Ion Mobility Mass Spectrometry of Isomeric Peptides

Brian Hauck[1], Christina Crawford[2], Herbert H. Hill[2]

1. Nazareth College of Rochester, Rochester, NY 14618

2. Washington State University, Pullman, WA, 99163

OVERVIEW

Purpose The purpose of this research was to investigate the difference in reduced ion mobility coefficients (K_o) of three isomeric peptides in different drift gases and determine the feasibility of distinguishing between peptides both on a standalone ion mobility spectrometer (IMS) and on an ion mobility spectrometry-time of flight mass spectrometer (IMS-tofMS). The effect of the polarizability of different drift gases on K_o was also investigated.

Method At least three mobility spectra of each peptide (WGY, WYG, and YWG) were collected over three days on a standalone IMS and on a IMS-tofMS in N_2 and CO_2. K_o values of all peptides in each gas were calculated on both instruments from their average drift times.

Results Initial results indicate that K_o values vary slightly between peptides within each drift gas and consistently follow a numerical order according to K_o values.

INTRODUCTION

- Ion Mobility Spectrometry (IMS) is a commonly used analytical technique, especially in security and defense applications.
- As a technique, IMS has the ability to resolve similar compounds, such as isomers, an advantage over traditional techniques such as GC-MS, which cannot distinguish between compounds of identical mass.
- Modern IMS instruments use length, temperature, voltage, and the drift times of sample ions to calculate the K_o values of each analyte:
  - $K_o = (L^2/Vt_d)(273.15/T)(P/760)$
  - This equation gives the reduced mobility coefficient of the sample ion, where L is the length of the drift tube, V is the gate voltage, and t_d is the drift time of the sample ion .
- This project investigated using IMS and IMS-tofMS as a means of distinguishing between isomeric structures by comparing K_o values and investigated the effect of a drift gas' polarizability on K_o.

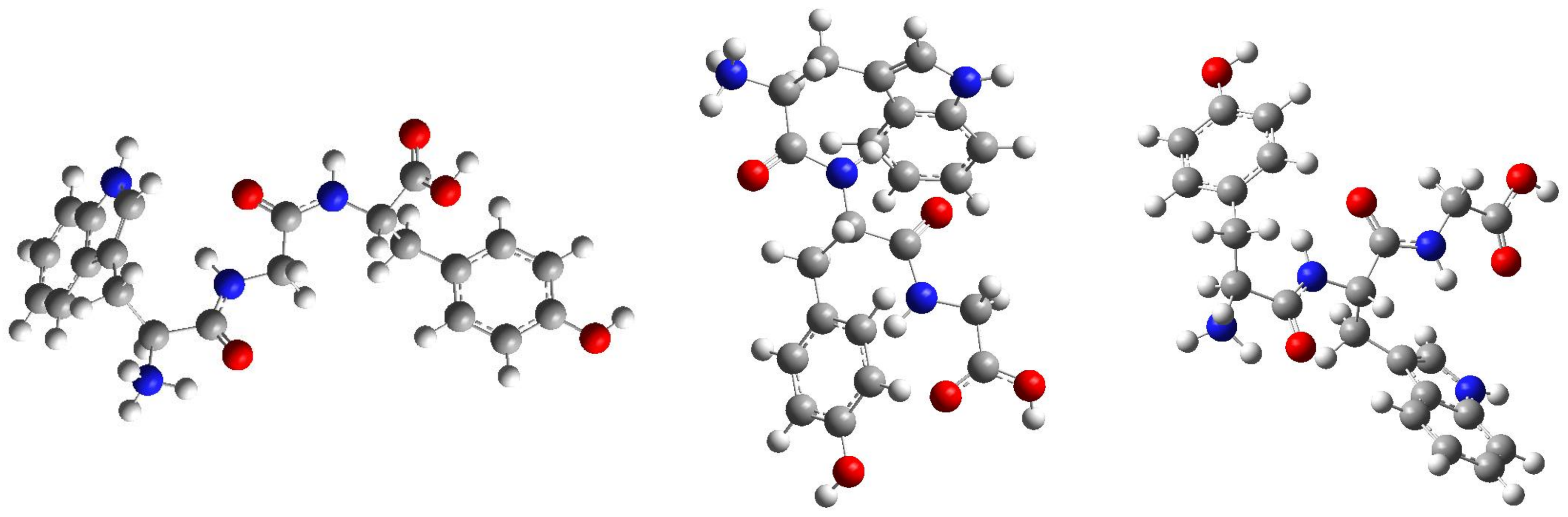

Figure 1: From left to right, chemical structures of n-terminus protonated WGY, WYG, and YWG.

EXPERIMENTAL METHODS

Figure 2: Standalone IMS used in this study.

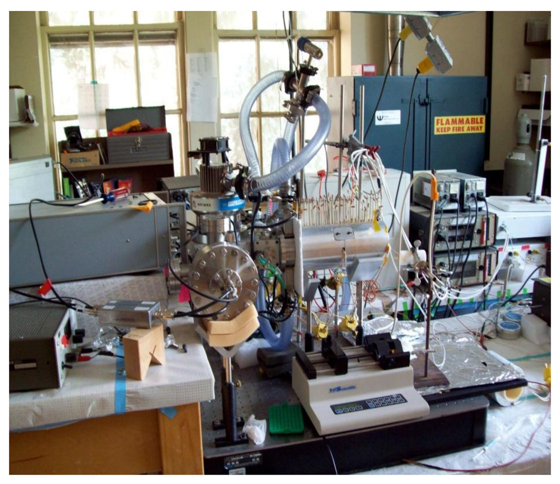

Figure 3: IMS-tofMS used in this study.

- Both instruments were set to operate at 200°C and at ambient pressure, with voltage monitored. An ESI spray solution of 45/45/5:MeOH/H_2O/AcOH was injected at 3μL/min.
- At least three mobility spectra of each peptide were collected in each drift gas over three days.

RESULTS

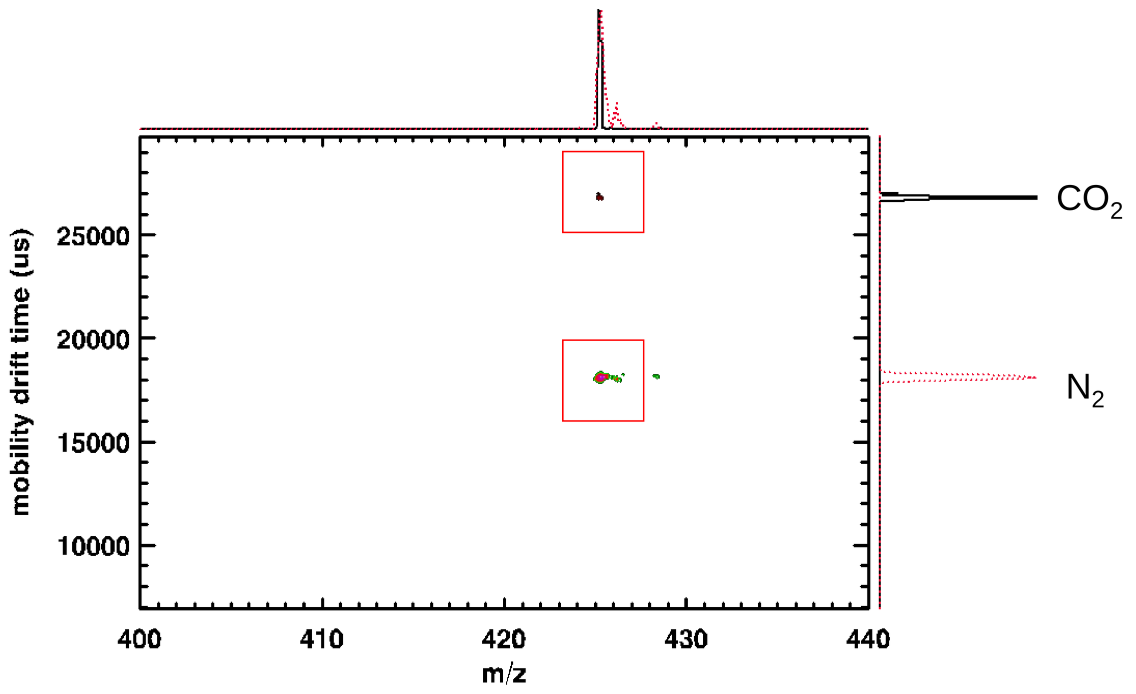

Figure 4: IMSTOF spectra of WGY in CO_2 and N_2.

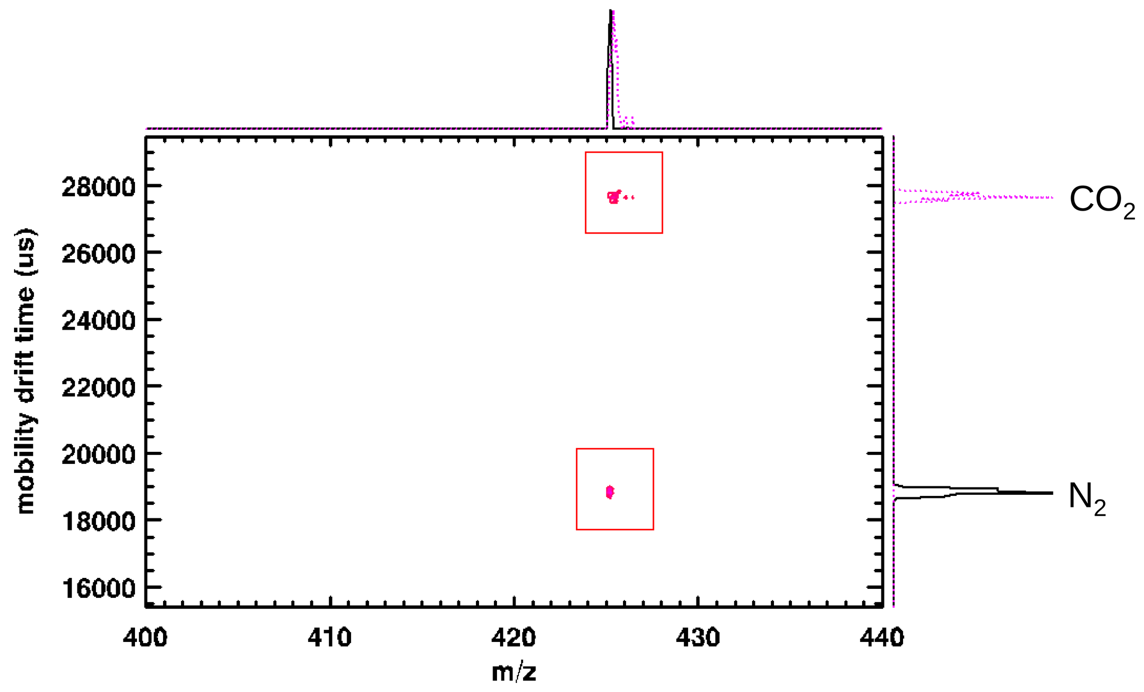

Figure 5: IMSTOF spectra of YWG in CO_2 and N_2.

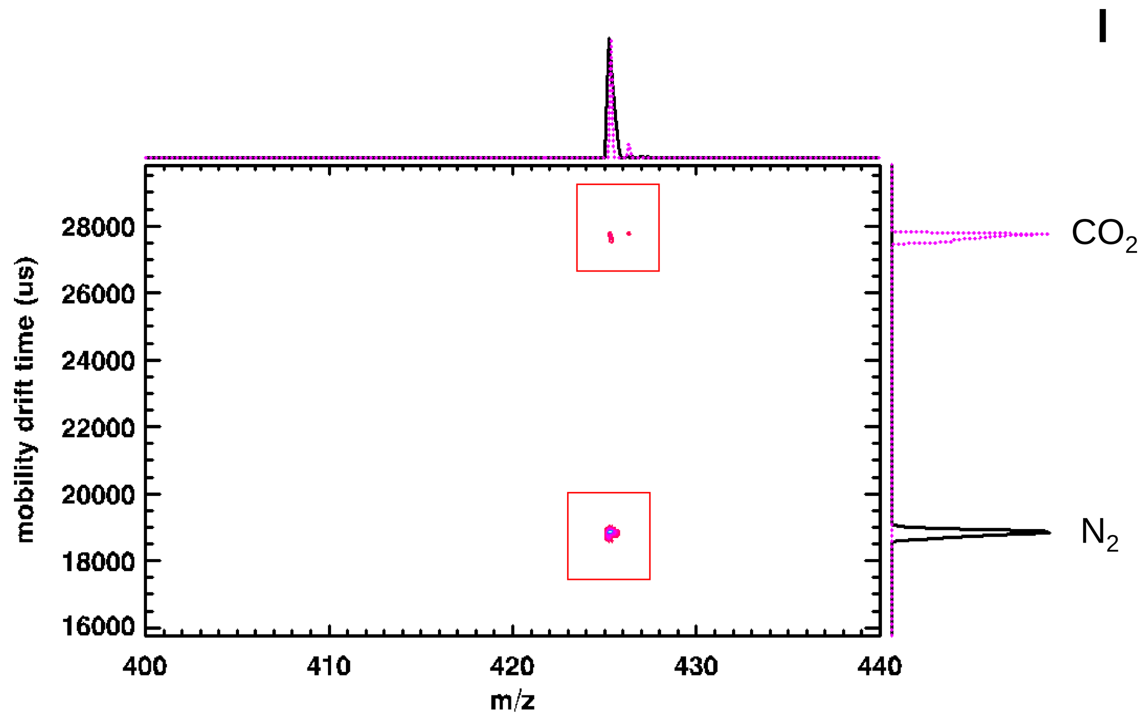

Figure 6: IMSTOF spectra of WYG in CO_2 and N_2.

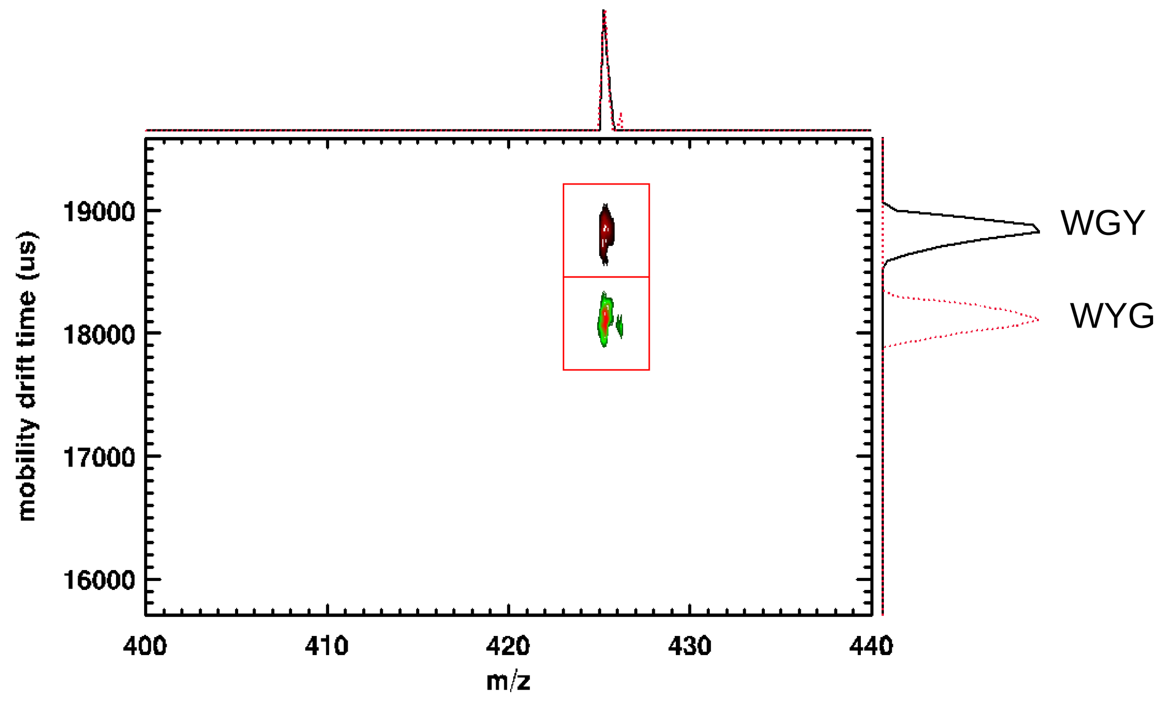

Figure 7: IMSTOF spectra of WGY and WYG in N_2.

Table 1. Reduced ion mobility coefficients (K_o) of three sample peptides in N_2 and CO_2 drift gases on WSU's standalone IMS and IMS-*tof*MS.

Peptide	K_o $cm^2V^{-1}s^{-1}$			
	IMS		IMSTOF	
	N_2	CO_2	N_2	CO_2
WGY	1.0154	0.6788	0.9749	0.6581
WYG	0.9756	0.6568	0.9380	0.6356
YWG	0.9762	0.6571	0.9398	0.6339

CONCLUSIONS

- He does not show to be a suitable drift gas on the standalone IMS due to inadequate separation between reactant ion peaks and sample ion peaks.
- WGY is consistently the peptide with the highest K_o, while K_o values for WYG, and YWG in CO_2 are too statistically similar to distinguish from one another.
- Initial results indicate that the polarizability of the drift gas and the K_o of the sample are inversely related.
- IMS and IMS-tofMS very well may be usefull techniques in distinguishing between isomers within a sample.
- Ultimately, this data will be compared with modeled predictions of the collision cross section properties of each peptide within an environment of zero polarizability in order to check the accuracy of such modeling.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation's REU program under grant number 0851502.

Peptide images were provided by Dr. Aurora Clark of Washington State University.