Mass Spectroscopy

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1 Operating Mechanism

The quadrapole mass spectrometer (QMS) accepts a gaseous input that is fed into a vacuum chamber through a variable leak valve. A schematic of the machine components is shown in Figure 1. The leak valve releases a trickle of gas molecules into the high-vacuum chamber that is maintained at vacuum by a turbo and roughing pump pair. Here we refer to the gas particulates as individual molecules instead of a volume encompassing gas because at such low pressure the mean free path of molecules gives them independent, ballistic, behavior. The turbo pump is the delicate, but also more capable, of the two pumps and is reserved for achieving further vacuum after the roughing pump has done the initial brute work. A turbo pump uses a number of rotary blades to collide with gas molecules, imparting mechanical energy with each collision and sending molecules speeding to the exhaust, reaching pressures down to approximately 10^{-8} Torr. This mechanism is naturally sensitive to high pressure and, depending on the axial blade separation, will only function once a sufficient vacuum has been reached. This pressure dependence arises due to the mean free path of individual gas molecules, because once molecules have gained momentum from a blade, they must be able to travel to the next blade or out the exhaust without being redirected by a molecular collision. This prerequisite pressure is obtained through the preliminary roughing pump, which operates by trapping a fixed volume of gas and forcefully displacing the entirety of that volume to an exhaust. This mechanism is reliable down to 10^{-3} Torr but fails to go further due to mechanical and structural limitations. Additionally, when the two pumps are placed in series, the roughing pump works to decreases the pressure of the turbo pump's exhaust region.

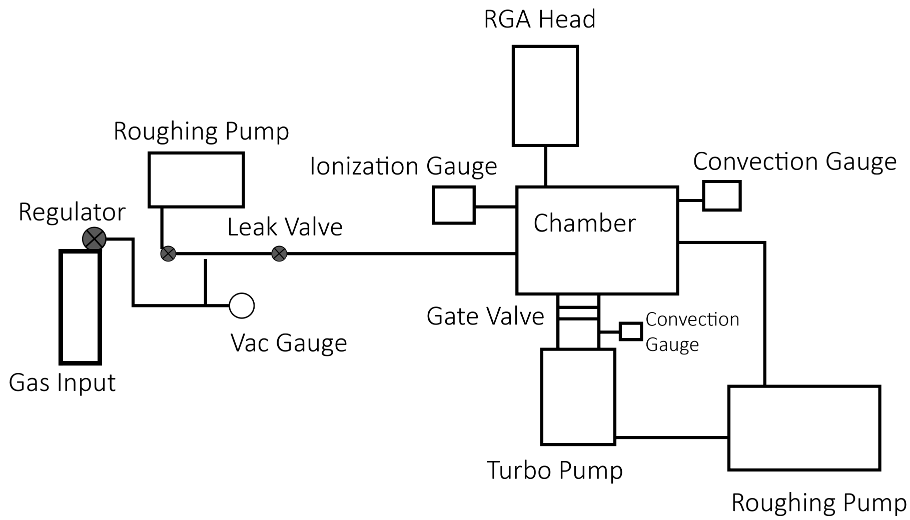

Figure 1: Block diagram of the vacuum chamber and QMS configuration.

The pressure at the turbo pump inlet is measured by a convection gauge, and another convection gauge measures the pressure in the chamber. The chamber gauge provides a preliminary measurement to ensure when it is safe to turn on the high precision pressure meter, called an ionization gauge. This is necessary because the RGA probe can be damaged when above 7×10^{-4} Torr, which is below the maximum sensitivity of a convection gauge, 6×10^{-4} Torr. A convection gauge works by maintaining a sensor wire at a certain temperature, where the power necessary to maintain that temperature is pressure dependent. Instead, the ionization gauge uses excited electrons to ionize gas molecules and measure the ion current, which performs well in the range $10^{-3} - 10^{-10}$ Torr, but would be overwhelmed and become damaged if turned on above this pressure.

The QMS uses a quadrapole filter, ionizer, and ion detector to sort molecules and atoms from the chamber by mass. The ionizer uses electrons boiled from a filament to ionize residual gas molecules, which then travel along the long z-axis of a quadrapole filter. The quadrapole filter is a set of four conducting rods that are maintained at a time varying potential, where two of the rods are at a negative potential and situated alternatively such that the time oscillating potential creates a crossed electric and magnetic field, which causes ions to oscillate in the x-y plane. With proper adjustment of voltage parameters, only atoms of a certain mass have stable trajectories that allow them to reach the ion detector, which is a shielded Faraday cup that measures the incident ion current and converts this value into a molecular chamber pressure [2].

2 Results and Discussion

We investigated Argon, Neon, Krypton, and laboratory air with background measurements prior to introducing each sample in order to minimize off-gassing related error. The raw Argon data is shown in Figure 2, and the background subtracted results are seen in Figure 4, where the background is from Figure 3. The first three ionization energies for Argon are 15.7 eV, 27.6 eV, and 40.7 eV, while the energy of the bombarding electron is in the range 25-105 eV, then we can predict all three of these ionization states are possible [1]. For Argon there is a peak at 40 amu, which is expected, and another at 20 amu, the ratio of the 40 amu peak height to the 20 amu peak height is 9.23.

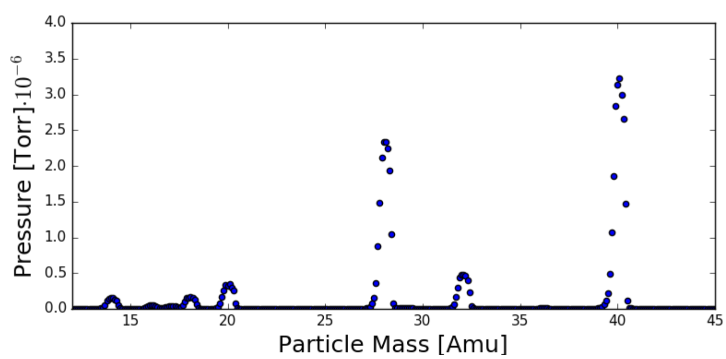

Figure 2: QMS results of an Argon sample without background subtraction. The peak at 14 amu is N, peak at 20 amu is possibly doubly ionized Argon, 28 amu is N_2, 32 amu is O_2, and 40 amu is Ar.

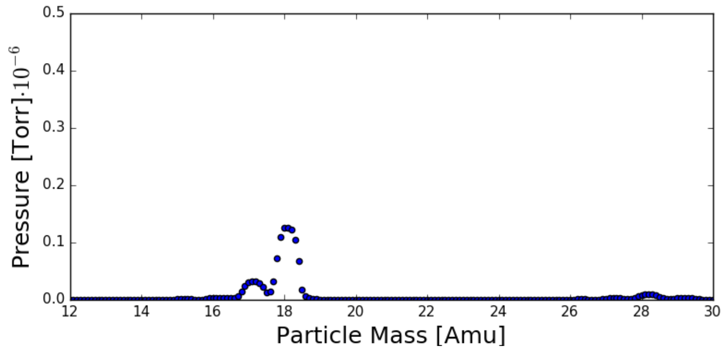

Figure 3: Background measurements taken prior to introduction of Argon into the chamber. The peak at 17 amu is OH^+ and 18 amu is H_2O.

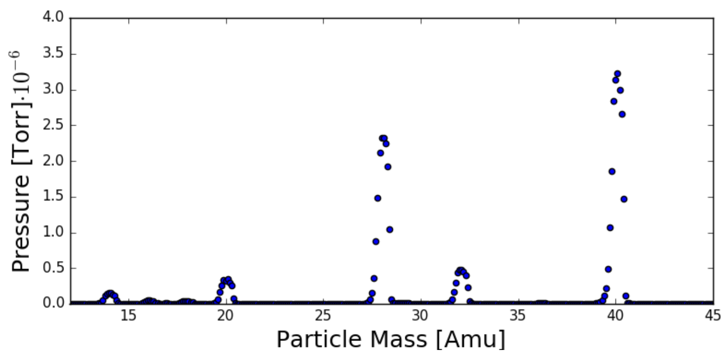

Figure 4: QMS results of an Argon sample with background subtraction.

The results for laboratory air are shown, with background subtraction, in Figure 5. Air is known to be approximately 78% N_2, 21% O_2, and 1% Ar. We found the ratio $N_2/O_2 = 4.6$ and $N_2/Ar = 181$, while the expected ratios are $N_2/O_2 = 3.7$ and $N_2/Ar = 89$.

We show the results for a sample of Neon gas in Figure 6. The first three ionization energies of Neon are 21.6 eV, 40.9 eV, and 63.5 eV, so again we can expect that all three ionization states are possible. In Figure 6, there is a clear peak at 20 amu, which corresponds to Neon, but there are no peaks at 10 amu or below.

Figure 7 shows the QMS results of a Krypton sample. The first three ionization energies of Neon are 14 eV, 24.3 eV, and 34.7 eV, which means we

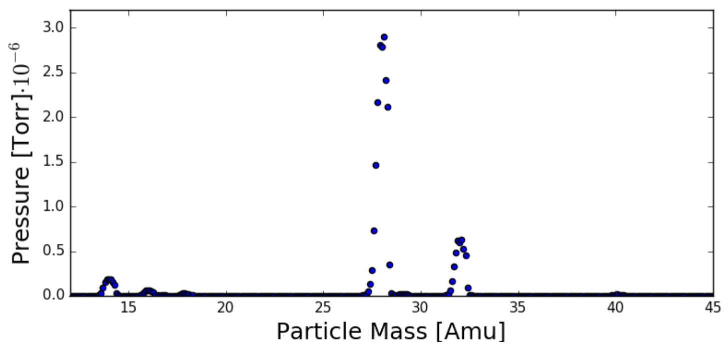

Figure 5: QMS results of laboratory air with background subtraction. Here the peak at 14 amu is N, at 16 amu is O, 17 amu is likely OH^+, 26 amu is N_2, and 32 amu is O_2.

can expect that all three ionization states are possible. Krypton is a heavy atom, of 84 amu, which is beyond the QMS capability and it does not appear that we detected any Krypton isotopes.

We also measured, shown in Figure 8, analysis of a human breath, comparing between breaths held in the lungs for two different amounts of time. Note that we were unable to guarantee that the leak valve was in the exact same position across these two measurements. Qualitatively, we can only extract that in the quick exhale situation the ratio of $N_2/O_2 = 4.68$, while in the holding of breath $N_2/O_2 = 4.51$. Not quite as expected. Lastly we investigated two different compressed air canisters, seen in Figure 9, but found no noticeable difference between the two and did not detect any molecules other than molecular oxygen and molecular hydrogen.

3 Conclusion

The QMS is capable of isolating and identifying the chamber pressure of molecular and atomic particles, which is sufficient information to determine the relative presence for each constituent of the input sample. We investigated three noble gases and were able to locate an expected peak for all but Krypton. By doing a background subtraction we were able to filter out any unwanted data that results from off-gassing within the chamber and we identified this off-gassing to be primarily water and water fragments.

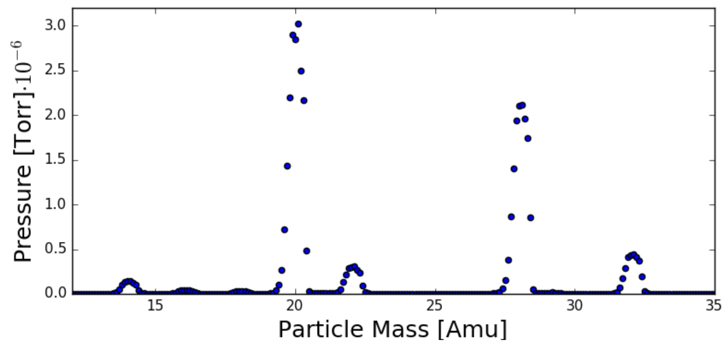

Figure 6: QMS results of a Neon sample with background subtraction. Of the new peaks unseen so far, 20 amu is clearly Ne, but there is another unknown peak at 22 amu.

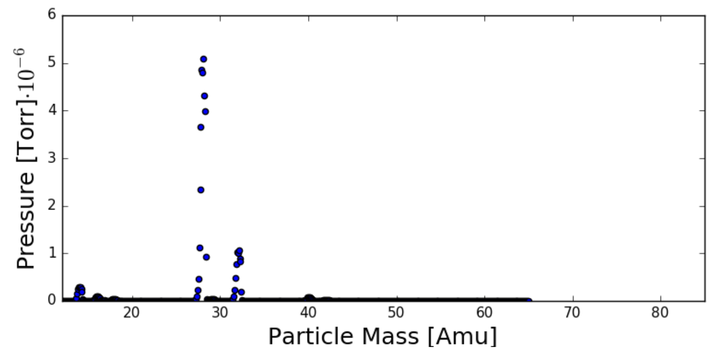

Figure 7: QMS results of a Krypton sample with background subtraction. This result looks similar to that of air, with a possible relic of Krypton at its half mass value near 40 amu.

References

[1] Ionization Energies (eV) of Atoms and Ions. URL `https://dept.astro.lsa.umich.edu/~cowley/ionen.htm`.

[2] Models RGA100, RGA200, and RGA300 Residual Gas Analyzer, 2009.

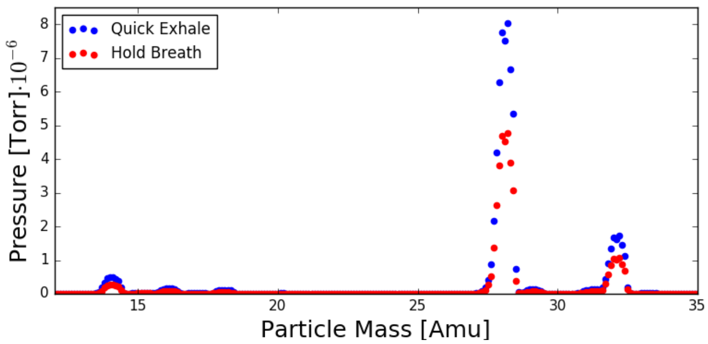

Figure 8: Comparison of the QMS results between two exhaled breaths. Blue dots represent a breath that was exhaled immediately and the red dots correspond to holding air in the lungs for approximately thirty seconds.

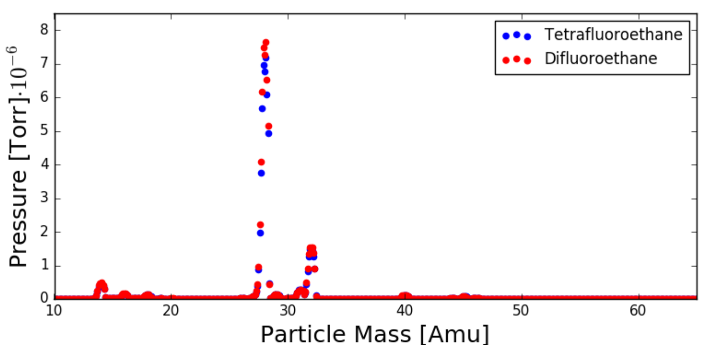

Figure 9: Comparison of the QMS results between two pressurized air canisters with a different propellant.