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) \( \text{C}_{12}\text{H}_{22}\text{O}_{11} \)

Saturated hydrocarbon has \( 2 \times (\# \text{ of C}) + 2 \) hydrogens; every degree of unsaturation means there’s a ring or a double bond, which corresponds to the loss of 2 H’s.

\[
\text{UN} = \frac{[2 \times (\# \text{ of C}) + 2 + (\# \text{ of N}) - (\# \text{ of H}) - (\# \text{ of X})]}{2} \\
= \frac{(12 \times 2 + 2) - 22}{2} = 2
\]

(b) \( \text{C}_{11}\text{H}_{12}\text{N}_{2}\text{O}_{2} \)

\[
((11 \times 2 + 2) + 2 - 12) / 2 = 7
\]

(c) \( \text{C}_{10}\text{H}_{15}\text{Br}_{2}\text{Cl}_{3} \)

\[
((10 \times 2 + 2) - 15 - 2 - 3) / 2 = 1
\]

2. A compound has a measured exact mass of 60.0119 \([\text{M}]^+\) using electron impact ionization. Identify the most likely molecular formula for the compound based on the following possible \([\text{M}]^+\) formulas and masses:

- \( \text{C}_3\text{H}_8\text{O} \) \( 60.0575 \)
- \( \text{C}_2\text{H}_4\text{O}_2 \) \( 60.0211 \)
- \( \text{C}_2\text{H}_8\text{N}_2 \) \( 60.0688 \)
C₂H₄O₂; This expected mass is the closest to the measured value

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

Noticeable peaks: 1700 cm⁻¹, 2900 cm⁻¹

Answer: B

Ketone Carbonyl @ 1700 cm⁻¹
Csp3-H @ 2900 cm⁻¹
4. You recovered a compound after setting up the reaction below. Using IR spectroscopy, explain how you would be able to determine if the reaction...

![Reaction diagram]

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

a) If the reaction did not occur, there would be a ketone C=O peak present at ~1700ppm.
b) If the reaction occurred, there would not be a C=O peak but rather an amine peak at ~3300ppm.

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.

![NMR spectrum diagram]

1 peak, all protons are equivalent; singlet

b.
5 peaks;

Hb, Hc, and Hd are not equivalent
Ha: broad singlet (doesn't participate in splitting)
Hb: enantiotopic, triplet
Hc: quintet
Hd: sextet
He: triplet

c.

3 peaks;
The molecule is symmetric, therefore Ha and Hb on both sides of the molecule are equivalent;
Ha: broad singlet
Hb: triplet
Hc: quintet

d.

6 peaks;
Hd and He are diastereotopic, therefore they will spit each other and show up as different signals.

Ha: doublet
Hb: broad singlet
Hc: sextet
Hd: multiplet (complex splitting)
He: multiplet
Hf: triplet

6. Which of the following molecules BEST corresponds to the following H-NMR spectra?
Answer: A

CH₃ signals @1.06, 0.87ppm; doublet & triplet
CH₂ signals @1.62ppm; diastereotopic, multiplet
H-C-NH₂ @ 2.63ppm; sextet
NH₂ signals @ 1.5ppm; singlet (does not contribute to splitting)