REPRESENTATIVE CARBON COMPOUNDS

A STUDENT WHO HAS MASTERED THE MATERIAL IN THIS SECTION SHOULD BE ABLE TO:

1. 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
     - Unsaturated - alkenes (olefins), alkynes, aromatics
   - Compounds containing halogens (with C and H)
     - 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
   - Compounds containing nitrogen: amines (1°, 2°, 3°), amides, nitriles

2. Classify hydrogens attached to sp^3 carbons as 1°, 2°, or 3°.

3. From a structural diagram of a molecule, predict whether or not it will have a dipole moment, and predict the direction of the dipole moment of the molecule if it exists.

4. Predict relative physical properties (including melting point, boiling point, and solubility) of compounds, based on the strength of the intermolecular forces and surface area of the compounds. Intermolecular forces include:
   - ionic
   - hydrogen bonding
   - dipole-dipole
   - London (Van der Waals attractive)

5. Define, recognize, and give examples of Bronsted-Lowry and Lewis acids and bases, including conjugate acids and bases. Also, predict the products of acid-base reactions. For some comments on how to do this see the next page.

6. Identify functional groups present in molecules from infrared (IR) spectroscopy data, and predict features of the IR spectra of molecules from their structures. Important IR absorption frequencies to know include:
   - O—H (alcohols, hydrogen bonded): 3200-3550 cm\(^{-1}\), strong and broad
   - N-H: 3300-3500 cm\(^{-1}\), medium intensity
   - O—H (carboxylic acids): 2500-3000 cm\(^{-1}\), broad peaks of variable intensity
   - C=O: 1630-1780 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.
General Comments on Acid-Base Reactions

Acid-Base reactions take place between a stronger acid and a stronger base to produce a weaker acid and a weaker base.

The newly formed acid is the conjugate acid of the starting base and the newly formed base is the conjugate base of the starting acid.

A conjugate acid is a stronger acid than the base it originated from and a conjugate base is a stronger base than the acid it originated from. For example, in the reaction

\[ \text{H}_2\text{O} + \text{HCl} \rightarrow \text{H}_3\text{O}^+ + \text{Cl}^- \]

\( \text{H}_3\text{O}^+ \) is a conjugate acid of water, so it is a stronger acid than water, and \( \text{Cl}^- \) is a conjugate base of \( \text{HCl} \), so it is a stronger base than \( \text{HCl} \).

Stronger acids have weaker conjugate bases and stronger bases have weaker conjugate acids and vice versa. In this chart, HX indicates the strong mineral acids such as HCl, HBr, and HI.

<table>
<thead>
<tr>
<th>Strongest Acid</th>
<th>Weakest Acid</th>
</tr>
</thead>
<tbody>
<tr>
<td>HX &gt; RCO2H &gt; H2O &gt; ROH &gt; RC≡CH &gt; R NH2 &gt; R2C≡CRH &gt; RH</td>
<td></td>
</tr>
<tr>
<td>X &gt; RCO2 &gt; OH &gt; RO &gt; RC≡C &gt; R NH &gt; R2C≡CR &gt; R</td>
<td></td>
</tr>
</tbody>
</table>

Electron-withdrawing groups make acids stronger and electron-donating groups make bases stronger.

Acidity and basicity can be predicted from the periodic table.

For elements of the same group, the one that is further down in the periodic table forms stronger acids. This can be illustrated on the following example: H2S is a stronger acid than H2O (sulfur is in the third row and oxygen is in the second). PH3 is a weaker base than NH3 (phosphorus is in the third row and nitrogen is in the second).

For elements in the same row, the strongest acid is to the right and the strongest base is to the left. HF is a stronger acid than H2O; CH3 is a stronger base than NH2. Be careful, however; CH4 is a weaker base than NH3 because CH4 has no pair of valence electrons.
### Simplified Table of Main IR Frequencies

<table>
<thead>
<tr>
<th>Wave number, cm(^{-1})</th>
<th>Functional Group</th>
<th>Peak Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3300 – 3600</td>
<td>O-H (alcohol)</td>
<td>Strong and broad</td>
</tr>
<tr>
<td>2500 – 3000</td>
<td>O-H (carboxylic acids)</td>
<td>Very broad (over ~ 500 cm(^{-1})), often looks like distorted baseline, can reach above 3000 cm(^{-1}).</td>
</tr>
<tr>
<td>3200 – 3500</td>
<td>N-H</td>
<td>Doublet in case of NH(_2) group of a primary amine or amide</td>
</tr>
<tr>
<td>3300</td>
<td>(\equiv C \equiv H) terminal alkyne</td>
<td>Usually sharp and strong</td>
</tr>
<tr>
<td>3000 - 3100</td>
<td>(\equiv C \equiv H) alkene or arene</td>
<td>Often weak, overlaps with CH alkane absorption</td>
</tr>
<tr>
<td>2800 – 3000</td>
<td>C-H (sp(^3) carbon)</td>
<td>Strong, broad and multi-banded</td>
</tr>
<tr>
<td>2250 - 2220</td>
<td>C≡N</td>
<td>Medium intensity</td>
</tr>
<tr>
<td>2100 - 2260</td>
<td>C≡C</td>
<td>Medium intensity for terminal alkynes, very weak for internal</td>
</tr>
<tr>
<td>1680 – 1820</td>
<td>C=O (amides, ketones, aldehydes carboxylic acid, esters)</td>
<td>Very strong; lower frequency for amides and when C=O is conjugated</td>
</tr>
<tr>
<td>1600 – 1650</td>
<td>C=C (alkene, aromatic ring)</td>
<td>Check to see if you have C-H unsaturated &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>1200</td>
<td>Ar-O</td>
<td>Strong (look for =C-H &amp; C=C first)</td>
</tr>
<tr>
<td>1050-1150</td>
<td>C-O</td>
<td>Strong (look for =C-H &amp; C=C first)</td>
</tr>
<tr>
<td>690 and 750</td>
<td>phenyl group</td>
<td>Strong (look for =C-H &amp; C=C first)</td>
</tr>
</tbody>
</table>
A STUDENT WHO HAS MASTERED THE OBJECTIVES ON THE PREVIOUS PAGE SHOULD BE ABLE TO SOLVE THE FOLLOWING PROBLEMS AND RELATED ONES:

1.1 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

1.2 Name the functional group or groups present in each of the following molecules. Indicate 1°, 2°, or 3° when appropriate.
   a) \( \text{CH}_3\text{CH}_2\text{CH}═\text{CH}_2 \)
   b) \( \begin{array}{c} \text{O} \\ \text{C-OH} \end{array} \)
   c) \( \begin{array}{c} \text{O} \\ \text{C-CH}_3 \end{array} \)
   d) \( \begin{array}{c} \text{O} \\ \text{C-N-H} \end{array} \)
   e) \( \text{CH}_3—\text{CH}—\text{C═C—CH}_3 \)
   f) \( \begin{array}{c} \text{O} \\ \text{CH}_3\text{C-OCH}_2\text{CH}_3 \end{array} \)

2.1 How many 1°, 2°, and 3° hydrogens are present in each of the following molecules?
   a) \( \text{(CH}_3)_2\text{CHCH}_2\text{CH}_3 \)
   b) \( \begin{array}{c} \text{O} \\ \text{C-CH} \end{array} \)
   c) \( \begin{array}{c} \text{C} \\ \text{CH}_2\text{CH}_3 \end{array} \)

3.1 Indicate directions of individual bond dipoles of the following compounds. Also indicate the directions of the overall dipoles, if appropriate, underneath the structures.
   a) \( \text{Br—C≡C—H} \)
   b) \( \text{Br—C=C—Br} \)
   c) \( \text{H—N—H} \)
   d) \( \text{H—C=O} \)
3.2 Draw the molecules in their approximate shapes, and indicate the overall dipoles, if appropriate, underneath the structures.

\[
\begin{align*}
\text{a) } & \text{CH}_2\text{Cl}_2 & \text{b) } & \text{Br}_2\text{C}=\text{CH}_2 & \text{c) } & \text{CH}_3\text{OH} & \text{d) } & \text{CH}_3\text{CCH}_3 \\
\end{align*}
\]

4.1 Which of these compounds has the highest boiling point? Which has the lowest?

\[
\begin{align*}
\text{A. } & \text{CH}_3(\text{CH}_2)_3\text{CH}_3 & \text{B. } & \text{CH}_3(\text{CH}_2)_4\text{OH} & \text{C. } & \text{CH}_3(\text{CH}_2)_4\text{Cl} & \text{D. } & \text{CH}_3\text{CH}_2\text{CCH}_2\text{CH}_3
\end{align*}
\]

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

\[
\begin{align*}
\text{A. } & \text{CH}_3(\text{CH}_2)_3\text{Br} & \text{B. } & \text{CH}_3(\text{CH}_2)_2\text{C-OH} & \text{C. } & \text{CH}_3(\text{CH}_2)_6\text{OH} & \text{D. } & \text{CH}_3(\text{CH}_2)_6\text{CH}_3
\end{align*}
\]

5.1 Give the conjugate acid and conjugate base of each of the following substances.

\[
\begin{array}{cc}
\text{Conjugate Acid} & \text{Conjugate Base} \\
\hline
\text{a) } & \text{H}_2\text{PO}_4^- \\
\text{b) } & \text{CH}_3\text{CH}_2\text{NH}_2 \\
\text{c) } & \text{C}_6\text{H}_5\text{OH} \\
\end{array}
\]

5.2 For each of the following reactions, identify which reactant is the acid and which is the base. Then give the product(s) of the reaction. It is useful to show unshared electron pairs.

\[
\begin{align*}
\text{a) } & \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{H}_2\text{SO}_4 \longrightarrow \\
\text{b) } & \text{AlCl}_3 + \text{Cl}^- \longrightarrow \\
\text{c) } & \text{CH}_3\text{CO}_2\text{H} + \text{CH}_3\text{CH}_2\text{C}=\text{C}^- \longrightarrow \\
\text{d) } & \text{CH}_3\text{CH}_2\text{OCH}_3 + \text{BF}_3 \longrightarrow \\
\text{e) } & (\text{C}_6\text{H}_5)_3\text{P} + \text{BF}_3 \longrightarrow \\
\text{f) } & \text{C}_6\text{H}_5\text{SO}_3\text{H} + \text{H}_2\text{O} \longrightarrow \\
\end{align*}
\]
5.3 For each of the following reactions, write the acid/base reaction product or indicate no reaction.

a) \( \text{CH}_3\text{Li} + \text{CH}_2=\text{CH}_2 \rightarrow \)

b) \( \text{CH}_3\text{CO}_2\text{Na} + \text{ClCH}_2\text{CO}_2\text{H} \rightarrow \)

c) \( \text{CH}_3\text{CH}_2\text{CH}_2\text{Li} + \text{H}_2\text{O} \rightarrow \)

d) \( \text{HC}≡\text{CNa} + \text{CH}_4 \rightarrow \)

e) \( \text{CH}_3\text{ONa} + \text{CH}_3\text{SH} \rightarrow \)

6.1 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 peaks present

b) A strong absorption at 1720 cm\(^{-1}\) and a broad absorption between 2500-3000 cm\(^{-1}\).

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

a) \( \text{CH}_3\text{CH}_2\text{OH} \) and \( \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 \)

b) \[\text{Structures} \]

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

A. \[\text{Structure A} \]

B. \[\text{Structure B} \]

C. \[\text{Structure C} \]

D. \[\text{Structure D} \]

6.4 An oxygen-containing compound does not have IR peaks in either the 3200-3600 cm\(^{-1}\) region or the 1630-1780 cm\(^{-1}\) region. Which of the following general formulas fits this IR spectrum?

A. \( \text{ROH} \)

B. \( \text{RCOOH} \)

C. \( \text{RCOR} \)

D. \( \text{ROR} \)
ANSWERS TO THE SAMPLE PROBLEMS:

1.1  a) alkane    CH₃CH₂CH₃  b) ether    CH₃-O-CH₂CH₃  c) 2° amine   CH₃-NH-CH₂CH₃
d) 3° alcohol   OH                  O                                    
               CH₃-C-CH₂CH₃                   CH₃CH₂CH₂C-H      CH₃CH₂CH₂Br
     CH₃                      CH₃

Note: There are many compounds that are correct answers to Question 1.1. Their structures may be drawn as complete Lewis structures, as condensed structures (as above), or as bond-line formulas.

1.2  a) alkene    b) carboxylic acid, aromatic ring  c) ketone, aromatic ring  d) amide
e) 2° alcohol, alkyne    f) ester

2.1  a) nine 1° H’s, 2 2°, and 1 3°; b) 6 1°, 10 2°, and 2 3° H’s; c) 3 1°, 10 2°, and 1 3° H

3.1  Bond dipoles and overall dipoles:

3.2  Shapes and overall dipoles:

4.1  B has the highest boiling point, and A has the lowest.

4.2  B is the most soluble in water, and D is the least soluble.
5.1 Conjugate acids and conjugate bases:

<table>
<thead>
<tr>
<th>Conjugate Acid</th>
<th>Conjugate Base</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) $\text{H}_2\text{PO}_4^-$</td>
<td>$\text{H}_3\text{PO}_4$</td>
</tr>
<tr>
<td>b) $\text{CH}_3\text{CH}_2\text{NH}_2$</td>
<td>$\text{CH}_3\text{CH}_2\text{NH}_3^+$</td>
</tr>
<tr>
<td>c) <img src="image" alt="Phenol" /></td>
<td><img src="image" alt="Phenol" /></td>
</tr>
<tr>
<td>d) $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$</td>
<td>$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$</td>
</tr>
<tr>
<td>e) <img src="image" alt="Phenol" /></td>
<td><img src="image" alt="Phenol" /></td>
</tr>
<tr>
<td>f) <img src="image" alt="Phenol" /></td>
<td><img src="image" alt="Phenol" /></td>
</tr>
</tbody>
</table>

5.2 Acids, bases, and reaction products.

a) $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{HSO}_4^-$

b) $\text{AlCl}_3 + \text{Cl}^- \rightarrow \text{AlCl}_4^-$

c) $\text{CH}_3\text{CO}_2\text{H} + \text{CH}_3\text{CH}_2\equiv\text{C}^- \rightarrow \text{CH}_3\text{CO}_2^- + \text{CH}_3\text{CH}_2\equiv\text{CH}$

d) $\text{CH}_3\text{CH}_2\text{OCH}_3 + \text{BF}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_3^+$

e) $(\text{C}_6\text{H}_5)_3\text{P} + \text{BF}_3 \rightarrow (\text{C}_6\text{H}_5)_3\text{P}^-\text{BF}_3$

f) $\text{C}_6\text{H}_5\text{SO}_3\text{H} + \text{H}_2\text{O} \rightarrow \text{C}_6\text{H}_5\text{SO}_3^- + \text{H}_3\text{O}^+$

5.3 a) $\text{CH}_3\text{Li} + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2=\text{CHLi}$

b) $\text{CH}_3\text{CO}_2\text{Na} + \text{ClCH}_2\text{CO}_2\text{H} \rightarrow \text{CH}_3\text{CO}_2\text{H} + \text{ClCH}_2\text{CO}_2\text{Na}$

c) $\text{CH}_3\text{CH}_2\text{CH}_2\text{Li} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{LiOH}$

d) $\text{HC}=\text{CNa} + \text{CH}_4 \rightarrow \text{no reaction}$

e) $\text{CH}_3\text{ONa} + \text{CH}_3\text{SH} \rightarrow \text{CH}_3\text{OH} + \text{CH}_3\text{SNa}$

6.1 a) Ketone, aldehyde, or ester  
b) Carboxylic acid

6.2 a) OH absorption  
b) C=C absorption

6.3 A  
6.4 D
1. Name the functional group in each of the following compounds, indicating 1°, 2°, or 3° if appropriate.

   a) CH₃CH₂CCH₂CH₃        b) CH₃—N—CH₃        c) (CH₃)₃C-CH₂C-OH

2. Give specific examples (don’t use R) for each of the following types of compounds.
   a) 3° alcohol          b) ester            c) aldehyde

3. Which of these compounds has a peak in its IR spectrum nearest 3030 cm⁻¹?

   A.  \[ \text{structure} \]   B.  \[ \text{structure} \]=O   C.  \[ \text{structure} \]OH   D.  \[ \text{structure} \]

4. Consider the following structure, and fill in the blanks.

   \[ \text{structure} \]

   This compound contains:  
   _____ 1° hydrogens  
   _____ 2° hydrogens  
   _____ 3° hydrogens

5. Indicate the direction of the dipole moment of the molecule shown.

   \[ \text{structure} \]

6. Which of the following compounds has the highest boiling point?

   A. CH₃CH₂CH₂CH₃    B. CH₃OCH₂CH₃    C. CH₃-C-CH₃    D. CH₃CH₂CH₂OH

7. Predict the product of each of the following reactions. Hint: Show unshared electron pairs as needed.

   a) H₂SO₄ + NH₃ ----→

   b) BF₃ + NH₃ ----→
1. Draw the structure of an example (do not use R) of each of the following classes of compounds.
   a) ether  
   b) amide  
   c) 2° alkyl bromide

2. What family does each of the compounds shown belong to? Be specific; indicate 1°, 2°, or 3° if appropriate.
   a)  
   b)  
   c) CH₃NHCH₃

3. Which of the following compounds has absorptions in the 3400-3650 cm⁻¹ and 1640-1680 cm⁻¹ regions of the IR spectrum?
   A.  
   B.  
   C.  
   D.  

4. Which of the compounds shown is the LEAST soluble in water?
   A. NaCl  
   B. CH₃OH  
   C. CH₃CCH₃  
   D. CH₃CH₂CH₃

5. Indicate the direction of the dipole moment of the molecule shown.

6. Which of the following compounds has the highest boiling point?
   A. CH₃C-OLi  
   B. CH₃CCH₃  
   C. CH₃C-OH  
   D. CH₃CHCH₃

7. Which of these molecules has the largest dipole moment?
   A. H-C≡C-H  
   B. Br-C≡C-Br  
   C. H-C≡C-Br

8. What is the strongest type of intermolecular force present in a pure sample of CH₃CH₂CH₂CH₂CH₃?