**Nuggets:** Drawing Organic Molecules, Functional Groups Part I, Naming organic molecules

### FUNCTIONAL GROUPS (Part I)

<table>
<thead>
<tr>
<th>Functional Group</th>
<th>Suffix</th>
<th>Formula</th>
<th>Other Important Info</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alkane</td>
<td>ane</td>
<td>C–C</td>
<td>saturated; tetrahedral; sp$^3$; $C_nH_{2n+2}$; free rotation around C–C $\sigma$-bond (see page 3 for naming examples)</td>
</tr>
<tr>
<td>Alkene</td>
<td>ene</td>
<td>C=C</td>
<td>unsaturated; trigonal planar; 120˚; sp$^2$; $C_nH_{2n}$; geometric isomers (cis/trans); alkene has a $\sigma + \pi$ bond in the double bond; can’t rotate thru C=C $\rightarrow \pi$ bond;</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Naming: e.g., trans-4-methyl-2-pentene</td>
</tr>
<tr>
<td>Alkyne</td>
<td>yne</td>
<td>C≡C</td>
<td>unsaturated; linear; sp; 180˚; $C_nH_{2n-2}$; $\sigma + 2\pi$ bonds in the triple bond; can’t rotate</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Naming: e.g., 4-methyl-1-pentyne</td>
</tr>
<tr>
<td>Cyclic</td>
<td>cyclo + (ane, ene, or yne)</td>
<td></td>
<td>cycloalkane: unsaturated, strained tetrahedral, sp$^3$; $C_nH_{2n}$; not planar</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Naming: e.g., 1,3-dichlorocyclopentane</td>
</tr>
<tr>
<td>Aromatic</td>
<td>benzene</td>
<td>$C_6H_6$</td>
<td>planar; triangular planar geometry at each C; sp$^2$ at each C; 120˚; resonance</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Naming: e.g., 1-bromo-3-chlorobenzene</td>
</tr>
</tbody>
</table>

**Hydrocarbon (H and C only) Functional Groups**

- **Alkanes:** only C–C single bonds = $\sigma$ bonds; **formula:** $C_nH_{2n+2}$; often denoted as “R”; C–C single bond **can rotate**; saturated molecules; **saturated** = no more H atoms can be added

- **Alkenes:** at least one C=C double bond = $\sigma + \pi$ bonds; **formula:** $C_nH_{2n}$ (for one double bond); R=R'; C=C double bond **can’t rotate because $\pi$ bond would need to be broken; cis/trans geometric isomers (see HelpSheet #3); unsaturated molecule; **unsaturated** = more H atoms could be added if multiple bond is broken

- **Alkynes:** at least one C≡C triple bond = $\sigma + 2\pi$ bonds; **formula:** $C_nH_{2n-2}$ (for one triple bond); R=R'; C≡C triple bond **can’t rotate because $\pi$ bonds would need to be broken; unsaturated molecule

- **Cyclic:** ring compounds; **formula:** $C_nH_{2n}$ (for one ring); 3-membered ring unstable; 4-membered ring somewhat stable; 5-membered ring stable; 6-membered ring stable puckered; unsaturated molecule

- **Aromatic:** for Chem 104 the focus is on benzene, $C_6H_6$, or a derivative of benzene; in benzene all C–C bonds are equivalent; $BO_{C-C} = 1.5$ in benzene; benzene is a planar molecule; unsaturated molecule
**DRAWING MOLECULES:** C – 4 bonds; N – usually 3 bonds; O – usually 2 bonds; H, F, Cl, Br, I – 1 bond

<table>
<thead>
<tr>
<th>Molecular formula</th>
<th>Lewis Dot – all bonds and lone pairs of e⁻ drawn</th>
<th>Condensed Structure</th>
<th>Dash-Wedge Bond Line Notation</th>
<th>Variations: Condensed Structures with some bonds drawn</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₃H₇Cl</td>
<td><img src="image" alt="Lewis Dot" /></td>
<td>CH₃CHClCH₃</td>
<td><img src="image" alt="Dash-Wedge" /></td>
<td><img src="image" alt="Variations" /></td>
</tr>
</tbody>
</table>

**BOND LINE Drawings**

**Example:**
- ![Bond Line Example](image)
  - Each point on the line is a C atom; there are 4 C present.
  - Each C must have 4 bonds; add H atoms to each C until each C has 4 bonds.

**Example:**
- ![Bond Line Example](image)
  - All atoms drawn; note how the bond connecting the O atom to the C atom does not have a C atom at the end of the line; rather the O atom is there.

**Adding substituents (branches) off the main chain**

**Where branches should not be placed**

- no substituents (branches) in these “triangle” regions

**Adding 1 branch**

- Drawn **correctly**: place branch vertical relative to the chain, and not in the “triangle” regions
- Drawn **incorrectly**: branch placed in incorrect “triangle” region

**Adding 2 branches**

- Drawn **correctly**: place branches at an angle relative to the chain (not “vertical”) and not in the “triangle” regions
- Drawn **incorrectly**: branches should be on the same side of chain and not in “triangle” regions

**Adding multiple branches**

- Drawn **correctly**: no branches in the “triangle” regions; single branch is “vertical” from chain; when 2 branches are on the same C atom they are at an angle relative to the chain

**3D Drawings (dash-wedge):**

- Wedge line is **coming out** of the plane of the paper towards you
- Dash line is **going behind** the plane of the paper away from you
- Regular/thin line is **in the plane** of the paper

**Example:**
- ![3D Drawings Example](image)
  - Both structures are **correct**: just drawn from a different perspective
NAMING MOLECULES:
1. Find longest C chain
2. **Number the longest C chain** to give smallest numbers for functional group or branches
3. **Prefix** = #carbon atoms:  
   - Meth = 1; Eth = 2; Prop = 3; But = 4; Pent = 5;  
   - Hex = 6; Hept = 7; Oct = 8; Non = 9; Dec = 10
4. **Suffixes** = functional group: “ane” for alkanes, “ene” for alkenes, “yne” for alkynes; use prefix “cyclo” for cyclic molecules; use “benzene” when a benzene ring is included
5. a. **Branches**: for C branches: prefix + “yl”; e.g., 1-C branch = meth+yl = methyl; 2-C branch = ethyl; etc.
   
   special branches: isopropyl:  
   tert-butyl:

   b. **Duplicate branches**: use: di = 2; tri = 3; tetra = 4; e.g., two (di) 1-C (methyl) branches = dimethyl ethyl before propyl; ethyl before dimethyl (alphabetize on “e” and “m” and ignore “di”)

d. **Every branch and functional group must have a number** identifying C chain position

e. Commas between numbers; dashes (“-”) between numbers and letters
6. Alkene functional group: check for cis/trans isomers (see HelpSheet #3 for what cis and trans mean)

### Example 1: Name the molecule shown.
1. Find longest C chain (dashed rectangular box) = 7 carbons long; prefix = hept
2. All C–C single bonds (alkane); suffix = ane
3. Find branches off longest C chain (dashed ovals); one branch = 1-C long = methyl; two branches = 2-C long = each is ethyl – since two identical branches = diethyl
4. **Number longest C chain** both ways; choose numbering scheme to yield smaller numbers for branches (bottom bold numbers are better). Functional groups (e.g., an alkyn) get higher priority in numbering chain; this molecule has no functional group (alkane not considered functional group)
5. Alphabetize branches (diethyl before methyl; alphabetize on “e” and “m”).
6. Each branch gets a number: 2-methyl; 3,4-diethyl (note the 2 numbers: one for each ethyl branch)
7. Commas () between numbers; dashes (-) between numbers and letters
**Answer 1:** 3,4-diethyl-2-methylheptane

### Example 2: Name the molecule shown.
1. Find longest C chain (dashed rectangular box) = 5 carbons long; prefix = pent
2. All C–C single bonds (alkane); suffix = ane
3. Find branches off longest C chain (dashed ovals); two branches = 1-C long = each is methyl – since two identical branches = dimethyl; two branches = Br = bromo – since two identical branches = dibromo
4. **Number longest C chain** both ways; choose numbering scheme to yield smaller numbers for branches (bottom bold numbers are better). Functional groups (e.g., an alkyn), get higher priority in numbering chain; this molecule has no functional group
5. Alphabetize branches (dibromo before dimethyl; alphabetize on “b” and “m”).
6. Each branch gets a number: 2,2-dibromo (note the 2 numbers: one for each Br); 3,3-dimethyl (note the 2 numbers: one for each methyl)
7. Commas () between numbers; dashes (-) between numbers and letters
**Answer 2:** 2,2-dibromo-3,3-dimethylpentane

### Example 3: Name the molecule shown.
1. Find longest C chain (dashed rectangular box) = 5 carbons long; prefix = pent
2. C=C double bond (alkene); suffix = ene
3. **Number longest C chain** so functional group gets smallest number. Functional group (e.g., the alkene) gets higher priority in numbering chain (bottom bold numbers are better). Alkene is in between C atoms 1 and 2 so it is in bond position 1. The other numbering places the alkene in bond position 4 (not as good!)
4. Find branches off the C chain (dashed ovals). Two branches = 1-C long = each is methyl – since two identical branches = dimethyl
5. Each branch and functional group gets a number. Functional group = double bond = 1; the branches are: 3,4-dimethyl (note the 2 numbers: one for each methyl)
6. Commas () between numbers; dashes (-) between numbers and letters
**Answer 3:** 3,4-dimethyl-1-pentene
1. Using the molecule shown, answer the following questions (another one of these problems similar to Help Sheet #1 but the structure is now drawn as a line diagram).
   a. How many lone pairs of electrons exist in this molecule?
   b. What is the angle labeled “b” in the diagram?
   c. What is the hybridization on the C atom labeled “c” in the diagram?
   d. What is the molecular geometry around the N labeled “d” in the diagram?
   e. What is the angle labeled “e” in the diagram?
   f. What orbitals were used to make the bond labeled “f” in the diagram?
   g. What is the electron domain geometry around the O atom labeled “g” in the diagram?
   h. What is the bond order for bond labeled “h” in the diagram?
   i. What orbitals were used to make the bond labeled “i” in the diagram?
   j. What is the molecular formula of this molecule?

2. Give the proper name for each of the following molecules drawn as condensed structures.
   a. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   b. \[
   \text{CH}_3-\text{CH}-\text{C}-\text{CH}_2-\text{CH}_3
   \]
   c. \[
   \text{CH}_2-\text{CH}_2-\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}_3
   \]
   d. \[
   \text{CH}_3-\text{CH}_2-\text{CH}-\text{CH}_2-\text{CH}_3
   \]
   e. \[
   \text{CH}_3-\text{CH}_2-\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}_3
   \]
   f. \[
   \text{CH}_2-\text{CH}-\text{C}-\text{CH}_3
   \]
   g. \[
   \text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}_3
   \]
   h. \[
   \text{CH}_3-\text{CH}_2-\text{CH}_3
   \]

3. Give the proper name for each of the following molecules drawn as bond line structures.
   a. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   b. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   c. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   d. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   e. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   f. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   g. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   h. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   i. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]
   j. \[
   \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H}
   \]

4. Draw the organic molecules in bond line notation given their names.
   a. 2,2,4-trimethylpentane
   b. 1,1,2-trichlorohexane
   c. 3,4,5-triethyl-2,6-dimethyloctane
   d. 1,1,2-trichlorocyclopentane
   e. 1-ethyl-2,4-dimethylbenzene
   f. 1,2-dichlorobenzene
   g. 4-methyl-2-hexyne
   h. 2,3,3-tribromo-1-butene
5. Which functional group could the molecule, C_{35}H_{70}, contain?
   a. alkane    b. alkene    c. alkyne    d. benzene    e. more info needed

6. Draw the two resonance structures using line notation that are used to represent benzene, C_{6}H_{6}.

7. Draw the **condensed structures** for the molecules given the names with bonds drawn between the groups (e.g., for ethane draw CH_{3}CH_{3}).
   a. 3-ethyl-2,2,4-trimethylpentane    b. 4,4-dibromo-2,3-dimethyl-2-pentene

8. From each of the following condensed molecular structures, draw the
   a) Lewis dot structure,
   b) bond line notation, and
   c) dash-wedge 3D structures.
   I. CH_{3}CH_{2}CH_{2}CH_{2}CH_{3}    II. CHCCH_{3}    III. CH_{3}CH_{2}CH(OH)CH_{3}    IV. CH_{3}HC=CClCH_{3}

**ANSWERS**
1. a. 7  {see the diagram below}

   ![Diagram](image1)

   b. 120°  {the vertex C atom has 3 domains (3 atoms attached + 0 lone pairs); hybridized as a sp^2 → triangular planar → 120°}

c. sp^2  {C atom has 3 domains (3 atoms attached + 0 lone pairs) → sp^2}

d. bent  {N atom has 3 domains (2 atoms attached + 1 lone pair) → sp^2 → bent}

e. ~109.5°  {S has 4 domains (2 atoms attached + 2 lone pairs) → sp^3 → tetrahedral → ~109.5°}

f. sp^3(C)−sp^2(C)  {C on the left has 4 domains (4 atoms attached) → sp^3; C on the right has 3 domains (3 atoms attached + 0 lone pairs) → sp^2; σ bond from HO−HO overlap: sp^3(C)−sp^2(C)}

g. tetrahedral  {O atom has 4 domains (2 atoms attached + 2 lone pairs) → sp^3 → tetrahedral}

h. 1.5  {C_{6}H_{5} group = benzene group → resonance → half the time single bond and half the time double bond; see diagram below}

   ![Diagram](image2)

i. sp^3(C)−sp^2(N)  {C on the left has 4 domains (4 atoms attached) → sp^3; N on the right has 3 domains (2 atoms attached + 1 lone pair) → sp^2; σ bond from HO−HO overlap: sp^3(C)−sp^2(N)}

j. C_{14}H_{13}NO_{2}S  {see the diagram below; it is helpful to draw in all of the atoms to get the correct molecular formula}
2. a. hexane  
b. 2-methylpentane  
c. 2, 4, 5-trimethylheptane  
d. 3-ethyl-2, 3-dimethylpentane  
e. 2, 2-dimethylpropane  
f. 4-propylheptane  
g. 2, 2, 3, 3-tetramethylbutane  
h. 3-ethylpentane

3. a. 2,2,4-trimethylpentane  
b. 3-methylpentane  
c. 2,2-dimethylpropane  
d. 1-hexene  
e. 1-butynе  
f. 3,4-dimethyl-1-pentyne  
g. 1,2-dimethylcyclopentane  
h. 1,3,5-triethylcyclohexane  
i. 1,3-dichlorobenzene  
j. 4-ethyl-2,3,5-trimethylheptane

4. a.  

b.  
c.  
d.  

2,3,3-tribromo-1-butene

e.  
f.  
g.  
h.  

5. b. \{the formula, \(C_{35}H_{70}\), matches \(C_nH_{2n}\); hence, it cannot be an alkane (\(C_nH_{2n+2}\)), nor an alkyne (\(C_nH_{2n-2}\)); it must be either an alkene or a cyclic compound (\(C_nH_{2n}\)\}

6.  

7. a. \(CH_3C(CH_3)_2CH(CH_2CH_3)CH(CH_3)CH_3\)  
b. \((CH_3)_2C=C(CH_3)(CBr_2CH_3)\)
8. I. a. b. c. It is helpful to assign hybridization to each atom; if the hybridization = sp³ then it’s a tetrahedral and a dash-wedge structure is needed; if it’s sp² or sp then it’s planar and no dash-wedge structure is needed:

\[
\begin{array}{c}
\text{sp}^3 \quad \text{sp}^3 \quad \text{sp}^3 \quad \text{sp}^3 \\
\text{sp}^3 \quad \text{sp}^3 \quad \text{sp}^3 \end{array}
\rightarrow

H - C - C - C - C - H
\]

II. a. b. c. It is helpful to assign hybridization to each atom; if the hybridization = sp³ then it’s a tetrahedral and a dash-wedge structure is needed; if it’s sp² or sp then it’s planar and no dash-wedge structure is needed:

\[
\text{sp} \quad \text{sp} \quad \text{sp}^3 \\
\rightarrow

H - C - C - C - H
\]

III. a. b. c. It is helpful to assign hybridization to each atom; if the hybridization = sp³ then it’s a tetrahedral and a dash-wedge structure is needed; if it’s sp² or sp then it’s planar and no dash-wedge structure is needed:

\[
\text{sp}^3 \quad \text{sp}^3 \quad \text{sp}^3 \\
\rightarrow

H - C - C - C - C - H
\]

IV. a. b. c. It is helpful to assign hybridization to each atom; if the hybridization = sp³ then it’s a tetrahedral and a dash-wedge structure is needed; if it’s sp² or sp then it’s planar and no dash-wedge structure is needed:

\[
\text{sp}^3 \quad \text{sp}^3 \\
\rightarrow

H - C - C - C - H
\]