Determination of Types of Fat Present in Cooking Oils Using Infrared Spectroscopy with an ATR Attachment

Introduction:

The electromagnetic spectrum has many different types of light other than just the visible light we see everyday. These types of light vary in wavelength (the distance from crest to crest in a wave). The wavelength of light affects the energy that each photon (individual packet of light) has. The shorter the wavelength, the greater the energy a photon of light has.

Spectroscopy is the study of the interaction of light with molecules or atoms. The specific interaction that a molecule has with light depends on the types of bonds in the molecule and the energy of the light. Shorter wavelengths of light in the ultraviolet and visible regions (~200-800nm) can cause bonding electrons to change orbitals when the light is absorbed; much longer wavelengths in the microwave region (~100,000-1,000,000nm) can cause bonds to rotate when the light is absorbed. The wavelengths of light between the visible region and microwaves are known as infrared (IR) (~1000-10,000nm) and can cause bonds to vibrate and/or rotate when the light is absorbed.

All of the interaction IR light has with molecules are based on very specific “selection rules.” The selection rules allow for identification of molecules based on the absorbance pattern of the wavelengths of light in the IR region. Also, the absorbance of IR light follows Beer’s law (at low enough concentrations), which means the concentration of molecules can be determined from the absorbance if a calibration curve is prepared.

Purpose:

Nutrition labels in the United States are required to provide accurate information on not only the amount of fat that food or drink contains, but the amount of that fat that is “saturated”. Some nutrition labels also provide information about the amount of fat present in the food that is “monounsatuated” or “polyunsaturated.” A saturated fat has a long chain of carbons that are attached to hydrogen atoms and all of the carbons are connected with “single” bonds. A monounsaturated fat has a long chain of carbons that are attached to only hydrogen atoms, but between two of the carbons in the chain there is a “double” bond, which reduces the total amount of hydrogen in the chain by two atoms. A polyunsaturated fat has at least two double bonds between the carbons in the chain which reduces the total amount of hydrogen by two atoms for every double bond present. Examples of all three types of fats are given below.
The infrared spectrum of each of these types of fats will be different due to the different bond types (i.e. it takes more energy to cause a double bond to vibrate than a single bond). By comparing the spectra of known types of fat, it is possible to determine the types of fat present in an unknown sample.

**Instrumentation:**
- Model M500 Infrared Spectrophotometer
- Model 57 ATR Attachment
- Grams/AI Software

**Supplies:**
- Standards of saturated, monounsaturated and polyunsaturated fats.

**Samples:**
- Obtain several varieties of cooking oil (safflower, vegetable, peanut, olive, walnut, coconut and shortening are good examples.)

**Procedure:**

**Instrument Setup:**
- Follow the specific instrument procedures in the manual for initial instrument set up
- Make sure the instrument warms up for at least an hour before beginning scans.

**Data Collection:**
NOTE: All scans can be performed on the 3 minute scan cycle. Longer cycles will not improve results a noticeable amount and will only increase analysis time.
- Run background scan from 4000 to 600 cm\(^{-1}\).
- Save the background scan and set it as the background scan. Make sure the instrument is set up to ratio future scans against the background scan.

**Qualitative Data Collection:**
- Place sample on salt plates or horizontal prism accessory.
- Take spectra of sample from 4000 to 600 cm\(^{-1}\).
- Compare the spectra of the various oils.

**Questions:**
- What peaks are present in all spectra?
- What peaks vary?
- Why do the spectra of all the oils look different? (What bonds are different)
- Could you determine which how many double bonds are present in a particular type of oil from an unknown oil? How would you do it?