# Unit 6: Identifying Compounds via Mass Spectrometry

Content Area: Science Course(s): Time Period: Marking Period 2 Length: 3 Weeks Status: Published

# **Brief Summary of Unit**

Working out a mechanism to synthesize a compound is important but without seeing the actual molecule, how do chemists know they have actually produced the compound they were trying to? Chemists can utilize specialized instrumentation to test their product in an attempt to identify the compound. Unlike some identification techniques, mass spectrometry is destructive which means the sample tested will be lost forever. The destruction serves a purpose as it is this destruction that creates fragments of the original molecule that can be used to determine the molecular mass, molecular formula, and a variety of structural features of the compound tests.

Updated June 2022

| Standards       |   |
|-----------------|---|
|                 |   |
| MA.S-ID.A       | Summarize, represent, and interpret data on a single count or measurement variable  |
| MA.A-SSE.A.1    | Interpret expressions that represent a quantity in terms of its context.  |
| TECH.K-12.1.1.c | use technology to seek feedback that informs and improves their practice and to demonstrate their learning in a variety of ways.  |
| MA.A-SSE.B.3    | Choose and produce an equivalent form of an expression to reveal and explain properties of the quantity represented by the expression.  |
| MA.N-Q.A.1      | Use units as a way to understand problems and to guide the solution of multi-step problems; choose and interpret units consistently in formulas; choose and interpret the scale and the origin in graphs and data displays. |
| MA.N-Q.A.2      | Define appropriate quantities for the purpose of descriptive modeling.  |
| MA.N-Q.A.3      | Choose a level of accuracy appropriate to limitations on measurement when reporting quantities.   |
| TECH.K-12.1.3.b | evaluate the accuracy, perspective, credibility and relevance of information, media, data or other resources.   |
| LA.RI.11-12.7   | Integrate and evaluate multiple sources of information presented in different media or formats (e.g., visually, quantitatively) as well as in words in order to address a question or solve a problem.                      |
| TECH.K-12.1.5.b | collect data or identify relevant data sets, use digital tools to analyze them, and represent data in various ways to facilitate problem-solving and decision-making.   |
| MA.A-CED.A.1    | Create equations and inequalities in one variable and use them to solve problems.   |
| TECH.K-12.1.6.a | choose the appropriate platforms and tools for meeting the desired objectives of their  |

|              | creation or communication.   |
|--------------|--|
| LA.W.11-12.1 | Write arguments to support claims in an analysis of substantive topics or texts, using valid reasoning and relevant and sufficient evidence.   |
| LA.W.11-12.7 | Conduct short as well as more sustained research projects to answer a question (including<br>a self-generated question) or solve a problem; narrow or broaden the inquiry when<br>appropriate; synthesize multiple sources on the subject, demonstrating understanding of<br>the subject under investigation.  |
| LA.W.11-12.8 | Gather relevant information from multiple authoritative print and digital sources, using advanced searches effectively; assess the strengths and limitations of each source in terms of the task, purpose, and audience; integrate information into the text selectively to maintain the flow of ideas, avoiding plagiarism and overreliance on any one source and following a standard format for citation. (MLA or APA Style Manuals). |
| LA.W.11-12.9 | Draw evidence from literary or informational texts to support analysis, reflection, and research.  |
| SCI.HS-PS2-6 | Communicate scientific and technical information about why the molecular-level structure is important in the functioning of designed materials.  |
| SCI.HS-PS4-1 | Use mathematical representations to support a claim regarding relationships among the frequency, wavelength, and speed of waves traveling in various media.  |
| SCI.HS-PS4-3 | Evaluate the claims, evidence, and reasoning behind the idea that electromagnetic radiation can be described either by a wave model or a particle model, and that for some situations one model is more useful than the other.   |
| SCI.HS-PS4-4 | Evaluate the validity and reliability of claims in published materials of the effects that different frequencies of electromagnetic radiation have when absorbed by matter.  |
| SCI.HS-PS4-5 | Communicate technical information about how some technological devices use the principles of wave behavior and wave interactions with matter to transmit and capture information and energy.   |
| WRK.K-12.P.3 | Consider the environmental, social and economic impacts of decisions.  |
| WRK.K-12.P.4 | Demonstrate creativity and innovation.   |
| WRK.K-12.P.5 | Utilize critical thinking to make sense of problems and persevere in solving them.   |
| WRK.K-12.P.8 | Use technology to enhance productivity increase collaboration and communicate effectively.   |

# **Essential Questions**

# **Essential Questions**

How does mass spectrometry work and how does it compare to similar techniques known as spectroscopy?

How is a mass spectra analyzed?

# **Enduring Understandings**

Mass spectrometry is a destructive analytical technique that can be used to determine the mass of a molecule and associated fragments.

Mass spectrometry is sensitive enough to detect the presence (or absence) of isotopes.

Analytical techniques, like mass spectrometry and IR/NMR spectroscopy, are often used together in order to

identify unknowns (it is very difficult to identify an unknown with only 1 analysis technique and no context).

### **Objectives**

Students will know that spectrometry does not use electromagnetic radiation while spectroscopy (IR/NMR) does.

Students will know that the mass spectrometer works by ionizing a molecule.

Students will know that the spectra displays the mass of the individual fragments produced.

Students will be skilled at identifying the peak of the molecular ion.

Students will be skilled at identifying peaks of the same fragment with different masses due to isotopes.

Students will know the limitations of mass spectrometry as an analytical technique.

Students will know that low- and high-resolution mass spec can be used to differentiate similar-mass compounds.

Students will know how fragmentation of a molecule occurs with respect to functional groups.

Students will be skilled at identifying fragments from functional groups on a mass spectra.

Students will know the conditions necessary for a McLafferty rearrangement to occur.

Students will be skilled at reading a mass spectra and determine the identity of the substance that produced it when given a list of candidates.

# **Learning Plan**

Preview essential questions and connect them to the concepts we will cover in the unit.

Diagram the mass spectrometer and discuss how it works (can use video(s) on the topic).

Analyze low-resolution mass spectra by identifying base peaks and molecular ion peaks.

Being the Simple Mass Spec Packet.

Examine the effect that isotopes have on the spectra.

Study fragmentation at functional groups: halides, ethers, alcohols, and ketones.

Exam the spectra of alkyl halides, ethers, alcohols, and ketones.

Complete the Predicting and Analyzing Mass Spectra Activity.

Lab "Analysis" Activity: given an experimental procedure (or proposed mechanism), determine if an experimental result was plausible through analysis of given mass spec [virtual/paper lab]

#### Assessment

#### **Formative Assessment**

Completion of practice problems assigned by teacher (textbook or otherwise).

Analyze low-resolution mass spectra for base peaks and molecular ion peaks.

Analyze low-resolution mass spectra for isotopes.

Identify fragmentation patterns and similarities between functional groups.

Identify spectra as those containing alkyl halide, ether, alcohols, or ketones.

Completion of the Lab "Analysis" Activity.

#### **Benchmark Assessment**

Completion of the Simple Mass Spec Packet.

Completion of the Predicting and Analyzing Mass Spectra Activity.

MidTerm Exam

#### **Alternative Assessment**

Develop a diagram detailing how a molecule produces its spectrum.

#### Summative Assessment

Unit Quizzes

Unit Test

#### **Materials**

Guided notes or teacher handouts

Organic Chemistry (Bruice, 2007) – electronic textbook

Activity/Lab Handouts (Includes materials specific to each activity: Lab "Analysis" Activity [Free Database: <u>https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre\_index.cgi</u>])

Molecular Modeling Kits (teacher provided)

Molecular Modeling Websites (an example: https://molview.org)

Safety Supplies (specifics to when they are required included in lab handouts)

# Integrated Accommodations and Modifications Spec Ed., ELL, At-Risk, G&T, Career Education, 504s

https://docs.google.com/spreadsheets/d/1WPR9w7-UpEeDhl7-1U\_EjbNwTuqMkUj8KIJdNwAS0Es/edit?usp=sharing