Nuggets: Functional Groups (Part I), Drawing Organic Molecules, 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>
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</thead>
<tbody>
<tr>
<td>Alkane</td>
<td>ane</td>
<td>C–C</td>
<td>saturated; tetrahedral; (sp^3); 109.5°; (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; Naming: e.g., (\text{trans-4-methyl-2-pentene})</td>
</tr>
<tr>
<td>Alkyne</td>
<td>yne</td>
<td>C≡C</td>
<td>unsaturated; linear; 180°; (C_nH_{2n-2}); (\sigma + 2\pi) bonds in the triple bond; can’t rotate Naming: e.g., (4)-methyl-1-pentyne</td>
</tr>
<tr>
<td>Cyclic</td>
<td>cyclo + (ane, ene, or yne)</td>
<td>cycloalkane: unsaturated, strained tetrahedral, (sp^3); (C_nH_{2n}); not planar Naming: e.g., (1,3)-dichlorocyclopentane</td>
<td></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 Naming: e.g., (1)-bromo-3-chlorobenzene</td>
</tr>
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</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 molecule; 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>
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<tr>
<th>Molecular formula</th>
<th>Lewis Dot – all bonds and lone pairs of e⁻ drawn</th>
<th>Condensed Structure</th>
<th>Dash-Wedge</th>
<th>Bond Line Notation</th>
<th>Variations: Condensed Structures with some bonds drawn</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₃H₇Cl</td>
<td></td>
<td>CH₃CHCICH₃</td>
<td></td>
<td></td>
<td>[Cl] (\text{CH}_3\text{CHCH}_3)</td>
</tr>
</tbody>
</table>

**BOND LINE Drawings**

**Example:**

\[\text{\textbullet~}\text{\textbullet~}\text{\textbullet~}\] = \[\text{\textbullet~}\text{\textbullet~}\text{\textbullet~}\]

Each point on the line is a C atom; there are 4 C present

\[\text{\textbullet~}\text{\textbullet~}\text{\textbullet~}\] = \[\text{\textbullet~}\text{\textbullet~}\text{\textbullet~}\]

Each C must have 4 bonds; add H atoms to each C until each C has 4 bonds

\[\text{\textbullet~}\text{\textbullet~}\text{\textbullet~}\] = \[\text{\textbullet~}\text{\textbullet~}\text{\textbullet~}\]

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

C chain

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

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

   c. **Alphabetize multiple branches**: do not alphabetize on the di, tri, or tetra 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)

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**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); three branches = 1-C long = methyl; since there are three identical branches = **trimethyl**
4. **Number longest C chain** both ways; choose numbering scheme to yield smaller numbers for branches (bottom blue 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. Each branch gets a number: the three methyl groups are on C #2, C #2, and C #3; 2,2,3-trimethyl (note the 3 numbers for the 3 branches)
6. Commas (,) between numbers; dashes (-) between numbers and letters

**Answer 1: 2,2,3-trimethylheptane**

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**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 there are two identical branches = dibromo
4. **Number longest C chain** both ways; choose numbering scheme to yield smaller numbers for branches (bottom blue 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** (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**

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**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 blue 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 pair 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 alkane molecules drawn as a Lewis dot structure, condensed structure, or a variation of condensed structure.

   a. \[\text{CH}_3\text{CH}_2\text{CH}_3\]
   b. \[\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3\]
   c. \[\text{CH}_3\text{CH}_2\text{CH}_3\]
   d. \[\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3\]
   e. \[\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3\]
   f. \[\text{CH}_3\text{CH} \text{CH}_2\text{CH}_3\]
   g. \[\text{CH}_3\text{C(CH}_3\text{)}_2\text{CH}_3\]
   h. \[\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3\]
   i. \[\text{CH}_3\text{C(CH}_3\text{)}_2\text{C(CH}_3\text{)}_2\text{CH}_3\]
   j. \[\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3\]
   k. \[\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3\]
   l. \[\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_3\]

3. Give the proper name for each of the following molecules drawn as bond line structures.

   a.
   b.
   c.
   d.
   e.
   f.
   g.
   h.
   j.
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-methyloctane
   d. 1,1,2-trichlorocyclopentane  
   e. 1,2-dichlorobenzene  
   f. 4-methyl-2-hexyne
   g. 2,3,3-tribromo-1-butene

5. Which functional group could the molecule, C\textsubscript{35}H\textsubscript{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\textsubscript{6}H\textsubscript{6}.

7. I. Draw the **condensed structures** for each molecular name given (e.g., for ethane the condensed structure would be CH\textsubscript{3}CH\textsubscript{3}).
   II. Write the molecular formula for each molecule given (e.g., for ethane the molecular formula would be C\textsubscript{2}H\textsubscript{6}).
   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
   I. Lewis dot structure, 
   II. bond line notation, and 
   III. dash-wedge 3D structures.
   a. CH\textsubscript{3}CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{3}  
   b. CHCCH\textsubscript{3}  
   c. CH\textsubscript{3}CH\textsubscript{2}CH(OH)CH\textsubscript{3}  
   d. CH\textsubscript{3}HC=CClCH\textsubscript{3}

*For more practice identifying functional groups, naming and drawing chemicals, see Practice Sheet #1.*
ANSWERS
1. a. 7 \{see the diagram below\}

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

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

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

e. \sim 109.5° \{S has 4 domains (2 atoms attached + 2 lone pairs) \rightarrow \text{sp$^3$} \rightarrow \text{tetrahedral} \rightarrow \sim 109.5°\}

f. sp$^3$(C)–sp$^2$(C) \{C on the left has 4 domains (4 atoms attached) \rightarrow \text{sp$^3$}; C on the right has 3 domains (3 atoms attached + 0 lone pairs) \rightarrow \text{sp$^2$}; \sigma$ bond from HO–HO overlap: sp$^3$(C)–sp$^2$(C)\}

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

h. 1.5 \{C_6H_5 group = benzene group \rightarrow \text{resonance} \rightarrow \text{half the time single bond and half the time double bond}; \text{see diagram below}\}

i. sp$^3$(C)–sp$^2$(N) \{C on the left has 4 domains (4 atoms attached) \rightarrow \text{sp$^3$}; N on the right has 3 domains (2 atoms attached + 1 lone pair) \rightarrow \text{sp$^2$}; \sigma$ bond from HO–HO overlap: sp$^3$(C)–sp$^2$(N)\}

j. C_{14}H_{13}NO_2S \{see the diagram below; it is helpful to draw in all of the atoms to get the correct molecular formula\}
2. a. hexane { ; could also have numbered the chain: }  
   \[CH_2-CH_2-CH_2-CH_2-CH_2-CH_1\] 5C = pent  
   1C = methyl

b. 2-methylpentane { }  
   \[CH_2-CH_2-CH_2-CH_2-CH_3\] 3C = prop  
   1C = methyl

b. 2-methylpentane { }  
   \[CH_2-CH_2-CH_3\] 3C = prop  
   1C = methyl

b. 2-methylpentane { }  
   \[CH_2-CH_3\] 1C = methyl

c. 2,2-dimethylpropane { ; could also have numbered the chain: }  
   \[CH_2-CH_3\] 3C = prop
   1C = methyl
   \[CH_2-CH_2\] 1C = methyl

d. 4-propylheptane { ; could also have numbered chain: }  
   \[CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3\] 4C = but  
   1C = methyl

e. 2,2,3-trimethylbutane { 1C = methyl; 1C = methyl }  
   \[CH_2-CH_3\] 3C = prop  
   1C = methyl

f. 3-methylpentane { ; could also have numbered chain: }  
   \[CH_3-CH_2-CH_2-CH_2-CH_3\] 4C = but

g. 2,2-dimethylpropane { ; same as question “c” }  
   \[CH_2-CH_2-CH_2-CH_3\] 4C = but

h. 2-methylbutane { }  
   \[CH_2-CH_2-CH_2-CH_3\] 4C = but
   1C = methyl

i. 2,2,3,3-tetramethylbutane { ; could also have numbered the chain: }  
   \[CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3\] 6C = hex
   1C = methyl

j. 3-ethylhexane { }  
   \[CH_3-CH_2-CH_2-CH_2-CH_2-CH_3\] 5C = pent
   1C = methyl

k. 2,3-dimethylpentane { }  
   \[CH_2-CH_2-CH_2-CH_2-CH_2-CH_3\] 6C = hex
   1C = methyl
   \[CH_2-CH_2-CH_2-CH_2-CH_3\] 4C = but
   1C = methyl

l. 3,4-diethylhexane { ; could also have numbered chain: }  
   \[CH_3-CH_2-CH_2-CH_2-CH_2-CH_3\] 6C = hex
   1C = methyl
3. a. 3-methylpentane { could also have numbered the chain:

b. 2,2,4-trimethylpentane { }

c. 1-hexene { }

d. 3-methyl-1-butene { }

e. 1-butyne { }

f. 3,4-dimethyl-1-pentyn { }

g. 1,2-dimethylcyclopentane { ; could also have numbered the ring:

h. 1,3,5-triethylcyclohexane { ; could also have numbered the ring several other ways: }

i. 4-ethyl-2,3,5-trimethylheptane { }

1C = methyl
5C = pent
6C = hex
4C = but
2C = ethyl
6C = cyclohex
2C = ethyl
2C = ethyl
1C = methyl
1C = methyl
1C = methyl
1C = methyl
2C = ethyl
2C = ethyl
7C = hept
4. (In the structures below, the longest C chain has been numbered to assist in showing how the name was translated into the bond-line structure. Normally, the numbering would not be included when going from a name to a structure.)

a. 

b. 

c. 

d. 

e. 

f. 

g. 

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

6. 

7. Start by drawing a bond-line diagram of the molecule:
  a. 3-ethyl-2,2,4-trimethylpentane

Add "groups" for each C group: to help write the condensed structure:

I. a. CH_{3}C(CH_{3})_{2}CH(CH_{2}CH_{3})CH(CH_{3})CH_{3}

Count the C and H atoms to determine the molecule formula:

II. a. C_{10}H_{22}

b. 4,4-dibromo-2,3-dimethyl-2-pentene

Add "groups" for each C group: to help write the condensed structure:

I. b. (CH_{3})_{2}C=C(CH_{3})CBr_{2}CH_{3}

Count the C and H atoms to determine the molecule formula:

II. b. C_{7}H_{12}Br_{2}
8. a. I. II. III. It is helpful to assign hybridization to each atom; if the hybridization = sp³ (4 domains) then it’s a tetrahedral and a dash-wedge structure is used; if it’s sp² (3 domains) or sp (2 domains) then it’s planar and no dash-wedge structure is needed:

```
| sp³ | sp³ | sp³ |
```

b. I. II. III. It is helpful to assign hybridization to each atom; if the hybridization = sp³ (4 domains) then it’s a tetrahedral and a dash-wedge structure is used; if it’s sp² (3 domains) or sp (2 domains) then it’s planar and no dash-wedge structure is needed:

```
| sp | sp | sp³ |
```

c. I. II. III. It is helpful to assign hybridization to each atom; if the hybridization = sp³ (4 domains) then it’s a tetrahedral and a dash-wedge structure is used; if it’s sp² (3 domains) or sp (2 domains) then it’s planar and no dash-wedge structure is needed:

```
| sp³ | sp³ | sp³ |
```

d. I. II. III. It is helpful to assign hybridization to each atom; if the hybridization = sp³ (4 domains) then it’s a tetrahedral and a dash-wedge structure is used; if it’s sp² (3 domains) or sp (2 domains) then it’s planar and no dash-wedge structure is needed:

```
| sp³ | sp³ |
```