Estimating Vapor Pressures of Pheromone Compounds Using Gas Chromatographic Retention

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Overview

Accurate determination of the vapor pressures of organic materials is important for predicting the sample's environmental impact. It is difficult to directly measure accurate and precise vapor pressures of chemical compounds with direct experimental methods. Thus, indirect or predictive models for estimating vapor pressures are used. In this study we are following a gas−liquid chromatography (GLC)-based approach, where retention data is correlated with vapor pressure using multiple reference standards. The method (GLC-RTyS) requires temperature-dependent retention factors (k-values) for test compounds and reference standards with known vapor pressures at matching temperatures. It has been observed that reference standards selected according to functional group compatibility are expected to have better estimation accuracy. The study will contribute to vapor pressure modeling methods, which could be a cost and labor-effective alternative to experimental techniques in environmental scientific fields.

Objectives

To follow the GLC-RTyS method for estimating vapor pressures of pheromone analogs from retention times of organic compounds, particularly alkanes and Fatty acid methyl esters.

Materials & Methods

A set of reference compounds with known vapor pressures

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Temperature Dependence: at the same temperature range as sample

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Plot the retention factors (k) of reference compounds against their known vapor pressures.

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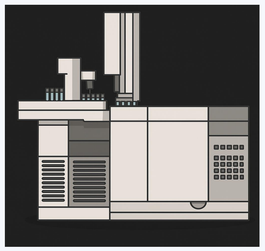
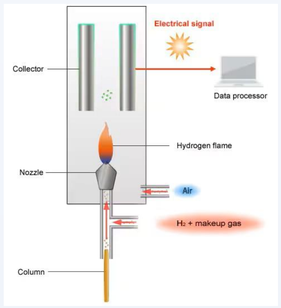
Use the calibration curve to estimate the vapor pressure of your unknown liquid based on its retention factor

Instrumentation



- Shimadzu GC-2010 Plus with FID detector
- In split mode in constant pressure Helium gas
- 1 µL of liquid sample injected with AOC autosampler

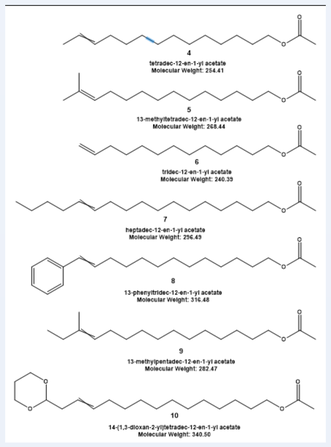
Rtx-1 GC Capillary Column, 30 m, 0.25 mm ID, 0.25 µm



Flame Ionization principle

Sample

Commercially available pheromone samples of Asian Corn Borer (***Ostrinia furnacalis)*** and its synthetic analogs were studied. Among them 4Z is the commercial sample and rest are analogs.Their details are given below:

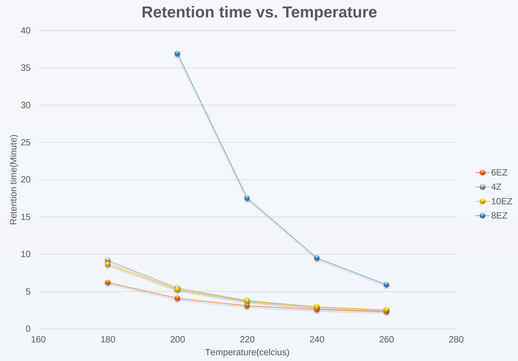


Standards

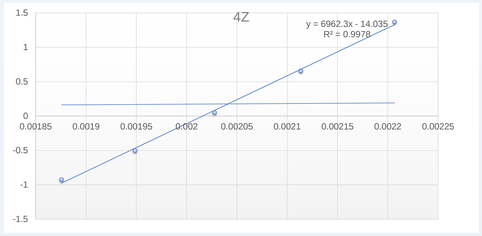
- n Alkanes
- FAMEs

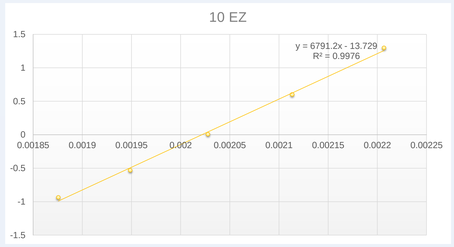
Data Analysis

After finding the retention temperature of the commercial standard and synthesized sample from comparing with n alkanes and FAMEs, they were run in a specific temperature range to observe if the samples follow the trend or not.



From the above plot, it is evident that the 10 and 6 numbered samples show the same chromatographic behavior as the commercial sample, whereas 8 shows showing anomalous trend. The reason might be due to a change in the functional group and a difference in molecular weight. Then these data were considered to calculate the retention factor and fit them in van't Hoff equation enthalpy of vaporization is obtained. Then, using Antoine equation, we can get vapor pressure of samples which need to be verified using standard dataset.





Approximate Enthalpy of vaporization of 4Z, 6EZ, 10EZ, 8EZ are 57884,53758,,56475 and 74426 J/mol.

Future Work

- Plot and compare the retention factor of unknown samples with standard datasets to determine vapor pressure.
- Follow the same procedure with the rest of the analogs.
- In current instrumentation, distinguishing E and Z isomers is not possible. GC-VUV could be a possible solution for that.
- Optimize the chromatographic conditions (column type, carrier gas flow rate, temperature gradient) to achieve the best separation of compounds.
- Validate the method by assessing its sensitivity (limit of detection, limit of quantitation), specificity, precision, and accuracy.
- Analyze data for finding possible errors in methodology or sampling or in the model.

References

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