Mass Spectrometry Worksheet
CHEM 212

1. What is separated and detected by mass spectrometers?

2. Below is a generalized schematic of the components of a mass spectrometer.

Circle and label each of the above phases in the figure below.

![Diagram of mass spectrometer components](image)

**Ionization Methods**

3. Define the following terms:
Base peak

Molecular ion
There are several (many) ways to generate ions that can be detected for mass spectrometry. These methods vary in aggressiveness and effectiveness.

4. The GC-MS available in the department (and used in the CHEM 212 lab) uses **electron ionization** (aka electron impact) to ionize molecules after separation by gas chromatography and prior to detection.

   a. Write the reaction of a molecule with an electron to form the molecular ion.

   b. What is a typical ionization energy for a valence electron? If the electron gives up 12-15eV of kinetic energy in colliding with the molecule, is that enough to result in loss of a valence electron?

   c. Diagram an **electron ionization** setup. Describe the function of each component.

5. Describe how a chemical ionization cell is different from electron ionization cell.

6. Explain why the following MS spectra of the SAME COMPOUND have different peaks and different peak abundances
7. You collect a mass spectrum of a known compound using electron ionization but do not observe a M^+ peak. What’s likely happened? Suggest two methods of increasing the detected M^+ ion abundance?

8. Is chemical or electron ionization the more aggressive method? What does it mean if an ionization method is more aggressive?

Mass Spectrometer- Selection of Ions
9. Diagram a magnetic sector mass spectrometer and describe how it selects a specific m/z ratio ion to impact the detector.

10. Diagram and describe how a quadrupole mass spectrometer works.
11. Diagram and describe how a TOF works.

![Diagram of TOF mass spectrometer](image)

**Mass Spectrometer - Detecting Ions**

12. Diagram an electron multiplier. What is the typical amplification?

![Diagram of electron multiplier](image)

13. Diagram and describe how a Channeltron converts ions into a measureable current.

![Diagram of Channeltron](image)
http://www.chem.arizona.edu/massspec/

<table>
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<tr>
<th>Ionization method</th>
<th>Typical Analytes</th>
<th>Sample Introduction</th>
<th>Mass Range</th>
<th>Method Highlights</th>
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<tbody>
<tr>
<td>Electron Impact (EI)</td>
<td>Relatively small volatile</td>
<td>GC or liquid/solid probe</td>
<td>to 1,000 Daltons</td>
<td>Hard method versatile provides structure info</td>
</tr>
<tr>
<td>Chemical Ionization (CI)</td>
<td>Relatively small volatile</td>
<td>GC or liquid/solid probe</td>
<td>to 1,000 Daltons</td>
<td>Soft method molecular ion peak [M+H]^+</td>
</tr>
<tr>
<td>Electrospray (ESI)</td>
<td>Peptides Proteins nonvolatile</td>
<td>Liquid Chromatography or syringe</td>
<td>to 200,000 Daltons</td>
<td>Soft method ions often multiply charged</td>
</tr>
<tr>
<td>Fast Atom Bombardment (FAB)</td>
<td>Carbohydrates Organometallics Peptides nonvolatile</td>
<td>Sample mixed in viscous matrix</td>
<td>to 6,000 Daltons</td>
<td>Soft method but harder than ESI or MALDI</td>
</tr>
<tr>
<td>Matrix Assisted Laser Desorption (MALDI)</td>
<td>Peptides Proteins Nucleotides</td>
<td>Sample mixed in solid matrix</td>
<td>to 500,000 Daltons</td>
<td>Soft method very high mass</td>
</tr>
</tbody>
</table>

**Applications of Mass Spec:**

Identification of pure compounds:

1. Molecular masses

2. Molecular formula from exact molar masses

3. Molecular formula from isotopic ratios

4. Structural information from fragmentation patterns

5. Compound identification based on comparison of spectra

Analysis of mixtures- hyphenated techniques:

GC-MS, CE-MS, HPLC-ICP-MS, ICP-MS, tandem MS
Gas Chromatography (GC)

14. State the function of each of the components of a GC-MS.

Carrier gas

Sample injection-

Headspace injection-

Liquid injection-

Injector chamber-

Column

Detector options:

Gas Chromatography-Mass Spectrometry (GC-MS)
Inductively Coupled Plasma-Mass Spectrometry (ICP-MS)

15. State the function of each of the components labeled below.

Plasma

Sampling cone

Skimmer cone

High voltage extraction lens

Octapole reaction cell

Deflector plates

Quadrupole mass separator

Electrostatic deflector plates
16. Draw a nebulizer and describe how the plasma is generated and how sample is introduced.

What did you learn today?

What remains unclear?