Determination of Caffeine Content in Coffee Beverages Using Fourier Transform Infra-Red Spectroscopy

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Introduction

Caffeine is a chemical substance that is a component in many beverages that are a part of so many people's daily routines. Its chemical formula is $C_8H_{10}N_4O_2$ and it can be naturally sourced through a variety of plants. Because an excessive consumption of caffeine (greater than 400 mg a day)can lead to serious health complications, it is important to be aware of how much caffeine is in different caffeinated beverages. In this experiment, the concentration of the caffeine contained in Cold Brew, Espresso, Decaffeinated coffee and Tea was analyzed and determined.

Discussion

In this experiment all spectrums had noises that might have occurred due to the flasks not being properly clean, meaning that the wavelengths were interacting with other substances besides the targeted one. That could also indicate why there were other peaks besides the peak of the targeted wavelength of 1665 cm^-1, and why there was a small error in Figure 1. The results of this experiments showed that a higher absorption indicated a higher concentration. Espresso presented the highest concentration with (93.350 ppm) of caffeine, the second highest was the Cold Brew sample (54.948 ppm), then Tea (25.783 ppm), and lastly, Decaffeinated coffee (16.842 ppm).

Results

Different molecule bonds vibrate in different frequencies, in which light can be absorbed into in different wavelengths. In this experiment, what is being analyzed is the concentration of caffeine, therefore the absorption band which was given was at around 1655 cm^-1, which is about the same as the carbonyl of caffeine. Then, to calculate the concentration, each sample was plugged into an equation as x (y=1360.2x-2.5164).

Results showed that Espresso has the highest caffeine concentration, followed by Cold Brew, then Tea, and lastly, Decaffeinated coffee, which surprisingly, is not caffeine free.

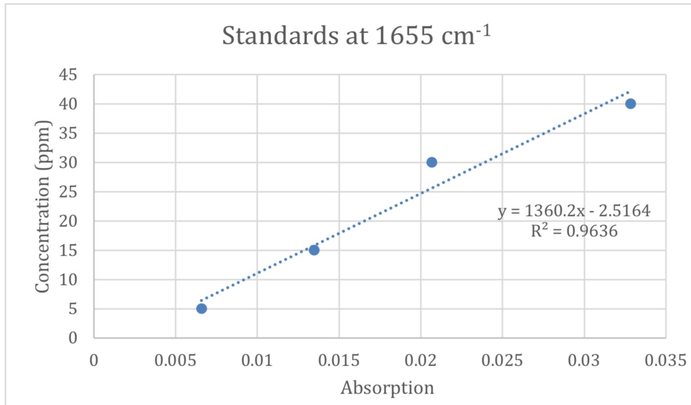

Figure 1. Four standard samples at wavelength 1665 cm^{-1}

Sample	STD1	STD2	STD3	STD4	CB	DE	ESP	TEA
Absorption	0. 006577	0. 013468	0. 02069	0. 03283	0. 0422475	0. 014232	0. 0704795	0. 020805
Concentration (ppm)	5	15	30	40	54. 9486495	16. 841966	93. 3498159	25. 782561

Table 2. Concentration and Absorption for all samples.

Methods

It was through using Fourier transform infra-red (FT-IR) spectroscopy, specifically the Shimadzu IR Affinity-1 with PIKE MIRacle, *single Reflection* that the concentration of caffeine in these beverages. However, because water is a strong IR absorber, it had to be extracted from the samples in order to obtain accurate results. In addition to that, chloroform was used to extract the analyte caffeine, but this solvent was allowed to evaporate prior to the acquisition of the FTIR spectrum of the solid.

References

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