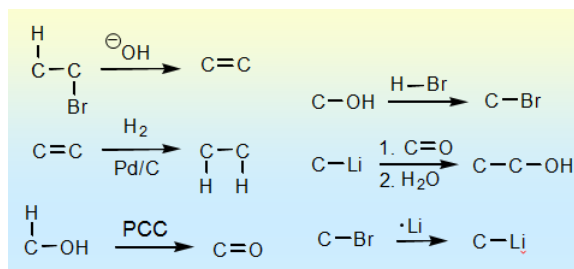
## Degrees of Unsaturation

- A degree of unsaturation is either  $\pi$  bond or a ring structure

Formula:  $\frac{2C + 2 + N - H - X}{2}$  where the variables are carbons, nitrogens, hydrogens, and halogens, respectively

## Synthesis

- There is a so-called “library” of organic reactions that are given on every exam. They are, for reference, as follows:



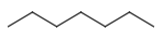
- To create a synthesis reaction, one starts with the desired product and works backward

\*The procedure is best explained using examples, so a few are shown on the following page.

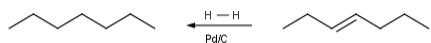
<sup>2</sup>An ionic compound forms with an electronegativity difference between atoms of  $> 1.7$ . Polar bonds are for differences of  $0.5 - 1.7$ , and a nonpolar bond is for differences  $< 0.5$

Synthesis Example 1: Synthesize heptane from reactants containing four carbon atoms or less

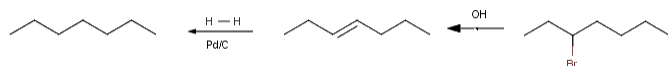
Step 1: Draw the structure of heptane



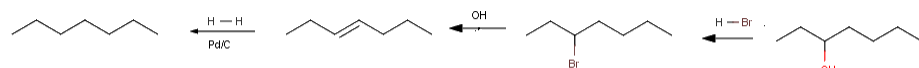
Step 2: Fill in the first reaction



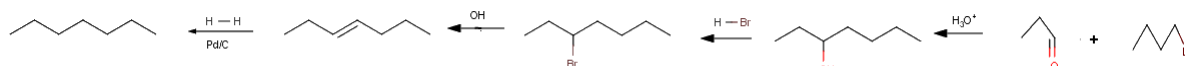
Step 3: Fill in the next reaction



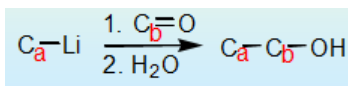
Step 4: Fill in the next reaction

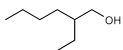


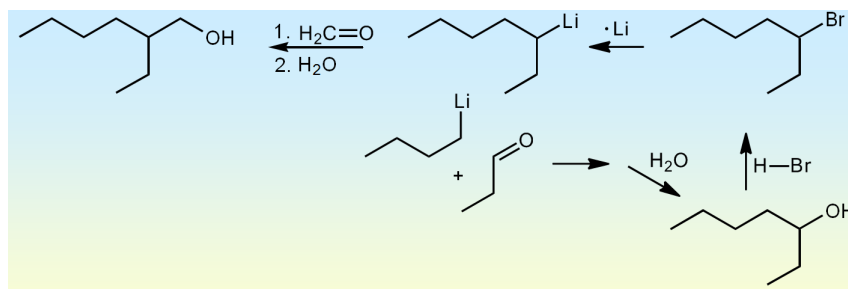
Step 5: Fill in the next reaction



\*Note: The only “tricky” reaction is the one involving the carbonyl group and the hydronium ion addition. For this, be careful of where to cut the molecule, and try to cut it efficiently because this “cutting” reaction can be done differently. Also, the carbon attached to the hydroxide group in the product side comes from the C=O carbon. To keep track of the carbons, they should be as follows<sup>3</sup>:



Synthesis Example 2: Synthesize  from reactants containing four carbon atoms or less



<sup>3</sup>The C=O over the reaction arrow simply represents a carbonyl group. It does not mean that *just* a C=O is added. Also, if the carbonyl group molecule is written out structurally, do not write it over the arrow.