Supplemental Information

Example original week 5 activity

The following 6 pages is an example activity from the original set from week 5 that focuses on analyzing submicroscopic representative, the quantitative relationships between mass, number of moles, and number of particles, and determine chemical formulas.

DISCUSSION ACTIVITY FOR WEEK #5

Group Members:

Manager	**Recorder**
Presenter	**Reflector**

iClicker Activity (5-10 min)

THE PLAN: We are going to use experimental data to determine the atomic composition of the particles that make up a substance, and extend the particulate model of matter to describe the composition and relative mass of different particles, as well as quantify their number in a sample of a substance.

The learning objectives for today's session are for you to:

- Analyze submicroscopic representations of a chemical system
- Determine the quantitative relationships between mass, number of moles, and number of particles in a solid, liquid, or gaseous sample based on information about the chemical composition of the particles that make up the substance
- Infer the relative mass, the average relative mass, or the molar mass of a substance using mass spectrometry data
- Determine the empirical and molecular formula of a chemical compound based on experimental information about its elemental composition and mass spectrum

As explained in week 1, each member of the team will be assigned to a specific role. Print your team members' names at the top of the page in the space of their assigned roles.

Recorder: Records answers for the team and submits the team report.

Reflector: Reads the questions and checks that the final conclusion makes sense and ensures that all members have consistent answers.

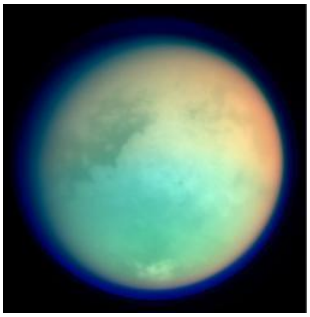
Spokesperson: Presents answers (or questions) to the class, instructor, or other teams.

Manager: Keeps the team on task and on schedule. Considers how the team is working and how it could improve in the future.

Exploring Titan: (30-35 min)

You should have watched the video on Titan before class. (https://youtu.be/TMxL3ZhO8A8) There is also information about the exploration of Titan at https://theconversation.com/the-secrets-of-titan-cassini-searched-for-the-building-blocks-of-life-on-saturns-largest-moon-83441.

Titan is the largest moon of Saturn. It has a dense atmosphere and there is data that suggests that stable bodies of liquid are present on its surface.The Cassini-Huygens robotic spacecraft mission arrived in Saturn in 2004 and studied the chemical composition of the planet and its moons, including Titan, until September 2017.

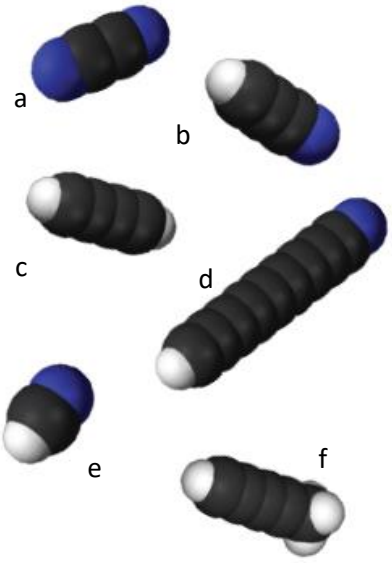


https://photojournal.jpl.nasa.gov/catalog/PIA06139

Titan's Haze

Titan's atmosphere has a characteristic haze that seems to absorb high energy radiation from the Sun, in a similar way as the ozone layer in our planet. The space filling representations of the molecules that seem to be present in this haze are shown below. (Note: Black = carbon, light grey = hydrogen, blue = nitrogen)

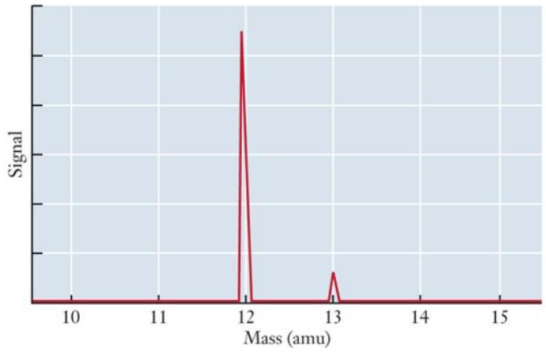
1. What is chemical formula of each of these substances?



Titan's Environment

The compounds on the surface of Titan are primarily hydrocarbons.

2. Consider a hypothetical mass spectrum of carbon. Use the graph to estimate the average atomic weight of carbon for this distribution. Document your thought process and work.



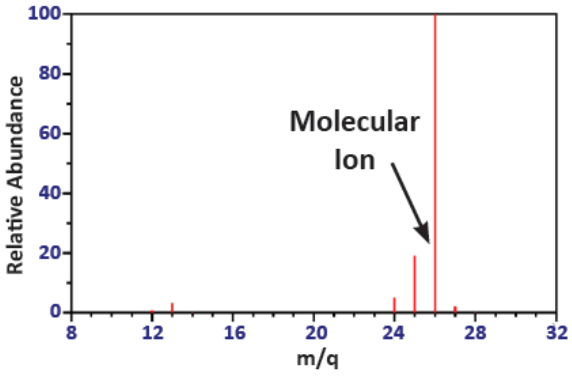
Some Data

TITAN		Additional Information
Average surface temperature	**93.7 K**	**This temperature does not vary much during the day or the seasons (min ~90 K; max 94 K)**
Average surface pressure	**1.47 atm**	**The atmospheric pressure on Earth is close to 1 atm.**
Air density at ground level	**5 kg/m^3**	**The air density on Earth is 1.2 kg/m^3**
Atmosphere composition (% in Volume)	**80-85% N_2; 5-25% Ar; 3-6% CH_4**	**Compared to 78% N_2; 21% O_2 in our planet**
Hydrosphere composition (% in Mass)	**72% C_2H_6 22.4% CH_4; 5.6% N_2**	**Compared to ~100% H_2O in our planet**

3. If you separated the components of a 10.0 g sample of the hydrosphere, how many times more molecules of ethane (C_2H_6) than of methane (CH_4) would you find in that sample? Show your work.

4. A sample of the bottom of Titan's ocean shows that one of the main components is a solid hydrocarbon. The analysis of this substance by mass spectrometry leads to the spectrum that is shown below. Elemental analysis reveals the following compositions: 92.26% C and 7.74% H.
    a. What is the empirical formula of this substance? Show your work.

b. What is the molecular formula of this substance? Provide evidence of how you arrived at your answer.



REFLECTING ON SKILLS

An important part of developing skills that are important for supporting your learning (and that are highly valued by employers) is to assess your progress and identify areas where you can improve. Reflect on your group's interpersonal communication so far today, particularly the way in which you worked together to make progress on the activity.

Critical Thinking	**Forming an argument or reaching a conclusion supported with evidence by evaluating, analyzing, and/or synthesizing relevant information.**

<table>
<tr><th>Category</th><th colspan="2">Ratings</th><th colspan="2">Observable Characteristics</th></tr>
<tr><td rowspan="4">Forming Arguments (Structure)</td><td colspan="2" rowspan="2">Made an argument that includes a claim (or position), supporting information, and reasoning</td><td></td><td>Stated the conclusion or the claim of the argument</td></tr>
<tr><td></td><td>Listed the evidence used to support the argument</td></tr>
<tr><td colspan="2">0 1 2 3 4 5

No evidence Incomplete Partial Complete</td><td></td><td>Linked the conclusion/claim to the evidence with focused and organized reasoning</td></tr>
<tr><td></td><td>State any qualifiers that limit the conditions for which the argument is true</td></tr>
<tr><td colspan="4">Suggestions for Improvements
a) Review the original goal—what question were you trying to answer?
b) Clearly state your answer to the question (your claim or conclusion).
c) Review the information you previously evaluated, analyzed, and/or synthesized, and decide what evidence supports your claim.
d) State/summarize the evidence clearly, including: what samples are being studied, how the results from the samples compare with one another (e.g. "faster than", "smaller than"), relevant statistical information (e.g. mean, standard deviation, statistical test used, and p-value), and how much difference was measured (e.g. "10% faster", "three times larger")
e) Explain how each piece of information links to and supports your answer.
f) Make sure the claim, supporting information/data, and reasoning are all present in your answer, and that the claim/conclusion answers the question.
g) List the conditions for which the claim holds true or is no longer valid</td></tr>
</table>

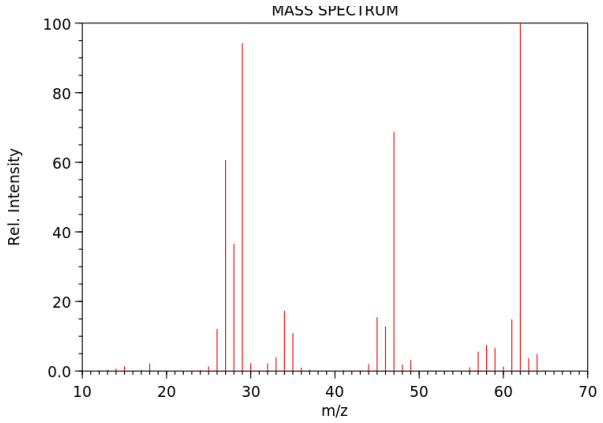
Indicate the number on the rubric you think best characterizes your level of forming arguments.

Why did you give your team this rating? Provide specific evidence related to your interactions an observer would have seen to support this rating.

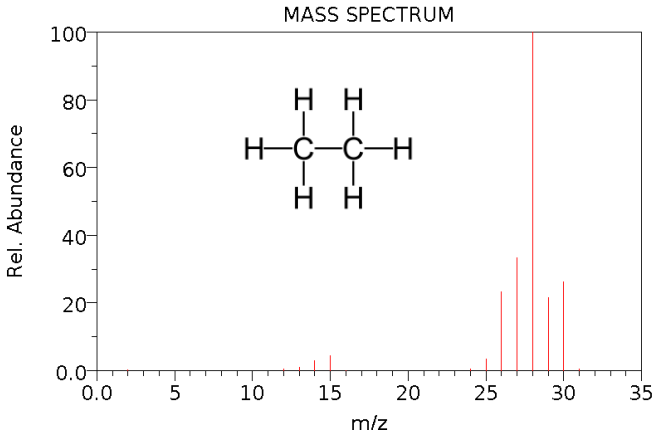
What is one way you can improve your performance next week? How do you plan to achieve this?

IF YOU HAVE TIME OR ON YOUR OWN

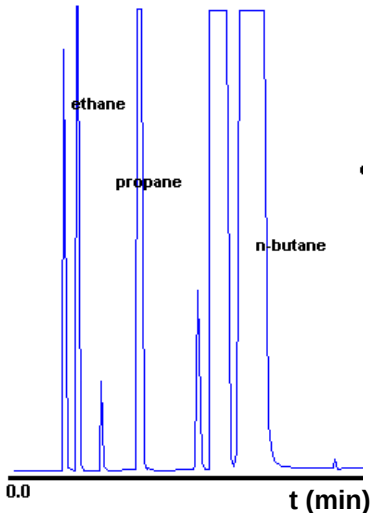
5. Analysis of a sample of liquid petroleum gas (LPG) shows the presence of a third substance with a strongly disagreeable smell that resembles that of leeks or onions. The substance seems to be intentionally added to LPG to impart an easily noticed smell to this otherwise odorless fuel. Elemental analysis of this compound reveals the following chemical composition: 38.66% **C**, 9.73% **H**, 51.61% **S**. The mass spectrum for this substance is shown in the figure. Determine the empirical and molecular formulas of this compound.



6. Ethane (C_2H_6) is commonly present in LPG in small amounts. Its mass spectrum is shown. Propose structures for the ions responsible for the peaks at an m/z ratio of 15 and 30.



7. The following image shows the results of the analysis by gas chromatography (GC) of a sample of LPG. The x-axis shows the time it took for the different substances to leave the chromatographic column (i.e., ethane exits first from the separation column). How would you explain these results using the particulate model of matter?



Example revised week 5 activity

The following 8 pages is an example activity from the original set from week 5 that focuses on analyzing submicroscopic representative, the quantitative relationships between mass, number of moles, and number of particles, and determine chemical formulas. This version of the activity has been edited in accordance to the methods section to integrate local research and explicitly promote meaningful learning.

DISCUSSION ACTIVITY WEEK #5

Group Members:

Manager	**Recorder**
Spokesperson	**Reflector**

iClicker Activity (5-10 min)

THE PLAN: We will be looking at a study conducted by researchers at the University of Iowa and using experimental data to determine the atomic composition of the particles that make up a substance. We will then extend the particulate model of matter to describe the composition and relative mass of different particles, as well as quantify their number in a sample of a substance.

The learning objectives and skills for today's session are for you to:

Learning Objectives	Skills
Analyze submicroscopic representations of a chemical system to identify the different phases present and characterize the properties different components	Know symbols for atomic, molecular, and ionic representations
Determine the quantitative relationships between mass, number of moles, and number of particles in a solid, liquid, or gaseous sample based on information about the chemical composition of the particles that make up the substance	Use molar mass relationships
Infer the relative mass, the average relative mass, or the molar mass of a substance using mass spectrometry data	Use relative intensity of the mass spectroscopy data to calculate the average relative atomic mass
Determine the empirical and molecular formula of a chemical compound based on experimental information about its elemental composition and mass spectrum	Relate percent composition to empirical formula
	Use empirical formula and molar mass to calculate molecular formula
	Relate molar mass to data from mass spectrum

As explained in week 1, each member of the team will be assigned to a specific role. Print your team members' names at the top of the page in the space of their assigned roles.

- **Recorder:** Records answers for the team and submits the team report.

- **Reflector:** Reads the questions and checks that the final conclusion makes sense and ensures that all members have consistent answers.
- **Spokesperson:** Presents answers (or questions) to the class, instructor, or other teams.
- **Manager:** Keeps the team on task and on schedule. Considers how the team is working and how it could improve in the future.

Organosulfate Quantification near Lake Michigan (30-35 min)

Last week, we discussed particulate matter composition and identified some of the molecules that make up atmospheric particulate matter near Lake Michigan from their structures and formulas. This week we will discuss the methods for how the researchers determined what molecules composed the samples collected.

You should have watched the video that discusses how the mass spectrometer instrument works: (https://uicapture.hosted.panopto.com/Panopto/Pages/Viewer.aspx?id=2f2ea2a7-ce32-42a1-b5e5-ae3701755cd0)

Take the first few minutes to talk about major points as a group and then work together to answer the following questions.

The recorder of the group should write down the responses to these questions and submit to Gradescope after class – make sure to record the names of team members present at the top of the page and select those team members when you submit the assignment.

1. What did your group know about mass spectrometry before watching the video?

2. How does your group think about mass spectrometry differently after watching the video compared to what you have learned in class?

3. Scientists can use mass spectrometry to determine the molecular formula of an analyte, which can then be used to calculate the average atomic weight of an analyte. Organosulfates analyzed in this study are primarily made up of organic molecules with an attached sulfate group. We know that at the center of a sulfate group is a sulfur atom. Consider hypothetical mass and isotopic abundance data for of sulfur.

Isotope	Atomic Mass (atomic mass units)	Natural Abundance (%)
^{32}S	31.972	94.99
^{33}S	32.971	0.75
^{34}S	33.968	4.25
^{36}S	35.967	0.01

a. Use the data to estimate the average atomic weight of sulfur.

b. Explain your thought process of the work you did in part a.

4. We saw some examples of organosulfates seen in particulate matter last week. Particulate matter in this study was composed of 59% organic matter by weight on average. On average, the organosulfates analyzed accounted for approximately 3.7% of this organic matter by weight. But researchers want to know more specifically which organosulfates make up this organic matter.

   Consider the following data on organosulfates of a particulate matter sample.

Compound	Molecular Formula	Mass to charge ratio (m/z)	Percent of organic matter
methyltetrol sulfate	$C_5H_{11}SO_7^-$	215	2.2%
methyltrihydroxyaldehyde hemiacetal	$C_5H_9SO_7^-$	213	0.2%
methydihydroxylactone	$C_5H_7SO_7^-$	211	0.2%

   Atmospheric chemists often refer to these compounds by their mass to charge ratio (*m/z*), so we will do that from here on.

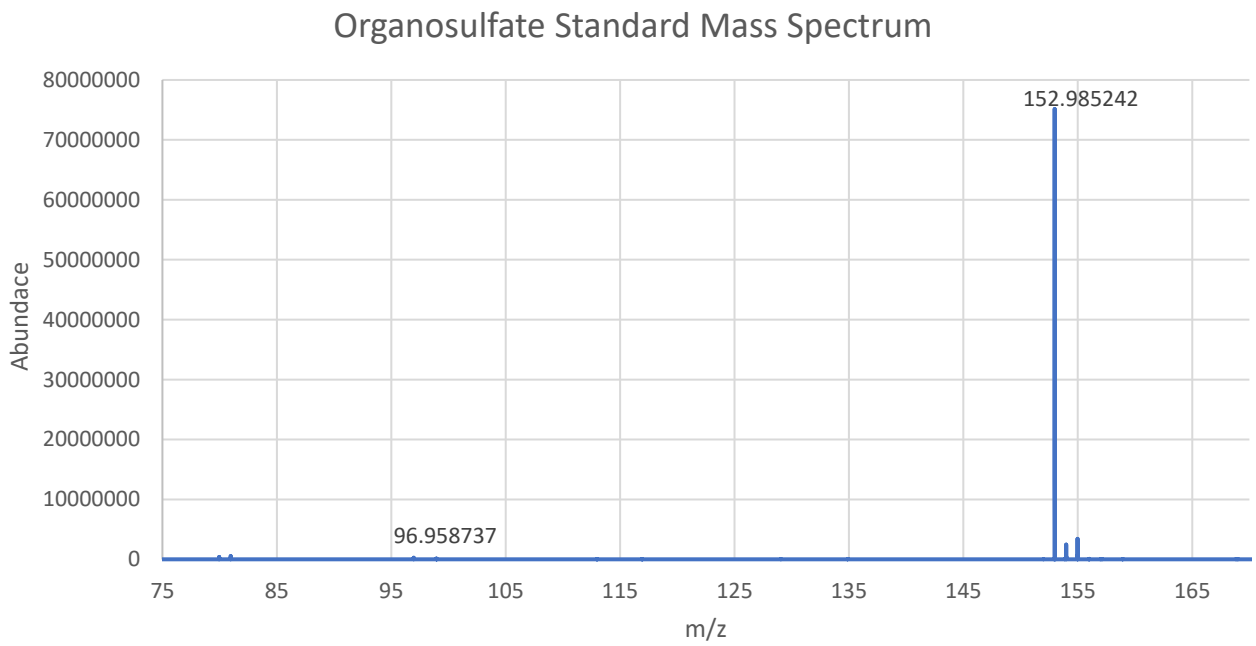
   a. Suppose a 3.2 µg sample of particulate matter that contained these three organosulfates was analyzed. Knowing that organosulfates make up 3.7% of organic matter in particulate matter samples, what percentage of the particulate matter is made up of these organosulfates?

b. How many times more molecules of *m/z* 215 would you find in this sample over *m/z* 213?

c. How many more molecules of *m/z* 215 would you find in this sample over *m/z* 211?

5. Particulate matter composition includes a wide variety of substances, as we saw last week. We know that this project uses tandem mass spectrometry, which was discussed in this week's video to track compounds by the sulfate functional group, which frequently fragments to bisulfate anion (HSO_4^-) and/or sulfate ion radical ($SO_4^{-\bullet}$) under MS/MS.

   After analyzing their samples, the researchers wanted to confirm the identity of one organosulfate. Researchers can use a standard to confirm the identity of an organosulfate. These standards are organosulfate salts with a potassium cation. The mass spectrum of this standard showed major MS peaks at *m/z* 152.9852 corresponding to the intact anion and *m/z* 96.9587 corresponding to a fragment ion can be seen below.



Elemental analysis was also completed on the organosulfate and revealed the following composition:

Element	Percent Composition
Potassium	20.34
Carbon	18.74
Hydrogen	2.62
Sulfur	16.68
Oxygen	41.60

a. What is the empirical formula of the substance?

b. What is the molecular formula of this substance?

c. Explain how you arrived at your answer to part b.

PAUSE TO REFLECT ON SKILLS AND HOW YOU CAN IMPROVE PERFORMANCE

An important part of developing skills that are important for supporting your learning (and that are highly valued by employers) is to assess your progress and identify areas where you can improve.

Teamwork	Interacting with others and building on each other's individual strengths and skills, working toward a common goal.

<table>
<tr><th>Category</th><th>Ratings</th><th colspan="2">Observable Characteristics</th></tr>
<tr><td rowspan="6">Progressing</td><td rowspan="2">Moved forward towards a common goal</td><td></td><td>Stayed on task, attentive to the assignment with only brief interruptions</td></tr>
<tr><td></td><td>Refocused team members to make more effective progress towards the goal</td></tr>
<tr><td rowspan="3">0 1 2 3 4 5

No evidence Rarely Sometimes Consistently</td><td></td><td>Checked time to monitor progress on task.</td></tr>
<tr><td></td><td></td></tr>
<tr><td></td><td></td></tr>
<tr><td colspan="3">Suggestions for Improvement:
a) Minimize distractions and focus on the assignment (close unrelated websites or messaging on phone or computer, turn off music, put away unrelated materials).
b) Redirect team members to the current task.
c) Ask other team members for their input on a task to move the discussion forward.
d) Ask for assistance if your team is stuck on a task and making little progress.
e) Compare progress on the task to the time remaining on assignment.
f) Communicate to team members that you need to move on.
g) As a team, list tasks to be done and agree on the order for these tasks</td></tr>
</table>

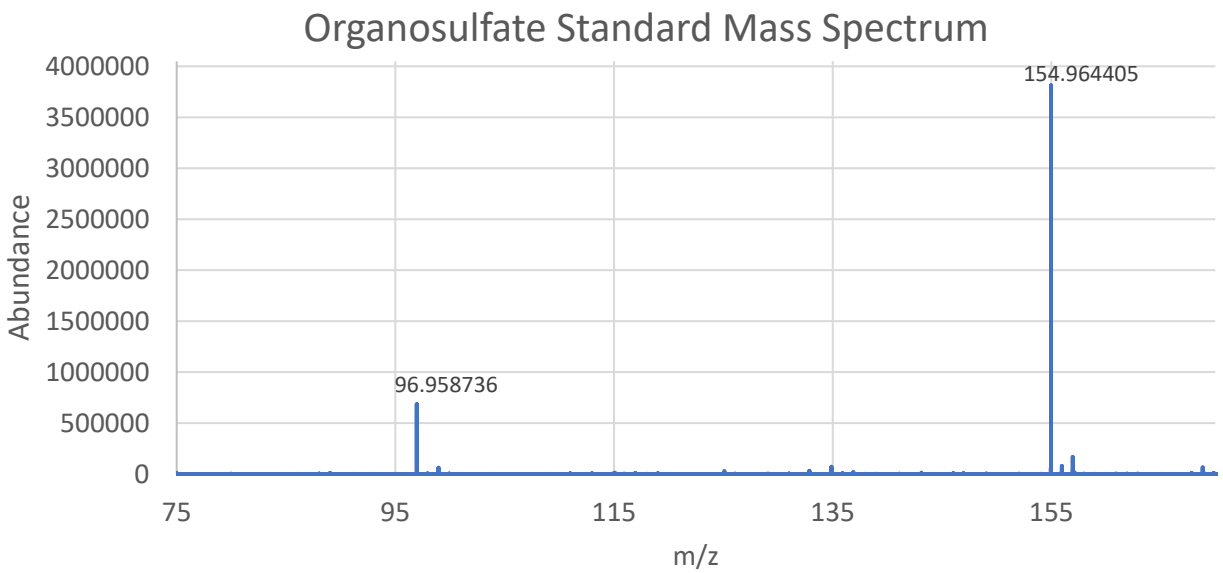
- As a team, choose a score that you think best characterizes your team's level of performance for today's category.

- Explain why the team chose this rating. Provide specific evidence based on the observable characteristics you discussed and at least one specific example team members discussed.

- Identify one way you can improve your performance next week. How do you plan to achieve this?

Continuing on..

6. As we have discussed, particulate matter is made up of a wide variety of organic matter. In addition to the molecule your group analyzed above, the research team found another organosulfate in some of their samples that they needed to confirm with a standard using the same procedure as described in question 5 using a potassium salt. Two major ions were observed (*m/z* 96.9587, fragment ion) and *m/z* 154.9644, intact anion) and can be seen below:



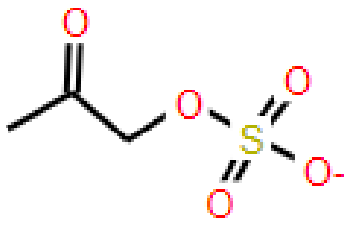
Elemental analysis was also completed on the organosulfate and revealed the following composition:

Element	Percent Composition
Potassium	20.14
Carbon	12.37
Hydrogen	1.56
Sulfur	16.51
Oxygen	49.42

a. What is the empirical formula of the substance?

b. What is the molecular formula of this substance?

7. As your group discovered in question 5, hydroxyacetone sulfate was found to be one of the organosulfates found in this study. The structure for the molecule is given below.



   a. Draw on the above structure where the molecule will fragment under electrospray ionization conditions encountered in the MS.

   b. How do you know that your answer for part a is correct? Use complete sentences to create an argument.

8. Calculate the molecular weight of hydroxyacetone sulfate ($C_3H_5SO_5^-$) accurate to four decimal places.

Element	Average Atomic Mass (atomic mass units)
Carbon	12.0107
Hydrogen	1.0078
Sulfur	32.065
Oxygen	15.9990

9. Using your answer from number 8 and knowing that *m/z* 152.9852 was observed by high-resolution MS, explain the similarities and differences between the molecular weight and ion observed by MS.

10. The two molecules you have identified in this worksheet from the mass spectral data are hydroxyacetone sulfate and glycolic acid sulfate. These compounds form in the atmosphere from reactions of gas phase precursors, particularly isoprene that is released from plants, and sulfuric acid that formed from the oxidation of sulfur dioxide in the atmosphere. Most sulfur dioxide originates in fossil fuels, like coal combustion. Following that hydroxyacetone sulfate and glycolic acid sulfate were among the most abundant organosulfates quantified at Zion, IL during LMOS 2017, what do they tell us about the sources of airborne particulate matter at that location?

Supplemental Figures

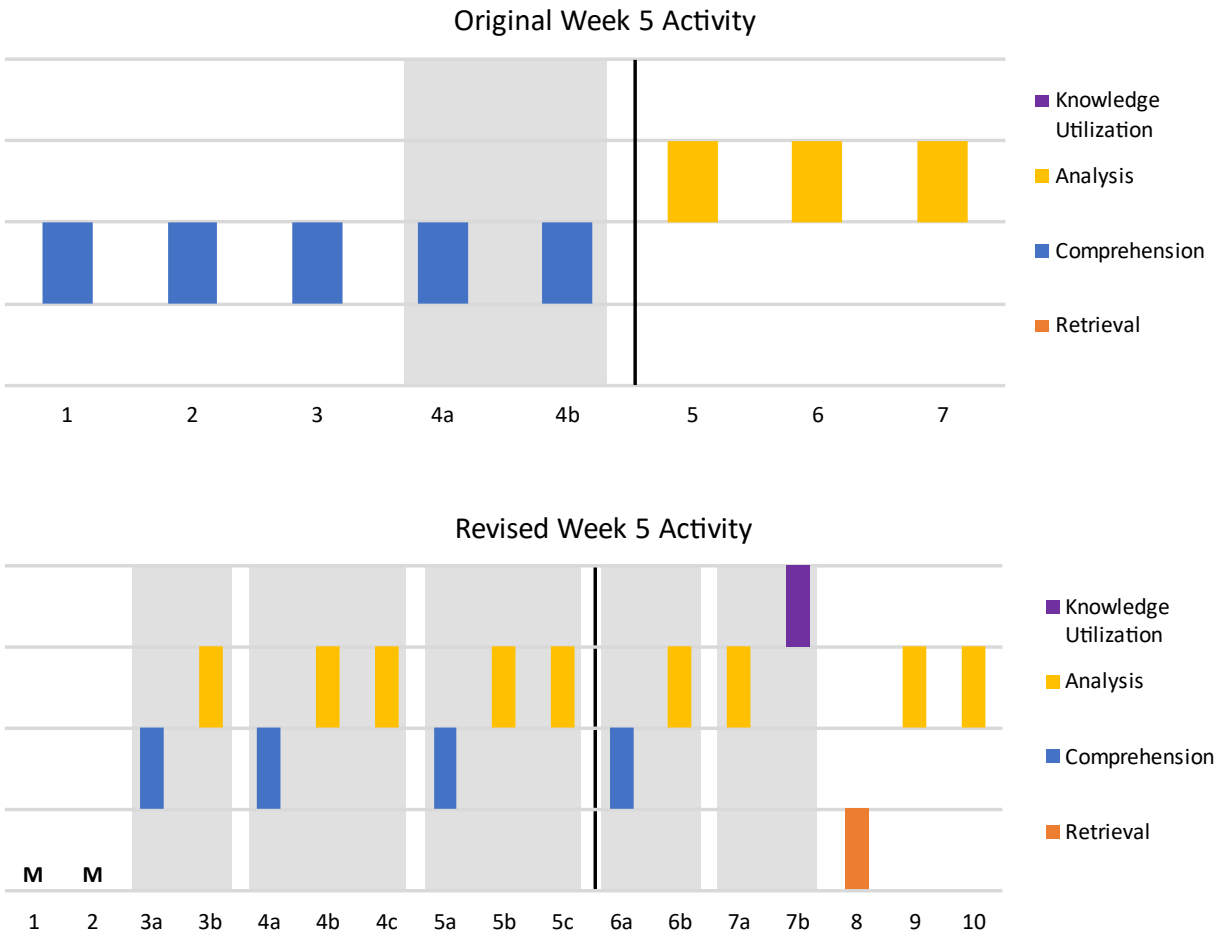


Figure S1. Marzano question level coding for the original and revised week 5 activities. The black line indicated the where the reflection is placed and question to the right are in the continuing on section. M indicated a metacognition question that is not leveled like the other four cognitive questions level. Grey boxes are used to highlight when questions are scaffolding for students to answers with parts a, b, c etc.

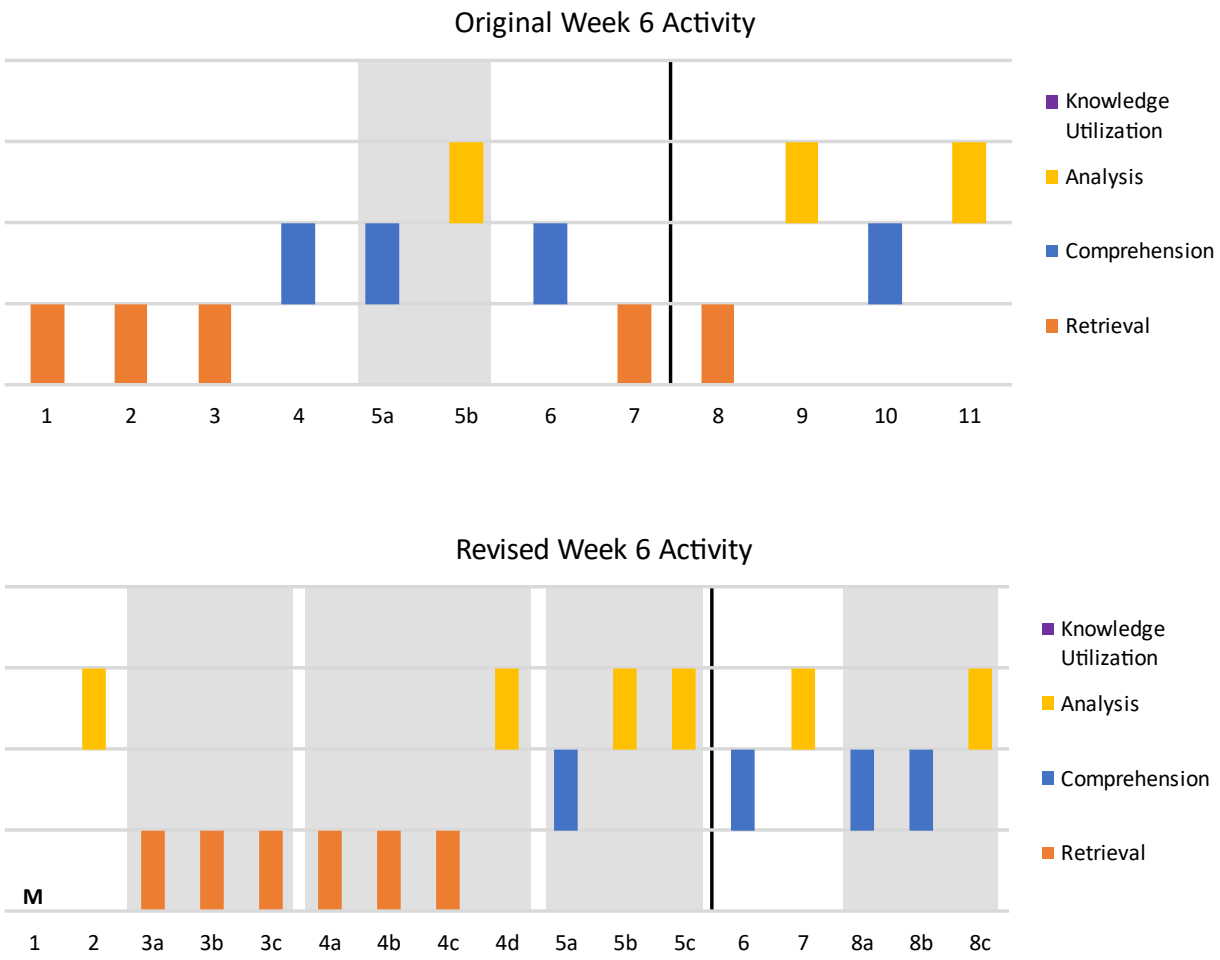


Figure S2. Marzano question level coding for the original and revised week 6 activities. The black line indicated the where the reflection is placed and question to the right are in the continuing on section. M indicated a metacognition question that is not leveled like the other four cognitive questions level. Grey boxes are used to highlight when questions are scaffolding for students to answers with parts a, b, c etc.

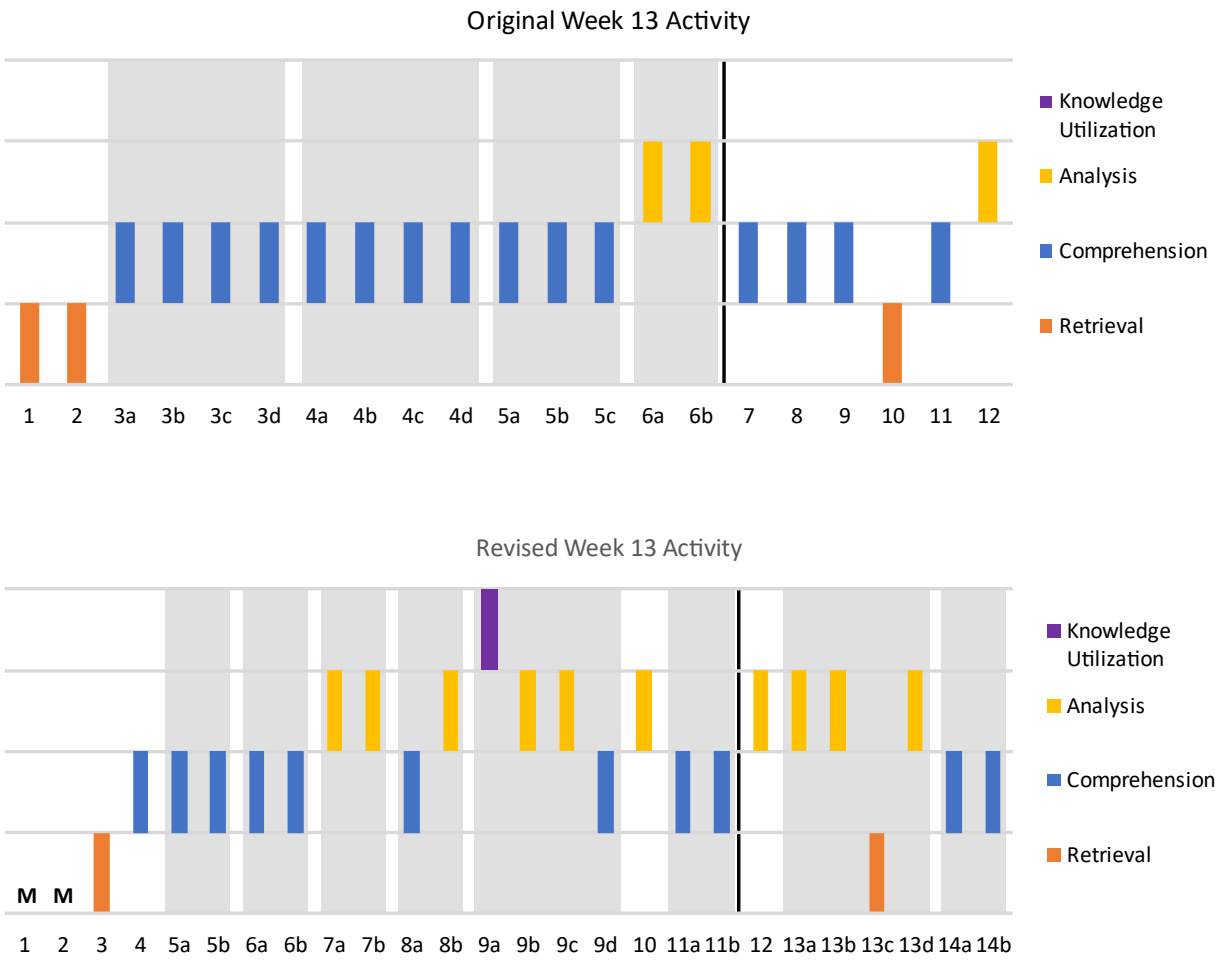


Figure S3. Marzano question level coding for the original and revised week 13 activities. The black line indicated the where the reflection is placed and question to the right are in the continuing on section. M indicated a metacognition question that is not leveled like the other four cognitive questions level. Grey boxes are used to highlight when questions are scaffolding for students to answers with parts a, b, c etc.