

Mass Spectrometry

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1 Conceptual Questions

1. *Concepts and Principles:* The important principles we considered regarding the lab were the process of ionization, the Lorentz force in the presence of a magnetic field, and the fragmentation of gases. Ionization, where an atom or molecule accumulates charge, occurred in the lab through the loss of electrons. The negatively ionized gas molecules then traveled through a magnetic field, causing them to be deflected by the magnetic force

$$F_{\text{magnetic}} = q(\vec{v} \times \vec{B}), \quad (1)$$

where q is the charge of an electron, \vec{v} is the velocity of the ionized molecule, and \vec{B} is our applied magnetic field. Because different gases (each with different masses) ionize differently, the gases experienced different deflections as a result of the Lorentz force and a varied charge accumulated and therefore were

differentiated by a mass to charge ratio.

In gas fragmentation, the molecules of a gas separate, which we observed as peaks at the values for the atomic mass units of the constituent atoms of the molecules as well as peaks at values that represent the molecule with one or more atoms removed.

2. *Experimental Parameters:* Because the force from Equation 1 acted as the magnetic field varied, the ionized molecules traveled in a spiral. Since different atoms with differing masses accumulated different numbers of electrons, they were pushed by the force to varying radii, allowing for the apparatus to differentiate between masses read based on radial distance. The apparatus then returned a plot of a particular pressure in Torr versus the mass in AMU. Here the pressure was used as a relative intensity of the sample. The peaks of the plots were then compared to the total mass of the sought-after gas molecule along with the masses of the gas' constituent atoms to account for fragmentation.

3. *Assumptions, Simplifications, and Limitations:* Equation 1 is a simplification of the more general Lorentz Force Law, or

$$F_{Lorentz} = q\vec{E} + q(\vec{v} \times \vec{B}), \quad (2)$$

where before we do not consider the electric field. We argued that the presence of the electric field would not produce large enough variation in the force to consider since we varied the magnetic field. One limitation of our experimental

setup was the inability to measure masses greater than 100 AMU. One difficulty in the experiment was the presence of atmospheric gases and water. These appear as extra peaks in the data, and obscure the peaks of the gases we investigated.

4. *Why this way in particular?* The experimental setup allowed us to extract different mass values for the molecules in the chamber by ionizing them through the accumulation of negative charge and separating them based on deflection radius from the magnetic force. By differentiating gases based off of a mass-to-charge ratio we were able to identify our gases and their individual atoms while also being able to recognize extraneous data from water and atmospheric gases.

2 Results and Data

Below, Table 1 displays each gas analyzed, as well as where each peak was located in terms of the mass read. Additionally, Table 1 displays the energy needed for an electron to singly, double, and triply ionize a particular gas. Since the energy of the ionizing electrons from our experiment was output from the spectrometer as 70 eV, each gas would have been singly ionized, as we see in the Figures below, but only Argon could feasibly be doubly ionized, which is consistent with our plots given that Argon did have a small peak at half its expected value of 40 AMU. Note that due to the turbo pump failing we were unable to measure the spectrum for atmosphere, but were able to extract the a Nitrogen to Oxygen ratio of 4:1 from the excess

atmospheric gas in our other measurements, which is consistent with the abundance of nitrogen we expect in the atmosphere.

Gas	Peaks [AMU]	Singly [eV]	Doubly [eV]	Triply [eV]
Helium	4	24.59	54.42	None
Argon	40, 20	15.76	27.63	40.74
Methane	17, 16, 15, 14, 13	12.61	None	None
Carbon Dioxide	44, 22, 16, 12	13.77	None	None

Table 1: Analyzed Gases, their peaks, and energy required for an electron to singly, doubly, and triply ionize the gas [1]

Displayed below are the Figures of each analyzed gas and the accepted data from NIST [2]. Appearing in each plot are peaks from excess atmospheric gases (at 28 AMU for diatomic Nitrogen and 32 AMU for diatomic Oxygen) and water and were therefore ignored when comparing the spectra to the expected result.

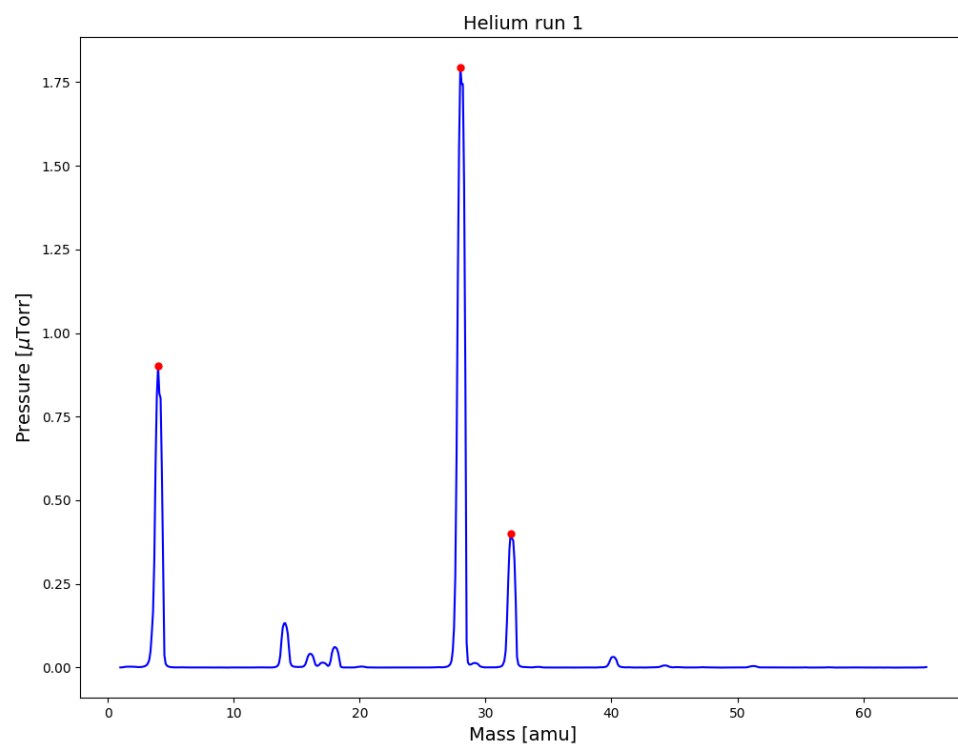


Figure 1: Mass Spectrum for Helium

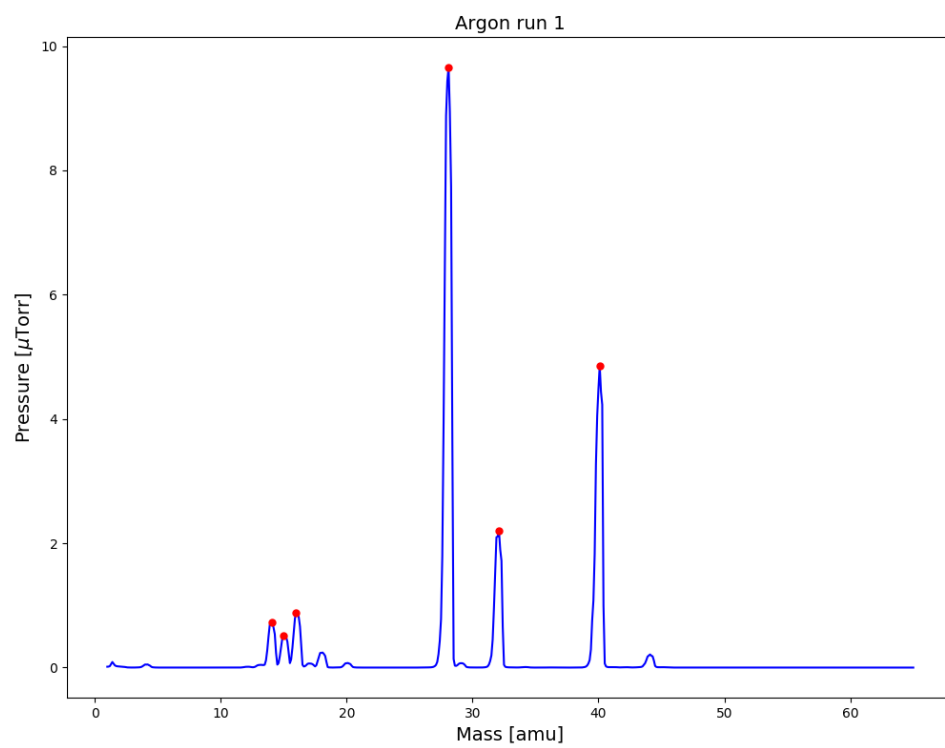


Figure 2: Mass Spectrum for Argon

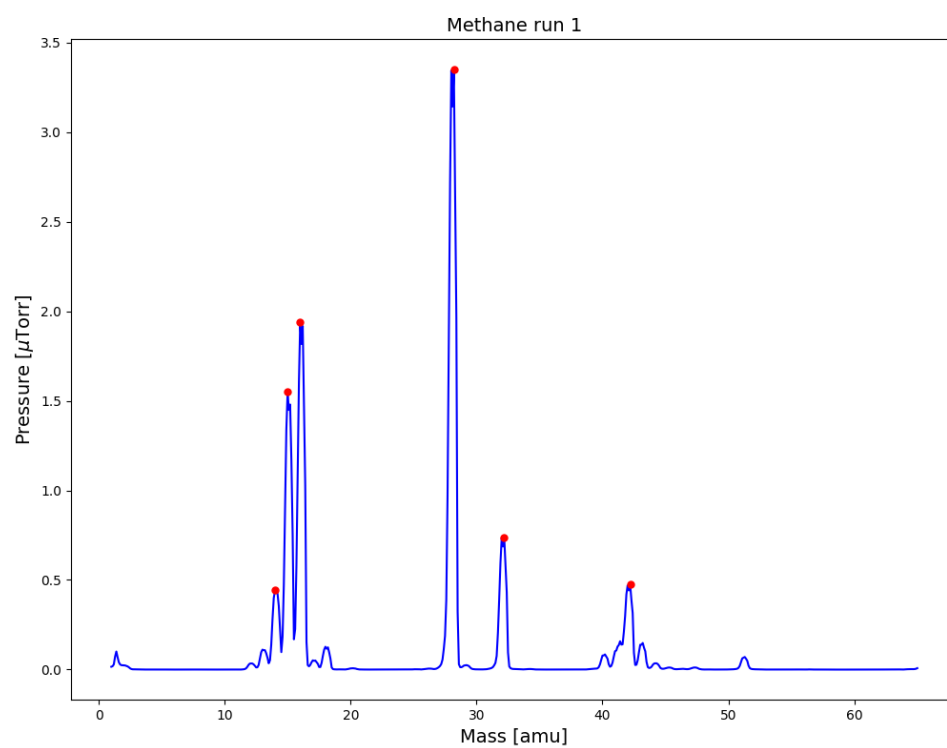


Figure 3: Mass Spectrum for Methane

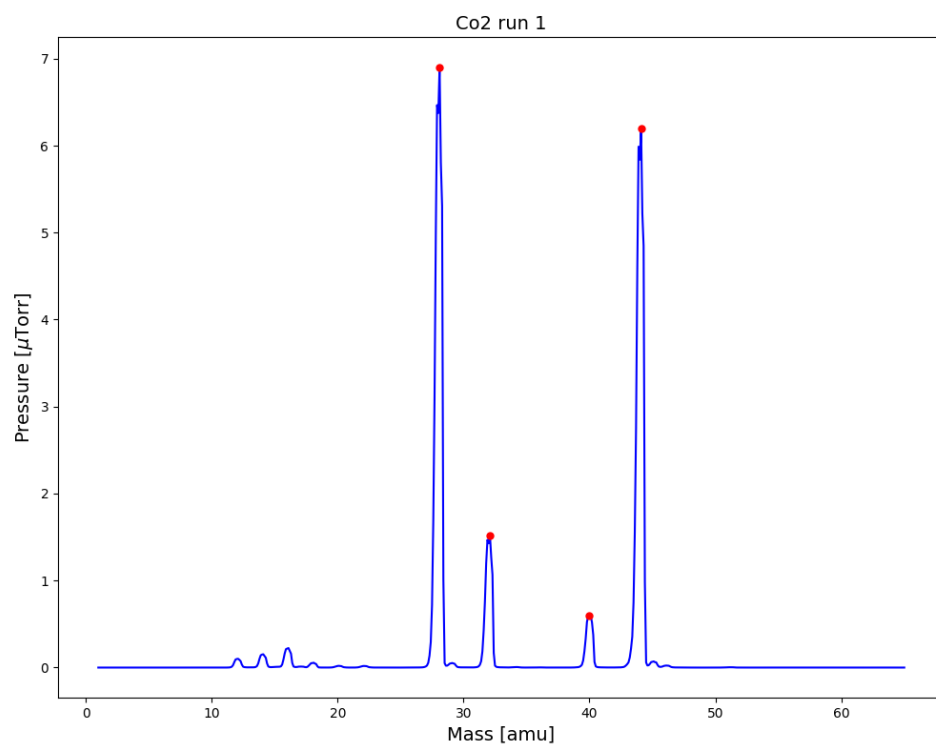
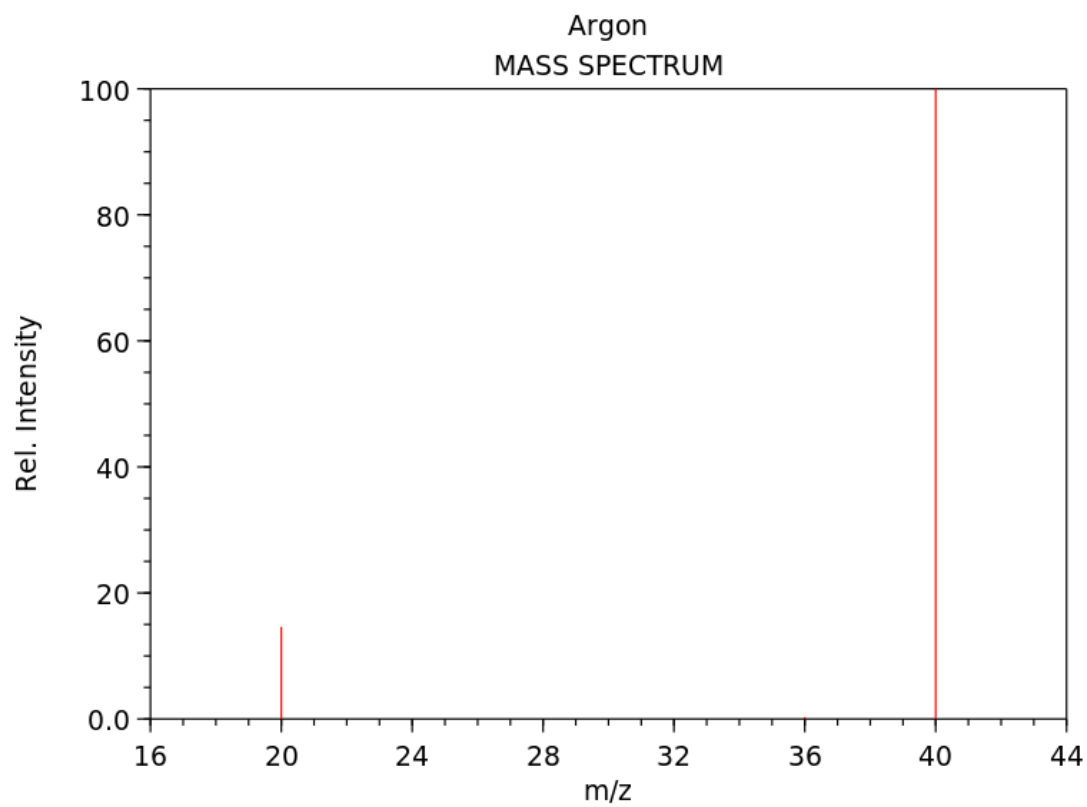
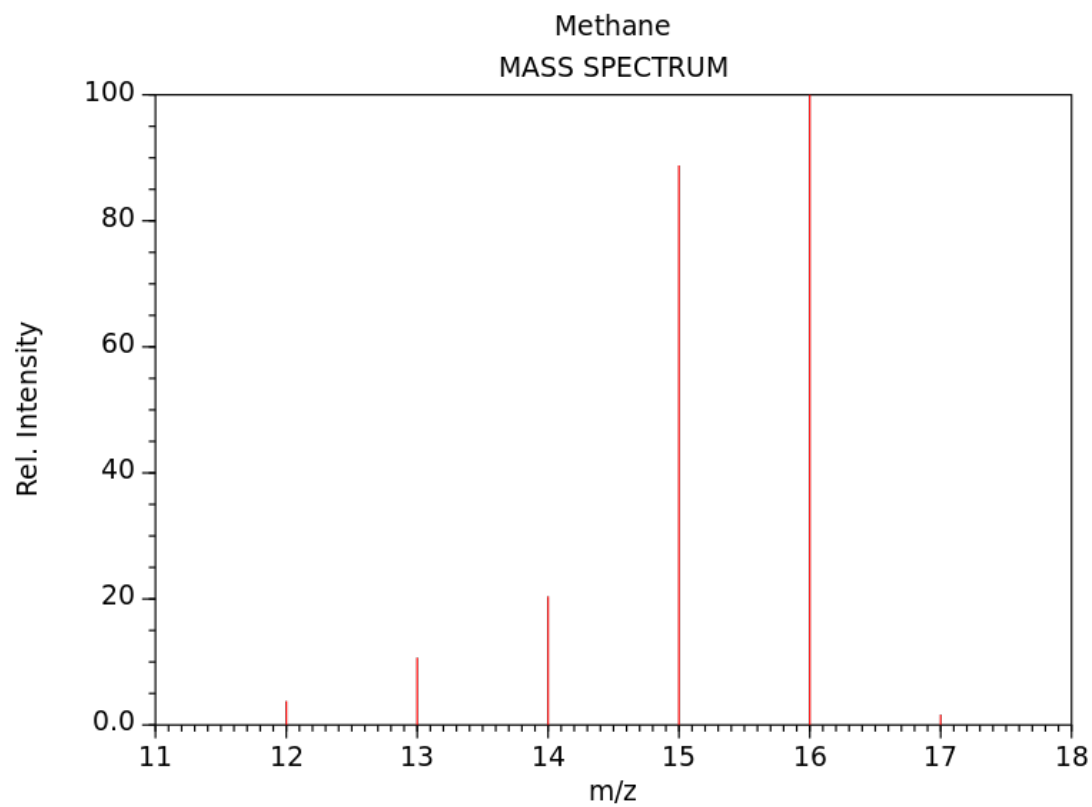


Figure 4: Mass Spectrum for Carbon Dioxide



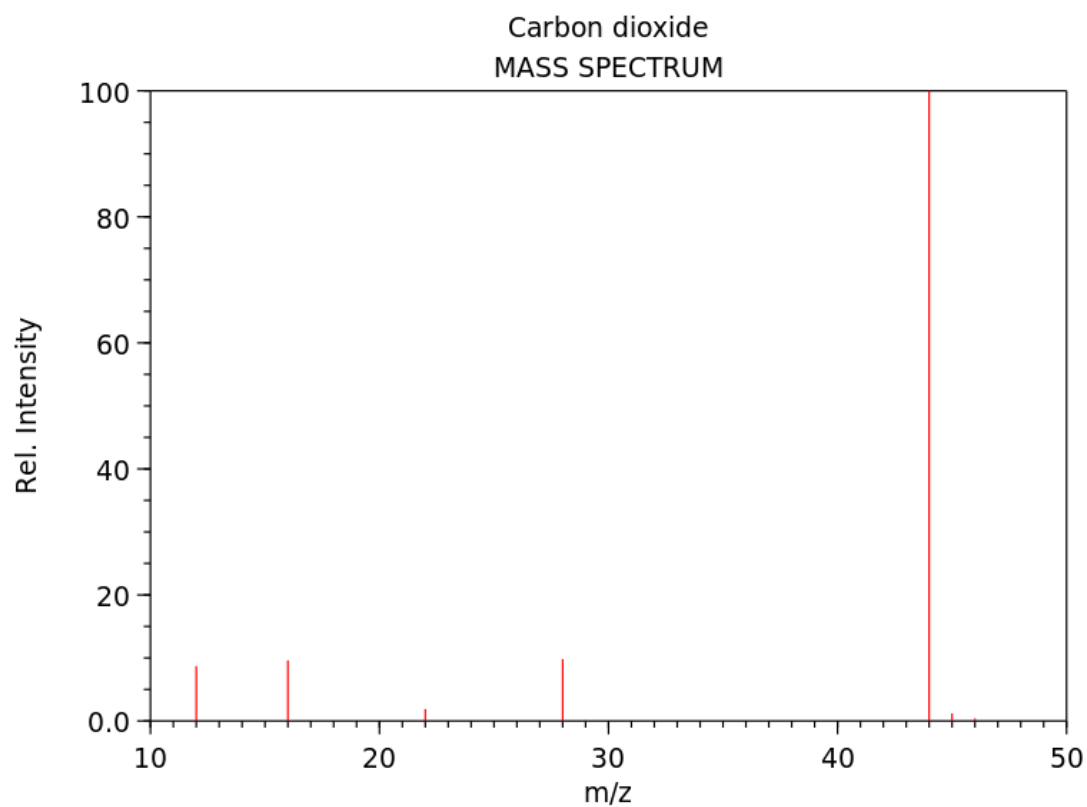
NIST Chemistry WebBook (<https://webbook.nist.gov/chemistry>)

Figure 5: NIST Spectrum for Argon



NIST Chemistry WebBook (<https://webbook.nist.gov/chemistry>)

Figure 6: NIST Spectrum for Methane



NIST Chemistry WebBook (<https://webbook.nist.gov/chemistry>)

Figure 7: NIST Spectrum for Carbon Dioxide

References

- [1] Ionization energies (ev) of atoms and ions. <http://www-personal.umich.edu/~cowley/ionen.htm>.
- [2] <https://webbook.nist.gov/chemistry/>.