A STUDENT SHOULD BE ABLE TO:

1. Given a Lewis (dash or dot), condensed, bond-line, or wedge formula of a compound draw the other representations.

2. Give examples of, and recognize when given the structure, representatives of the following classes of compounds. Also, draw isomers of given compounds.

   Hydrocarbons (compounds containing C and H only)
   - Saturated - alkanes (1°, 2°, 3° H and 1°, 2°, 3°, and 4° C)
   - Unsaturated - alkenes (olefins), alkynes, aromatics

   Organic compounds containing halogens
   - Alkyl halides (1°, 2°, 3°)

   Compounds containing oxygen:
   - C–O single bonds only: alcohols (1°, 2°, 3°), ethers
   - C=O compounds: aldehydes, ketones, carboxylic acids, esters, acyl halides, anhydrides

   Compounds containing nitrogen: amines (1°, 2°, 3°), amides, nitriles

   Compounds containing sulfur: thiols, sulfides

3. Identify functional groups present in molecules from infrared (IR) spectroscopy data, and predict features of the IR spectrum of molecules from their structures. Important IR absorption frequencies to know include:
   - O–H (alcohols, hydrogen bonded): 3200-3400 cm⁻¹, strong and broad
   - N–H: 3200-3500 cm⁻¹, medium intensity
   - O–H (carboxylic acids): 2500-3500 cm⁻¹, broad peaks of variable intensity
   - C=O: 1650-1800 cm⁻¹, strong absorption

   If you need to use other frequencies to identify other functional groups (and sometimes you will), a table of IR frequencies will be provided.

4. Apply concepts learned in Module 1.
### Simplified Table of Main IR Frequencies

<table>
<thead>
<tr>
<th>Wavenumber, cm(^{-1})</th>
<th>Functional Group</th>
<th>Peak Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3200 – 3600</td>
<td>O-H (alcohol)</td>
<td>Strong and broad</td>
</tr>
<tr>
<td>2500 – 3500</td>
<td>O-H (carboxylic acid)</td>
<td>Very broad (over ~ 500 cm(^{-1})); often looks like distorted baseline; can obscure C-H bands.</td>
</tr>
<tr>
<td>3200 – 3500</td>
<td>N-H (amine, amide)</td>
<td>Doublet in case of NH(_2) group in a primary amine or amide</td>
</tr>
<tr>
<td>3300</td>
<td>(\equiv)C-H terminal alkyne</td>
<td>Usually sharp and strong</td>
</tr>
<tr>
<td>3000 – 3100</td>
<td>=C-H alkene or aromatic</td>
<td>Often weak; overlaps with alkane CH absorption</td>
</tr>
<tr>
<td>2800 – 3000</td>
<td>C-H (sp(^3) carbon - hydrogen)</td>
<td>Strong, broad and multi-banded</td>
</tr>
<tr>
<td>2200 – 2300</td>
<td>C≡N nitrile</td>
<td>Medium intensity</td>
</tr>
<tr>
<td>2100 – 2250</td>
<td>C≡C(H) alkyne</td>
<td>Medium intensity for terminal alkynes, very weak for internal</td>
</tr>
<tr>
<td>1650 – 1800</td>
<td>C=O (amides, ketones, aldehydes carboxylic acids, esters, etc.)</td>
<td>Very strong; lower frequency for amides and when C=O is conjugated</td>
</tr>
<tr>
<td>1620 – 1680</td>
<td>C=C alkene, aromatic</td>
<td>Check to see if you have sp(^2) C-H &gt;3000 cm(^{-1}) (if not, it’s completely substituted)</td>
</tr>
<tr>
<td>~ 1600</td>
<td>-NH(_2) (bending) 1° amines and amides</td>
<td>Only if you have corresponding N-H peak at 3200 - 3500 cm(^{-1}) (this peak may be mistaken for C=C otherwise)</td>
</tr>
<tr>
<td>1000-1300</td>
<td>C-O</td>
<td></td>
</tr>
</tbody>
</table>
To best prepare for this module, please work Chapter 2 Skill Builder problems and Chapter 15 Skill Builder problems (IR problems only) in the textbook.

A STUDENT WHO HAS MASTERED THE OBJECTIVES FOR THIS UNIT SHOULD BE ABLE TO SOLVE THE FOLLOWING PROBLEMS AND RELATED ONES:

1.1  Draw complete structures (showing all atoms, bonds as lines, and non-bonding valence electrons as dots) for the following compounds. Also, name the functional groups.

   a) \((\text{CH}_3)_2\text{CHCH}_2\text{CH}_3\)  
   b) \(\text{CH}_3(\text{CH}_2)_3\text{CHOHCH}_3\)

   c) \[
   \begin{array}{c}
   \text{CH}_3 \\
   \text{CH}_2
   \end{array}
   \]

   d) \[
   \begin{array}{c}
   \text{CH}_2\text{OCH}_3
   \end{array}
   \]

1.2  Draw a bond-line structure for each of the following compounds. Use dashes and wedges to indicate three-dimensional geometry where appropriate.

   a) \((\text{C}_2\text{H}_5)_3\text{C(\text{CH}_2)_2\text{CH(C}_2\text{H}_5)\text{CH(\text{CH}_3)(\text{CH}_2)_2\text{CH}_3}}\)
   b) \(\text{CH}_3\text{CHCH(\text{CH}_3)(\text{CH}_2)_2\text{CH(C}_2\text{H}_5)(\text{CH}_2)_2\text{CH}_3}\)

   c)
   \[
   \begin{array}{c}
   \text{CH}_3 \\
   \text{CH}_2
   \end{array}
   \]

   d)
   \[
   \begin{array}{c}
   \text{H} \\
   \text{C} \\
   \text{H}
   \end{array}
   \]

   e) \((\text{CH}_3\text{CH}_2)_3\text{CO(\text{CH}_2)_2\text{CH=CH(CH}_2)_2\text{OC(\text{CH}_2\text{CH}_3)}_3}\)
   f) \((\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{CHCH}_2\text{CH}_2\text{C} \equiv \text{N}\)
1.3 Draw both condensed and bond-line structures for (a) and (b); draw a bond-line formula for (c); and name the functional groups present.

[a) \[\text{Condensed Structure} \]

[b) \[\text{Bond-Line Structure} \]

[c) \[\text{Bond-Line Structure} \]

1.4 Write condensed formulas for each of the following and name each functional group.

[a) \[\text{Condensed Structure} \]

[b) \[\text{Condensed Structure} \]

[c) \[\text{Condensed Structure} \]

[d) \[\text{Condensed Structure} \]

2.1 Draw the structure of an example of each of the following classes of compounds. **Do not use the symbol “R.”**

a) alkane 

b) ether 

c) 2° amine 

d) 3° alcohol 

e) aldehyde 

f) 1° alkyl halide 

g) thiol 

h) alkyne 

i) acyl chloride
2.2 Name the functional group or groups in each of the following molecules. Indicate 1°, 2°, or 3° where appropriate.

a) \( \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \)  
   b) \( \text{C}_6\text{H}_5\text{COOH} \)  
   c) \( \text{C}_6\text{H}_5\text{COCH}_3 \)  
   d) \( \text{H}_2\text{N}\text{C}_6\text{H}_4\text{H} \)  
   e) \( \text{CH}_3\text{CH}=\text{C}=-\text{CH}_3 \)  
   f) \( \text{H}_3\text{C}-\text{COCH}_2\text{CH}_3 \)  
   g) \( \text{C}_6\text{H}_5\text{CO} \)  
   h) \( \text{CH}_3\text{CHCH}_2\text{SH} \)  
   i) \( \text{H}_3\text{C}=-\text{S}-\text{CH}_2\text{CH}_3 \)

3.1 Based on the IR data given, what functional group(s) can be present in these compounds?

a) A strong absorption at 1710 cm\(^{-1}\), no N in the molecular formula, no O-H band present.

b) A strong absorption at 1720 cm\(^{-1}\) and a broad absorption between 2500-3500 cm\(^{-1}\).

c) An oxygen-containing compound with a strong absorption at 3200-3400 cm\(^{-1}\), no N in the molecular formula, no band at 1650-1800 cm\(^{-1}\).

3.2 An oxygen-containing compound does not have IR signals in either the 3200-3400 cm\(^{-1}\) region or the 1650-1800 cm\(^{-1}\) region. Which of the following functional groups fits this IR spectrum?

   a) ROH   b) RCOOH   c) RCOR   d) ROR
3.3 For each of the following compounds, determine whether or not you would expect the IR spectrum to exhibit a signal to the left of 3000 cm\(^{-1}\).

a) ![Image](image1.png) b) ![Image](image2.png) c) ![Image](image3.png)  
d) ![Image](image4.png) e) ![Image](image5.png) f) ![Image](image6.png)  
g) ![Image](image7.png) h) ![Image](image8.png)

3.4 What IR frequencies would enable a chemist to distinguish between these molecules?

a) CH\(_3\)CH\(_2\)OH and CH\(_3\)CH\(_2\)OCH\(_2\)CH\(_3\)

b) ![Image](image9.png) and ![Image](image10.png)

c) H\(_3\)CH\(_2\)CHC≡CHCH\(_2\)CH\(_3\) and ![Image](image11.png)

3.5 An unknown compound having the formula C\(_6\)H\(_{13}\)N had a peak in its IR spectrum at 3350 cm\(^{-1}\). Which of the following compounds is consistent with this?

a) ![Image](image12.png) b) ![Image](image13.png) c) ![Image](image14.png) d) ![Image](image15.png)
3.6 For each of the following IR spectra, identify whether it is consistent with the structure of a ketone, an alcohol, a carboxylic acid, a primary amine, or a secondary amine. Explain.

a) 

b) 

1470
1380

1400
1200
1100
1000
900
800
700
600

\( \bar{\nu} \text{ cm}^{-1} \)

100

0

% Transmission

3500
3000
2500
2000
1500
1000
500
0

3500
3000
2500
2000
1500
1000
500
0

% Transmission

3500
3000
2500
2000
1500
1000
500
0

% Transmission

3500
3000
2500
2000
1500
1000
500
0

\( \bar{\nu} \text{ cm}^{-1} \)

4.1 a) Draw all constitutional isomers of \( \text{C}_3\text{H}_9\text{N} \) and identify the functional group present in each one. Indicate 1°, 2°, or 3° if appropriate.
4.1 b) Draw at least four constitutional isomers of C₄H₆O₂ with as many functional groups as possible. Identify each functional group. Some molecules may have more than one.

4.2 Which of the following compounds is the most soluble in water? Which is the most soluble in hexanes?

a) CH₃CH₂NH₂    b) CH₃(CH₂)₄C-OH

c) CH₃(CH₂)₄CH₃    d) (C₂H₅)₂CHCH₂Br

4.3 Which compound has the highest boiling point? Which has the lowest?

a) (CH₃CH₂)₃N    b) \( \text{benzene} \)

c) \( \text{cyclpentane} \)    d) CH₃CH₂-S-CH₂CH₃

4.4 Provide hybridizations and approximate bond angles around the atoms that are in bold. You may need to add lone pairs to complete the octet.

a) \( \text{CH}_3-S-\text{CH}≡\text{CH}-\text{C}≡\text{H} \)    b) \( \text{CH}_3\text{N}+-\text{CH}_2-\text{C}≡\text{N} \)

hybridization _____ _____ _____ _____    _____ _____

bond angle _____ _____ _____ _____    _____ _____

SOLUTIONS TO SAMPLE PROBLEMS:
1.1 Functional groups: a) alkane; b) alcohol; c) alkene; d) ether.

a) H\( -\text{C} -\text{C} -\text{C} -\text{C} -\text{H} \)    b) H\( -\text{C} -\text{C} -\text{C} -\text{C} -\text{C} -\text{H} \)

H\( -\text{C} -\text{C} -\text{C} -\text{C} -\text{H} \)    H\( -\text{C} -\text{C} -\text{C} -\text{C} -\text{H} \)

H\( -\text{C} -\text{C} -\text{C} -\text{C} -\text{H} \)
1.1

1.2 Bond-line structures:

a) 

b) 

c) 

d) 

1.3 Functional groups: a) alkene; b) aldehyde, 2° alkyl halide; c) alkene, ketone

a) CH₃CH₂CH(CH₃)CH=CH₂  b) CHOCHCl(CH₂)₂CH(CH₃)₂

Note: when the carbon vertex points down, the attached groups point down.

1.4 a) alkene, 2° alcohol, carboxylic acid; b) alkyne; c) thiol, alkene; d) sulfide

a) CH₂=CH(CH₃)CH(OH)(CH₂)₂C(CH₃)₂CH₂CO₂H  b) (C₂H₅)₂CHC≡C(CH₂)₃CH₃

c) (CH₃)₂CHCH₂(SH)CH=CHC(CH₃)₃  d) (CH₃)₂CHCH₂S(CH₂)₂CH(CH₃)₂C(CH₃)₃

2.1 There are numerous other correct answers. These are just examples.

a) alkane  b) ether  c) 2° amine

CH₃CH₂CH₃  CH₃OCH₂CH₃  CH₃-NH-CH₂CH₃
2.1  
\[ \text{d) } 3^\circ \text{ alcohol} \quad \text{e) aldehyde} \quad \text{f) } 1^\circ \text{ alkyl halide} \]
\[ \begin{align*}
\text{CH}_3 & \quad \text{O} \\
\text{H}_3\text{C} - & \quad \text{CH} - \text{CH}_2\text{CH}_3 \\
\text{OH} & \quad \text{CH}_3\text{CH}_2\text{CH}_2\text{H} \\
\text{g) thiol} & \quad \text{h) alkyne} \quad \text{i) acyl chloride} \\
\text{CH}_3\text{CH}_2\text{CH}_2\text{SH} & \quad \text{CH}_3\text{CH}_2\text{C} & \quad \text{Cl} \\
\end{align*} \]

2.2  
\[ \text{a) alkene} \quad \text{b) aromatic, carboxylic acid} \quad \text{c) aromatic, ketone} \]
\[ \text{d) amide} \quad \text{e) } 2^\circ \text{ alcohol, alkyne} \quad \text{f) ester} \]
\[ \text{g) aromatic ring, anhydride} \quad \text{h) thiol} \quad \text{i) sulfide} \]

3.1  
\[ \text{a) aldehyde, ketone, ester, anhydride} \quad \text{b) carboxylic acid} \quad \text{c) alcohol} \]

3.2  
\[ \text{d) } \]

3.3  
\[ \text{a) no} \quad \text{b) no} \quad \text{c) yes} \quad \text{d) no} \quad \text{e) yes} \quad \text{f) yes} \quad \text{g) yes} \quad \text{h) no} \]

3.4  
\[ \text{a) } 3200-3400 \text{ cm}^{-1} (\text{OH}) \quad \text{b) } 1620-1680 \text{ cm}^{-1} (\text{C=C}) \quad \text{and} \quad 3000-3100 \text{ cm}^{-1} (=\text{C-H}) \quad \text{c) } 3000-3100 \text{ cm}^{-1} (=\text{C-H}) \]

3.5  
\[ \text{a) } \]

3.6  
\[ \text{a) primary amine (NH doublet, 3500 cm}^{-1}) \quad \text{b) alcohol (broad OH, 3350 cm}^{-1}) \quad \text{c) ketone (C=O, near 1700 cm}^{-1}) \]

4.1  
\[ \text{a) primary amine} \quad \text{primary amine} \quad \text{secondary amine} \quad \text{tertiary amine} \]
\[ \text{b) There are many other C}_4\text{H}_6\text{O}_2 \text{ isomers.} \]

4.2  
\[ \text{a) is most soluble in water; c) is most soluble in hexanes} \]

4.3  
\[ \text{b) has the highest BP; c) has the lowest BP} \]

4.4  
\[ \begin{align*}
\text{a) } & \quad \text{CH}_3 - & \quad \text{S} - & \quad \text{CH} = & \quad \text{CH} - & \quad \text{C} - & \quad \text{H} \\
\text{b) } & \quad (\text{CH}_3)_2\text{N} - & \quad \text{CH}_2 - & \quad \text{C} & \quad \text{=} & \quad \text{N} \\
\end{align*} \]

<table>
<thead>
<tr>
<th>hybridization</th>
<th>bond angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{sp}^3 )</td>
<td>( 109.5^\circ )</td>
</tr>
<tr>
<td>( \text{sp}^3 )</td>
<td>( 109.5^\circ )</td>
</tr>
<tr>
<td>( \text{sp}^2 )</td>
<td>( 120^\circ )</td>
</tr>
<tr>
<td>( \text{sp}^2 )</td>
<td>( 120^\circ )</td>
</tr>
<tr>
<td>( \text{sp}^3 )</td>
<td>( 109.5^\circ )</td>
</tr>
<tr>
<td>( \text{sp} )</td>
<td>( 180^\circ )</td>
</tr>
</tbody>
</table>
1. Name the functional group in each of the following compounds, indicating 1°, 2°, or 3° if appropriate.

   a) \[ \text{CH}_3\text{CH}_2\text{C} = \text{CCH}_2\text{CH}_3 \]  
   b) \[ \text{H}_3\text{C} - \text{N} - \text{CH}_3 \]  
   c) \[ \text{(CH}_3\text{)}_3\text{C} - \text{C} - \text{O} - \text{OH} \]

2. Give specific examples (do not use R) for each of the following types of compounds.
   a) 3° alcohol  
   b) ester  
   c) aldehyde  
   d) sulfide

3. Which of these compounds has a band in its IR spectrum nearest 3030 cm\(^{-1}\)?

   a) \[ \text{Cyclic structure} \]  
   b) \[ \text{Cyclic structure with O} \]  
   c) \[ \text{Cyclic structure with OH} \]  
   d) \[ \text{Cyclic structure with double bond} \]

4. Which of the following functional groups does not show any absorption bands in the 3200-3500 cm\(^{-1}\) region of the infrared spectrum?
   a) alcohols  
   b) primary amines  
   c) secondary amines  
   d) tertiary amines

5. What IR frequencies would enable a chemist to distinguish between these?

   \[ \text{(CH}_3\text{CH}_2\text{)}_3\text{N} \]  
   \[ \text{(CH}_3\text{CH}_2\text{)}_2\text{NH} \]

6. Which of the following compounds has the highest boiling point?
   a) \(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3\)  
   b) \(\text{CH}_3\text{OCH}_2\text{CH}_3\)  
   c) \(\text{CH}_3\text{CH}_2\text{CH}=\text{O}\)  
   d) \(\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}\)

7. Which of the following compounds is the most soluble in water? Which is the most soluble in hexanes?
   a) \(\text{CH}_3\text{CH}_2\text{-S-CH}_2\text{CH}_3\)  
   b) \(\text{CH}_3\text{(CH}_2\text{)}_3\text{CH}_3\)  
   c) \(\text{CH}_3\text{-O-CH}_2\text{CH}_3\)  
   d) \(\text{CH}_3\text{(CH}_2\text{)}_3\text{CH}_2\text{Br}\)
1. Draw structures as indicated.

a) Lewis structure of

b) an isomer of

- \[
\begin{array}{c}
N \\
\text{B} \\
H \\
H
\end{array}
\]

- \[
\begin{array}{c}
O
\end{array}
\]

c) condensed formula for

- \[
\text{CH}_3(\text{CH}_2)_3\text{CH(OH)}\text{CH}=\text{C(CH}_3)_2
\]

d) a bond-line formula for

\[
\text{O}
\]

2. Consider the molecule below. Give:

\[
\begin{array}{c}
\text{H} \\
\equiv \\
\text{C} \\
\text{C} \\
\text{H}_2 \\
\text{H}_3
\end{array}
\]

- a) the hybridization of C2 ______
- b) the hybridization of C4 ______
- c) the O-C4-C5 bond angle ______

3. Draw the structure of an example (do not use \( R \)) of each of the following classes of compounds.

- a) 1° amine
- b) acyl chloride
- c) ether
- d) 2° alkyl bromide

4. Name the functional group or groups present in each of the following molecules. Indicate 1°, 2°, or 3° when appropriate.

- a)

- b)

- c)

5. Draw at least four constitutional isomers of \( \text{C}_2\text{H}_10\text{NO}_2 \) with as many functional groups as possible. Identify each functional group. Some molecules may have more than one.
**Multiple Choice**

1. An oxygen-containing compound which shows no IR absorption at 1650-1800 cm\(^{-1}\) or 3200-3400 cm\(^{-1}\) is likely to be what type of compound?
   - a) an amide
   - b) an alcohol
   - c) a ketone
   - d) an ether

2. Which of these compounds has a band in its IR spectrum at 1650-1800 cm\(^{-1}\)?
   - a) 
   - b) 
   - c) 
   - d) 

3. Which of the following compounds has the **highest** boiling point?
   - a) CH\(_3\)CH\(_2\)CH\(_2\)CH\(_3\)
   - b) CH\(_3\)CH\(_2\)CH\(_2\)CH\(_2\)OH
   - c) CH\(_3\)OCH\(_2\)CH\(_3\)
   - d) CH\(_3\)CH\(_2\)CH\(_2\)OH

4. Which of the following compounds is the **least soluble** in water?
   - a) CH\(_3\)CH\(_2\)CH\(_2\)Br
   - b) (CH\(_3\))\(_2\)CHCH\(_2\)CH\(_2\)OH
   - c) CH\(_3\)CH\(_2\)CH\(_2\)OH
   - d) (CH\(_3\))\(_2\)CHCH\(_2\)CH\(_2\)Br

5. Indicate which of the four compounds below is responsible for the IR spectrum shown below. **Explain your answer.**
   - a) CH\(_3\)CH\(_2\)CH\(_2\)C\equivCCH\(_3\)
   - b) CH\(_3\)CH\(_2\)CH\(_2\)OH
   - c) CH\(_3\)CH\(_2\)CH\(_2\)C\equivCH
   - d) CH\(_3\)CH\(_2\)CH\(_2\)OH