Week 9 Worksheet

Topics Covered:
- Degrees of unsaturation
- Mass Spectroscopy
- IR
- NMR

1. Calculate the degrees of unsaturation from the molecular formula provided below.

   (a) $C_{12}H_{22}O_{11}$

   (b) $C_{11}H_{12}N_{2}O_{2}$

   (c) $C_{10}H_{15}Br_{2}Cl_{3}$
2. A compound has a measured exact mass of 60.0119 [M]$^+$ using electron impact ionization. Identify the most likely molecular formula for the compound based on the following possible [M]$^+$ formulas and masses:

- $C_3H_8O$: 60.0575
- $C_2H_4O_2$: 60.0211
- $C_2H_8N_2$: 60.0688

3. Which of the following molecules BEST corresponds to the following IR spectra?

Noticeable peaks: 1700 cm$^{-1}$, 2900 cm$^{-1}$

![IR spectra image]

a) ![Structure a)](image)  
b) ![Structure b)](image)  
c) ![Structure c)](image)  
d) ![Structure d)](image)
4. You recovered a compound after setting up the following reaction. Using IR spectroscopy, explain how you would be able to determine if the following reaction…

\[
\begin{array}{c}
\text{O} \\
\text{CH}_3 \\
1) \text{CH}_3\text{NH}_2 \\
2) \text{NaBH}_3\text{CN} \\
\end{array}
\]

\[
\begin{array}{c}
\text{NH} \\
\end{array}
\]

a) Did not occur  
b) Occurred to completion, assuming the compound is 100% pure.

5. (Klein 5e 3.4, 3.6, 3.7, 3.8) Identify the number of signals expected in the proton NMR spectrum of each of the following compounds. Then, predict the splitting pattern for each signal.

a. 

\[
\begin{array}{c}
\text{ } \\
\text{ } \\
\text{ } \\
\end{array}
\]
b. 

\[
\text{HO-CH}_{2}-\text{CH}_{2}\text{OH}
\]

c. 

\[
\text{HO-CH}_{2}-\text{CH}_{2}\text{OH}
\]

d. 

\[
\text{HO}-\text{CH}-(\text{CH}_{3})
\]
6. Which of the following molecules BEST corresponds to the following H-NMR spectra?

- a) \( \text{NH}_2 \)
- b) \( \text{OH} \)
- c) \( \text{NH}_2 \)
- d) \( \text{OH} \)
Appendix

**Interpretation of Infrared Spectra**

### X-H Region

<table>
<thead>
<tr>
<th>Phenol &amp; Alcohols</th>
<th>RO-H</th>
<th>3700 - 3500 sharp or 3200 - 3600 broad (H-bonded)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acids</td>
<td>R-OH</td>
<td>2800 - 3600 very broad</td>
</tr>
<tr>
<td>Amines &amp; Amides</td>
<td>R-NH</td>
<td>3300 - 3500 (2 bands: (-\text{N}_2^+H) primary, 1 band: (-\text{N}_2^-R) secondary)</td>
</tr>
<tr>
<td>C-H Bonds</td>
<td>C-H</td>
<td>3200 - 3300</td>
</tr>
<tr>
<td></td>
<td>C=C-H</td>
<td>3000 - 3200</td>
</tr>
<tr>
<td></td>
<td>C=C-H</td>
<td>2000 - 3000</td>
</tr>
</tbody>
</table>

### Sp Region

| Acetylenes       | C≡C | 2100 (weak or absent if highly symmetrical)     |
| Nitriles         | C≡N | 2200                                            |
| Carbon dioxide   | O=C=O| 2350                                           |

### Double Bond Region

| Alkenes          | C=C | 1600 - 1670 weak unless conjugated              |
| Imines           | C=N | 1600 - 1700                                      |
| Nitro            | NO\_2 | 1350 and 1550                                  |

### Carbonyl Groups

| Anhydrides       | \(\text{O}^\equiv\text{O}\) | 1800 - 1840 (2 bands) |
| Acid Chlorides   | \(\text{O}^\equiv\text{Cl}\) | 1800                  |
| Esters           | \(\text{O}^\equiv\text{O}\) | 1725 - 1750           |
| Acids            | \(\text{O}^\equiv\text{OH}\) | 1710                  |
| Amides           | \(\text{O}^\equiv\text{NH}_2\) | 1650                  |
| Aldehydes        | \(\text{O}^\equiv\text{H}\) | 1725                  |
| Carboxylate      | \(\text{O}^\equiv\text{O}\) | 1550-1610 and 1400    |

![Ketones: Acyclic (\(\text{O}^\equiv\text{O}\))](image1) and ![Ketones: Cyclic (\(\text{O}^\equiv\text{O}\))](image2) and ![Ring Contraction](image3) and ![Conjugation](image4)
<table>
<thead>
<tr>
<th>Type of proton</th>
<th>Chemical shift (ppm)</th>
<th>Type of proton</th>
<th>Chemical shift (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>RₘCₙHₘ</td>
<td>4.5–6</td>
</tr>
<tr>
<td>( R^3CH )</td>
<td>~1.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( R_2CH_2 )</td>
<td>~1.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( RCH_3 )</td>
<td>~0.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( Z = C, O, N)</td>
<td>1.5–2.5</td>
<td>R_C_H</td>
<td>9–10</td>
</tr>
<tr>
<td>( \equiv )</td>
<td>~2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( Z = N, O, X )</td>
<td>2.5–4</td>
<td>R_O_H</td>
<td>1–5</td>
</tr>
<tr>
<td>( \equiv )</td>
<td>~2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( Z = C, H )</td>
<td>0.9–2</td>
<td>( \equiv )</td>
<td>4.5–6</td>
</tr>
</tbody>
</table>