Alan Yu

Organic Lab 309:03

Santanu Malakar

Experiment 33: Spectral Identification of Monoterpenes

February 4, 2019

Purpose: The purpose of this lab is to use Infrared Spectroscopy to determine the unknown monoterpene within a sample.

Equations: NONE

Mechanisms: NONE

Amounts and Properties: Small sample of unknown monoterpene.

Hazards and Safety: Monoterpenes can irritate eyes and skin. Some monoterpenes are quite flammable, so avoid open flames near the monoterpenes. Deuterochloroform is harmful if inhaled or absorbed through skin. It is a suspected carcinogen. Wear gloves, goggles, and try to work inside the Hood or working quickly to insert the sample into the Spectrometer.
To Dispose: Turn the Monoterpenes back to the instructor and keep deuterochloroform in the designated waste container.

Procedure:

Infrared Spectrum:

1. Get an IR spectrum of the unknown monoterpene and record wave numbers for all significant absorbent bands in the spectrum.

Identification of Unknowns:

1. Look at the information gathered and decide what functional groups are present and any other relevant information.
2. Using the information decide what the monoterpene is from Figure 1.

Figure 1: List of Possible Monoterpenes

Discussion:

The Unknown that was received was Unknown 4. From the IR spectrum made from the spectrometer, the bands at the ~3000 range slightly resemble the peaks from an existing cyclohexene spectrum. This knocks out all the other monoterpenes that don't have a cyclohexene, which leaves carvone and limonene to be evaluated. At the ~3325 to ~3600 range the IR bands show a small resemblance towards an Ketone overtone. Since carvone has a ketone, it seems logical that the IR spectrum would best match carvone.

Conclusions:

Due to the bands and the similarity of most of the bands with specific known ranges, the unknown monoterpene from unknown 4 was identified as carvone.

Exercises:

2. A. For 1-butanol, a large OH stretch can be seen over the ~3000 to ~3600 wavenumber. For 2-butanol, a slightly smaller OH stretch can be seen over the ~3200 to ~3600 wavenumber with a slight peak after the OH stretch. For 2-methyl-2-butanol, no OH stretch could be seen, but a large peak at the ~2900/~3000 wavenumber.

B. For ortho-xylene, there are multiple sharp peaks at the ~2800 to ~3200 wavenumber which can represent like a mountain of peaks. For meta-xylene, there are about 3 peaks that are a little spread out with one being extremely prominent at the ~2850 wavenumber. The three peaks for meta-xylene span from ~2800 to ~3100 wavenumbers. For para-xylene, it has the characteristics of both of the other xylenes combined. There is a sharp peak that is distinguishable at around the 2800 to 2900 wavenumber and a mountain of peaks at the ~2750 to ~3100 wavenumber range.

C. For butanal, there are four peaks, with the first two being like a sine wave leading into a small peak which sharply turns into a larger peak. This range is found at ~2600 to ~3000 wavenumbers. For 1-butanol there is a large OH stretch seen from the ~3000 to ~3600 wavenumbers. For 2-butanone, there is a ketone IR band that could be seen at the ~3400 wavenumber with a few peaks at ~2800 to ~3000 wavenumbers, with the peak near the 3000 wavenumber being the tallest. For butanoic acid, there is a mini OH stretch that can be seen from the ~3050 wavenumber that is attached to a C-H bond wavenumber at ~2975 wavenumber. For butyl acetate, there is a range of 2 peaks in the IR spectrum where it first has a small peak following a large peak about 3x the size. These peaks are found at ~2700 and ~2950 wavenumbers respectively.