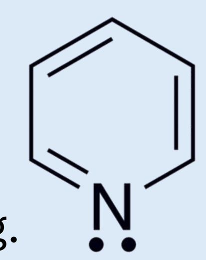
# Optimization of Ethanol and Acetone Reagent Ion Concentrations in a Chemical Ionization Mass Spectrometer (CIMS) for Improved Detection of Pyridine

**Uriel Aguilar Gutierrez**[1], Bri Dobson[2], Maxwell Lee,[2] Eleanor Browne[2]
[1]Research Experience for Community College Students, Aims Community College, Greeley, CO
[2]Department of Chemistry and Cooperative Institute for Research in Environmental Sciences, University of Colorado Boulder, Boulder, CO

## Introduction

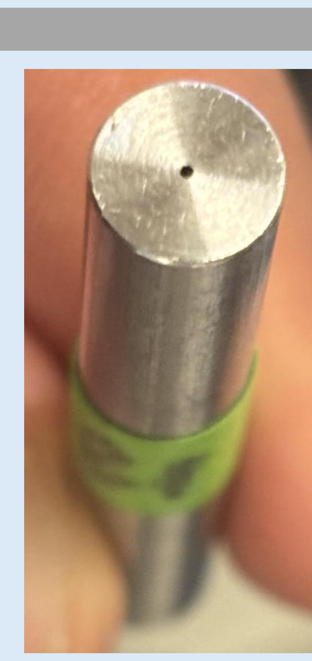
- The atmosphere is composed of many gases, some of which can be harmful to public health and could affect climate change.
- To identify and measure gases, a Chemical Ionization Mass Spectrometer (CIMS) can be used for high sensitivity detection.
- Pyridine is a gas we want to measure because it's toxic. It's released from industrial emissions, tobacco smoke, vehicle exhaust, and biomass burning.




- The CIMS first uses a reagent ion to ionize analyte gases. The optimal concentration of the reagent ion is unknown.
- **This study aims to determine how different concentrations of protonated ethanol and protonated acetone reagent ions affect the sensitivity of a CIMS to pyridine.**

## Methods

- **Various critical orifices (Fig 1) were used to dilute the flow and change the concentration of the reagent ion entering the CIMS (Fig 3).**
- The CIMS' sensitivity to pyridine was measured at multiple reagent ion concentration by flowing different amounts of pyridine into the CIMS.
- The data was analyzed, and calibration curves were made for each reagent ion concentration.



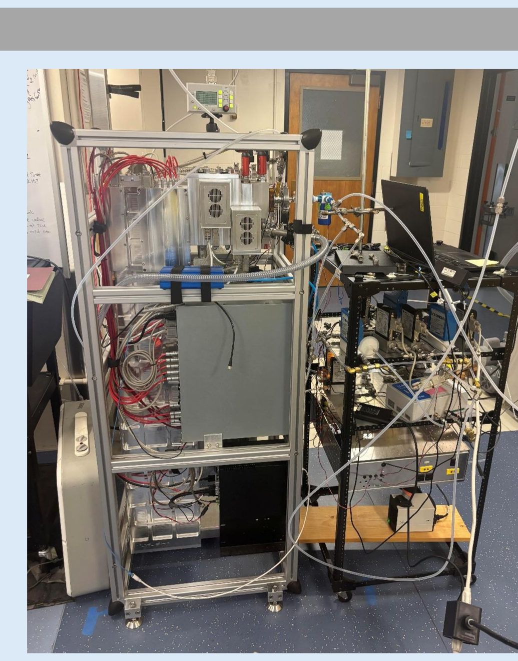


**Figure 1 (Left):** A critical orifice. It has a small hole on one end to limit the amount of gas flowing through. In this case, the gas flowing through is nitrogen.
**Figure 2 (Right):** The calibration system connected to the CIMS.

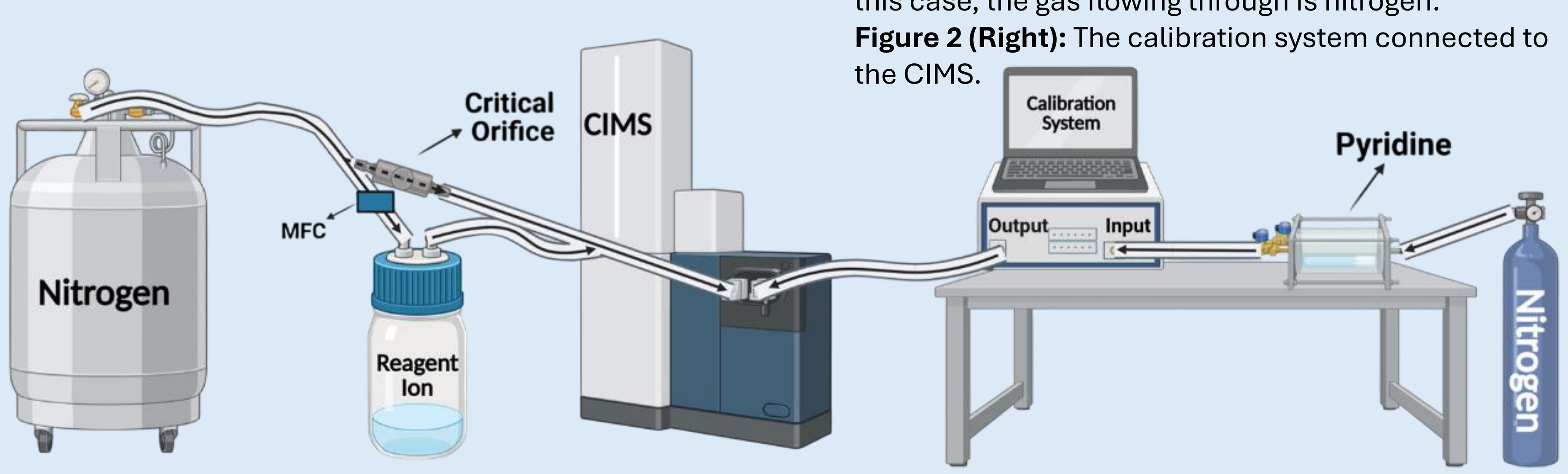



**Figure 3:** Starting from the left, $N_2$ is flowed through tubing and is split into a critical orifice and a mass flow controller (MFC). The $N_2$ flowing through the MFC carries the reagent ion out of the bottle. The $N_2$ flowing through the critical orifice dilutes the reagent ion into the CIMS. From the right, $N_2$ is flowed over a permeation tube of pyridine, through the calibration system, and into the CIMS. The calibration system is what controls how much pyridine is flowing into the CIMS.

## Results

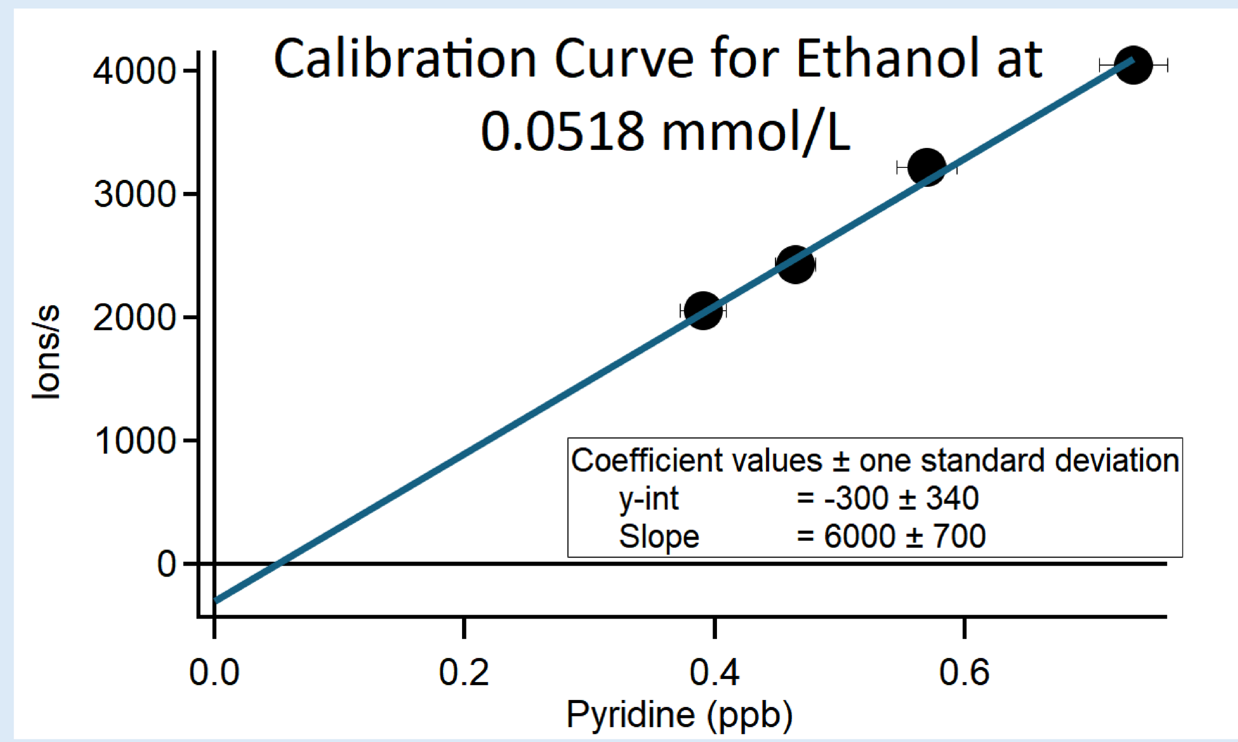



**Figure 4:** Calibration curve using protonated ethanol as a reagent ion. This slope represents the first point plotted in Figure 6.

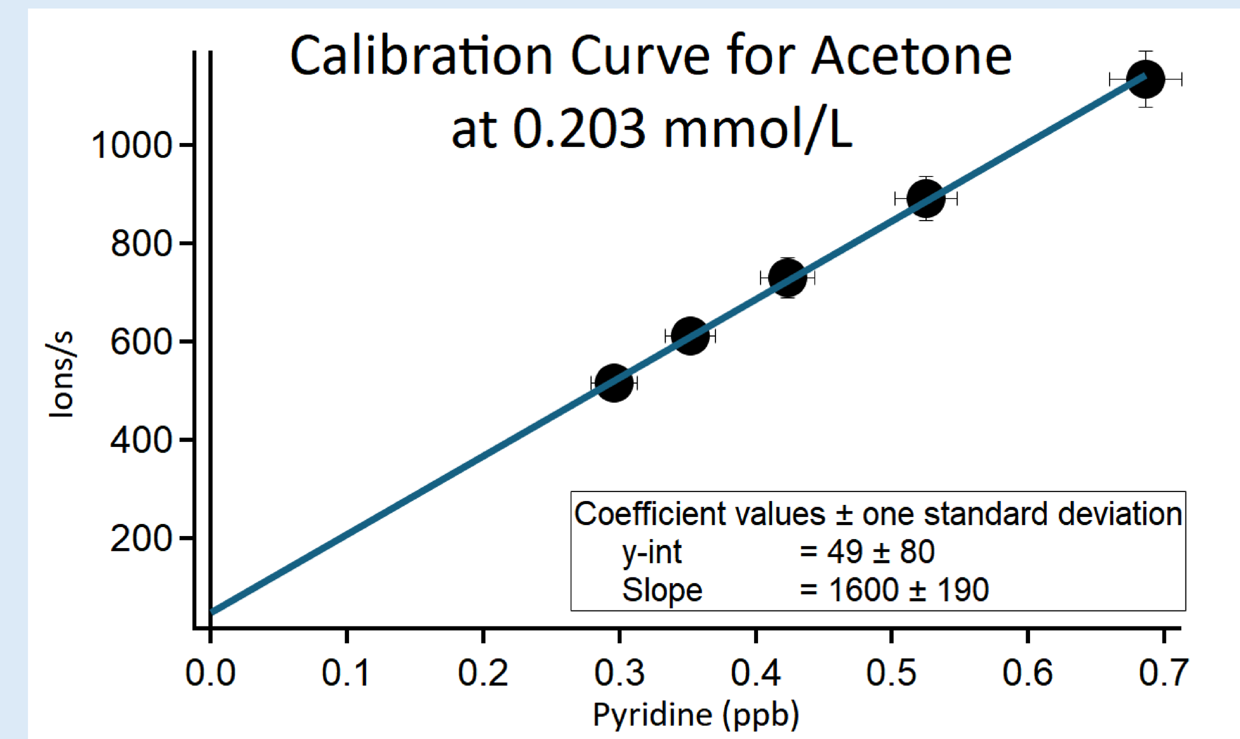



**Figure 5:** Calibration curve using protonated acetone as a reagent ion. This slope represents the first point plotted in Figure 7.

A calibration is done by keeping the concentration of the reagent ion constant and changing the concentration of the calibrant, pyridine in this case. This allows us to see how much pyridine is detected by the CIMS at that specific reagent ion concentration. The steeper the slope, the more sensitive the CIMS will be.

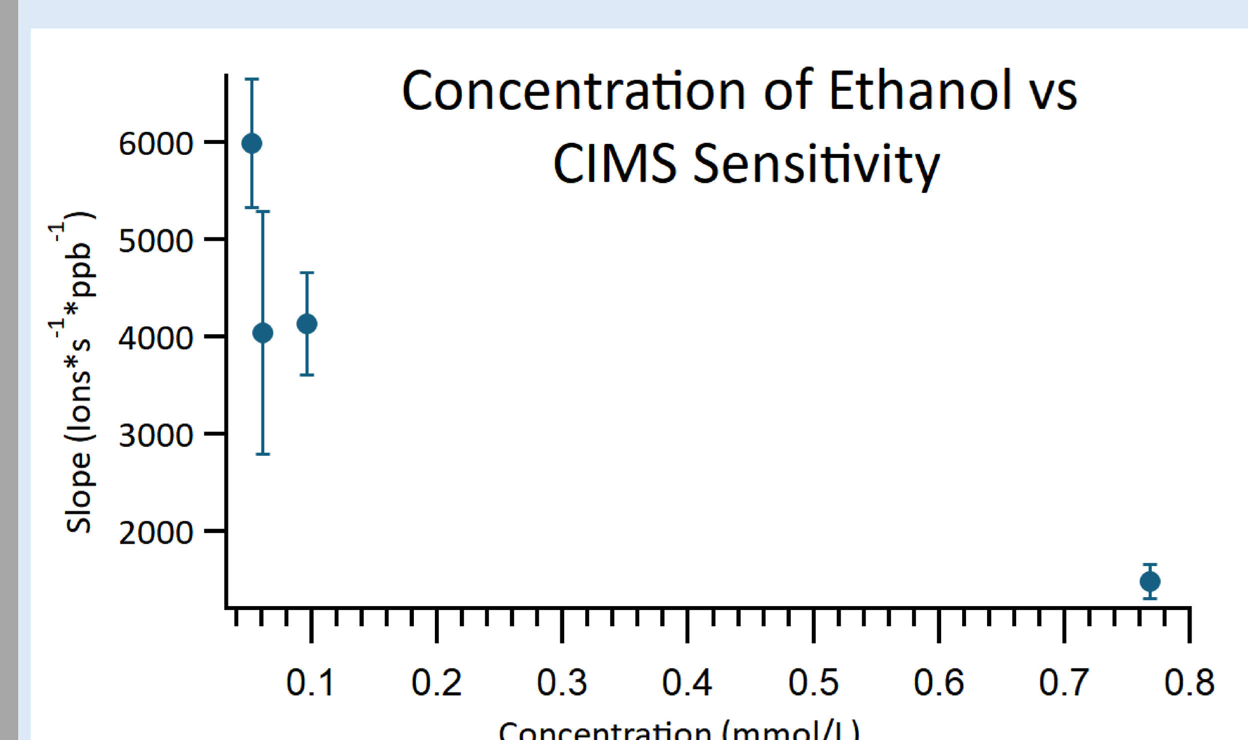
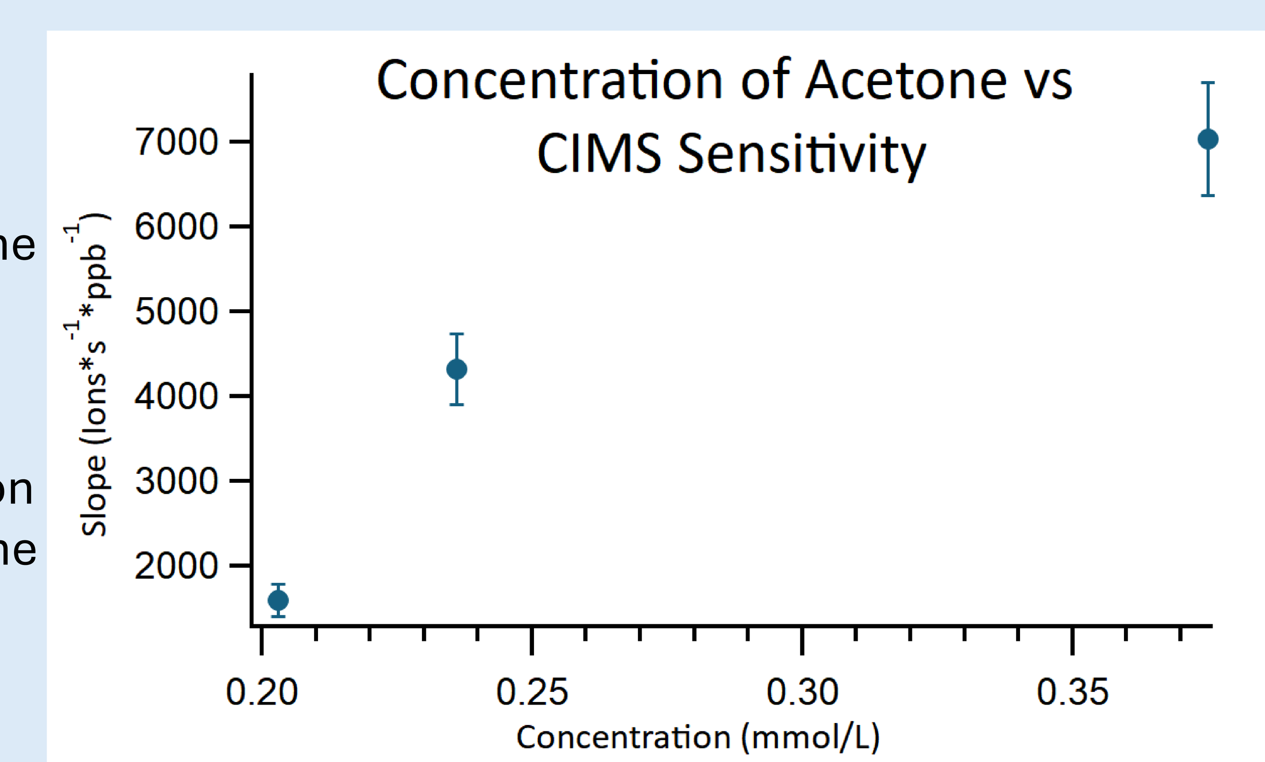



**Figure 6 (Left):** This graph shows the concentration of ethanol vs the slope of the calibration curve. From this graph, we can see that as the concentration of ethanol increases, the sensitivity **decreases**.

**Figure 7 (Right):** This graph shows the concentration of acetone vs the slope of the calibration curve. From this graph we can see that as the concentration of acetone increases, the sensitivity **increases**.




## Discussion & Conclusion

- **The data shows that as the concentration of the protonated ethanol reagent ion increases, the sensitivity of the CIMS to pyridine decreases. However, the opposite is true for the protonated acetone reagent ion.**
- This implies that there is a difference in the ionization mechanisms between the ethanol and acetone reagent ions.
- To make the CIMS most sensitive to pyridine, one should use higher concentrations of protonated acetone as the reagent ion.
- The results were unexpected. I hypothesized that the CIMS' sensitivity would increase if both reagent ion concentrations increased.
- Although ethanol may be less sensitive than acetone, using ethanol in a humid environment may be better since ethanol's sensitivity doesn't change with humidity as much as acetone's does.
- The CIMS can also identify other gases present in the atmosphere so, these results may also apply to other compounds.

Scan for Abstract and Acknowledgements

## References

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