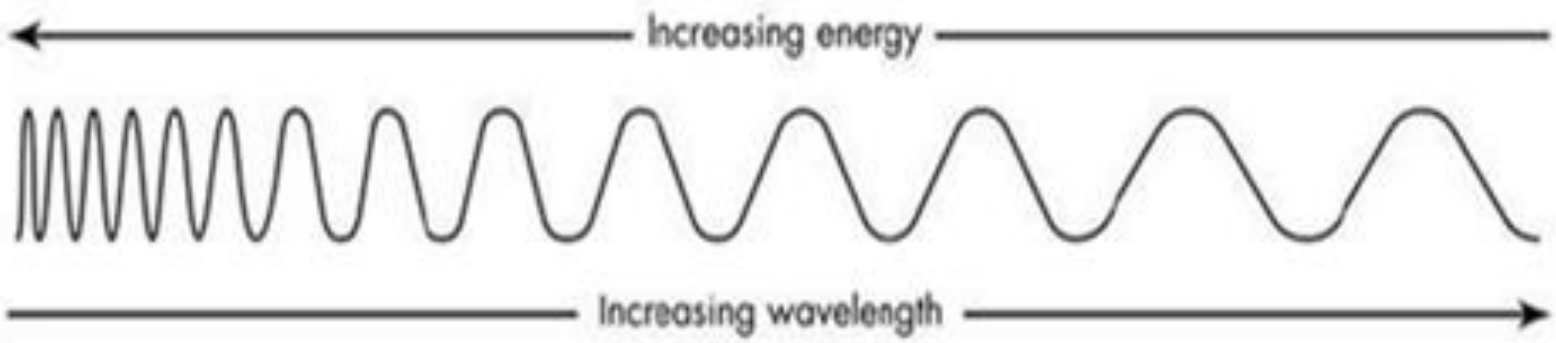
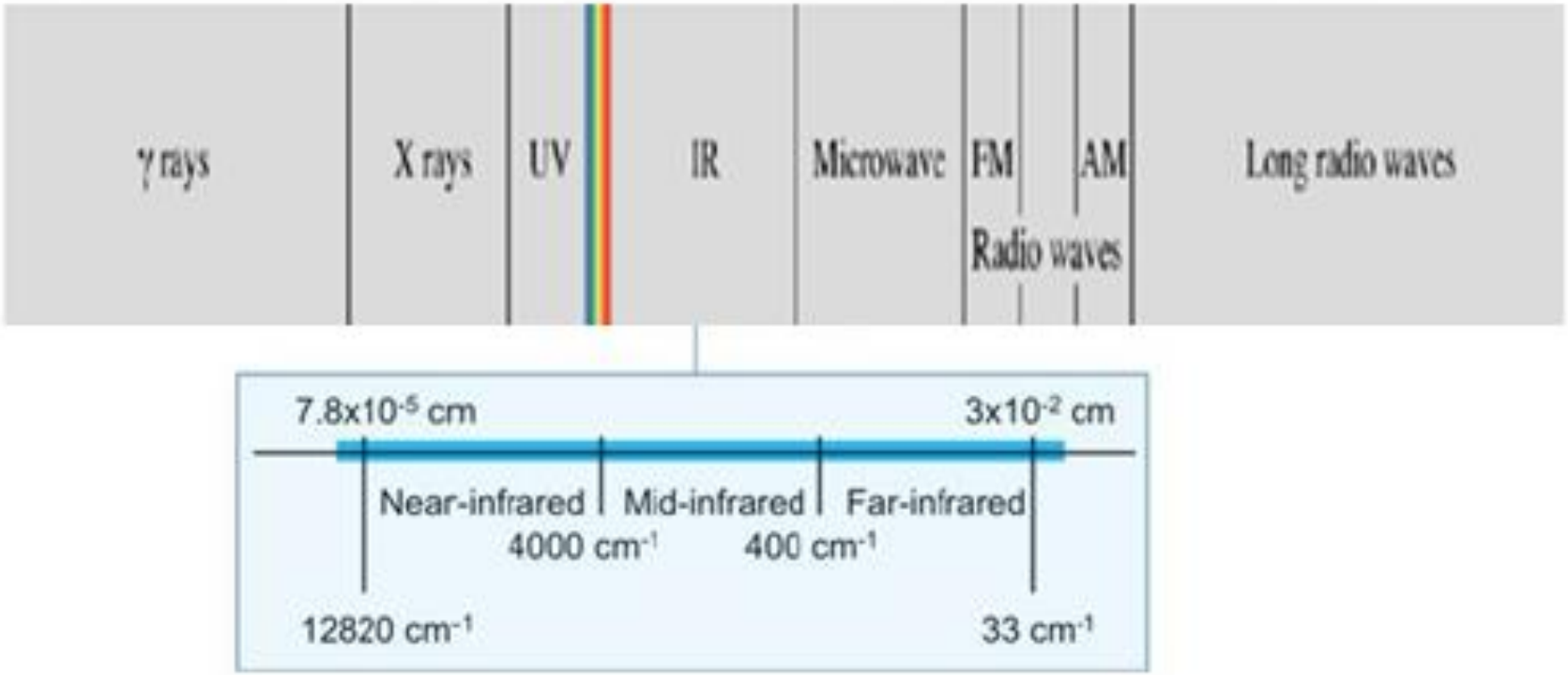
Fourier Transform Infrared (FT-IR) Spectroscopy

Prof. Dr. Çiğdem AYKAÇ

Electromagnetic Spectrum





There are three infrared regions; each has potential to provide different information:

1. Far-Infrared (400-33 cm^{-1}): molecules containing heavy atoms, molecular skeleton and crystal lattice vibrations
2. Mid-Infrared (4000-400 cm^{-1}): useful for organic analysis
3. Near Infrared (12820-4000 cm^{-1}): very useful for quantitative analysis

Wavelength and Wavenumber

In IR regionwavenumber is usedgenerallywhich can be defined as thenumber of wavelengths per unit distance:

$$Wavenumber = \frac{1}{Wavelength\ (in\ cm)}$$

- For the IR, wavelength is in microns.
- Wavenumber is typically in 1/cm, or cm^{-1}.
- 5 microns corresponds to 2000 cm^{-1}.
- 20 microns corresponds to 500 cm^{-1}.

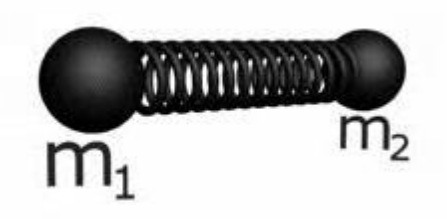
- The primary source of infrared radiation is thermal radiation (heat).
- For a molecule to absorb IR, the **vibrations** within a molecule must cause a net change in the **dipole moment** of the molecule.

Infrared radiation can obtain :

1. The type of atoms within the molecule.
2. The type of bonds between atoms.
3. The molecular structure (by additional techniques such as NMR, mass spectroscopy, etc.)
4. From a quantitative point of view, infrared spectroscopy has a very well gained reputation for its power, flexibility, and reliability.

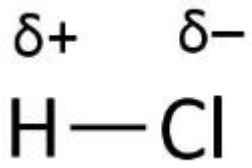
Molecular Vibrations

- In order to understand molecular vibrations, a bond can be treated as a simple harmonic oscillator composed of two masses (atoms) joined by a spring.
- Representation of a diatomic molecule with two generic atoms (of masses m1 and m2) connected by a spring.



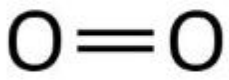
- If masses m1 and m2 are equal, no change in the dipole moment will occur as the molecule vibrates.

- The HCl molecule possesses a permanent dipole moment, so it is **infrared active**.



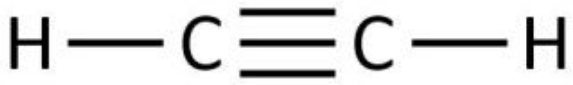
- Molecules with a permanent dipole moment, such as water, HCl, and NO, are **infrared active**.

- The O_2 molecule does not possess a permanent dipole moment, so it is **infrared inactive**.



Diatomic molecules such as Cl_2, H_2, N_2 are **infrared inactive.**

In the case of alkenes (C=C) and alkynes (C≡C) if the bond is symmetrically substituted no band will be seen in the IR spectrum, however, if the bond is asymmetrically substituted a stretching frequency corresponding to the alkene or alkyne bond will be present.

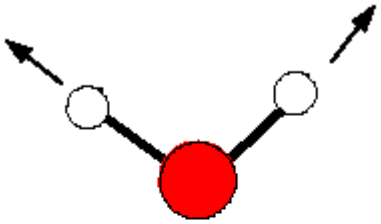
IR inactive: 

IR active: 

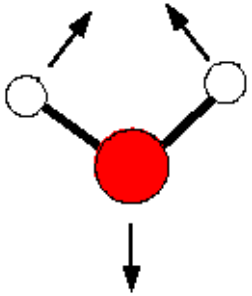
Vibration Types

- There are two different types of vibrational modes:

Vibrations can either involve a change in bond length (stretching) or bond angle (bending)

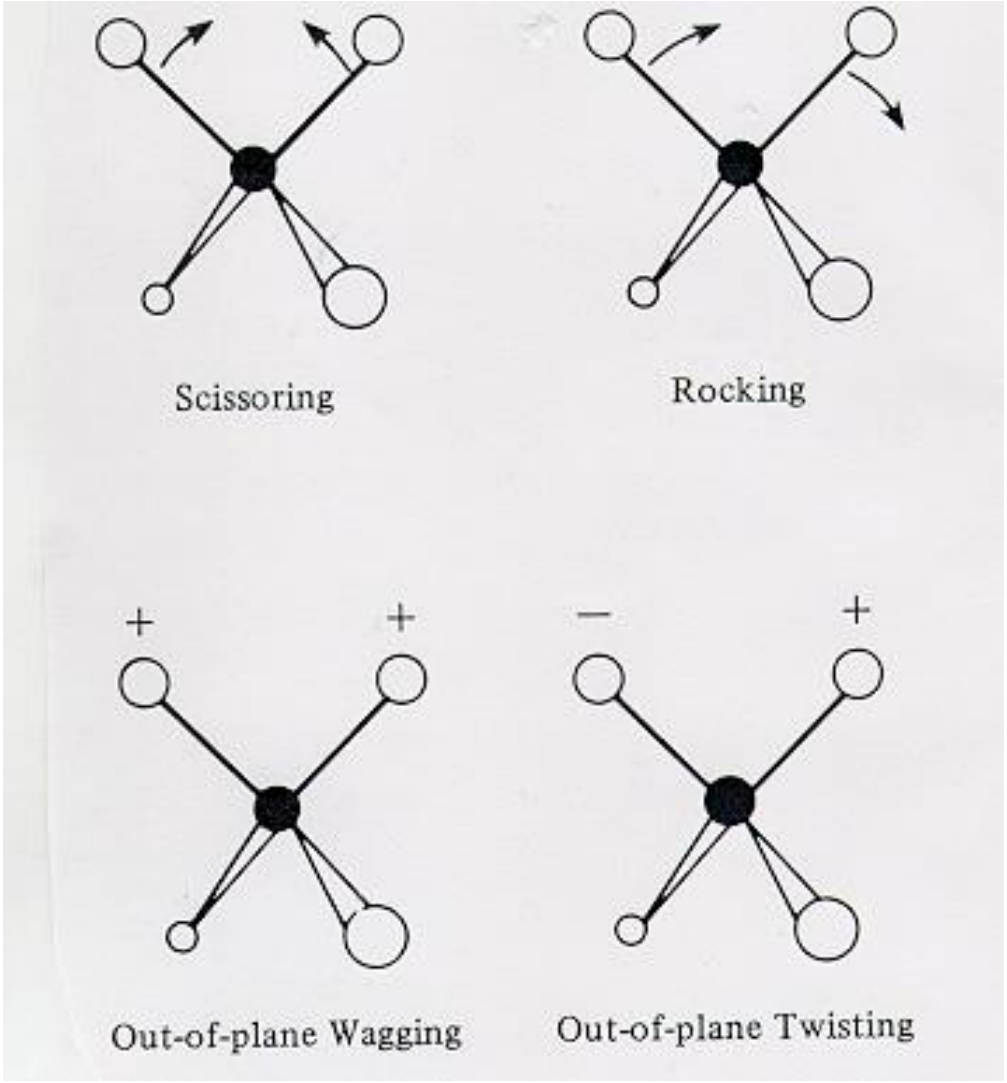


Stretching

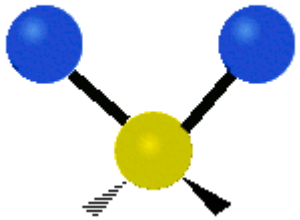


Bending

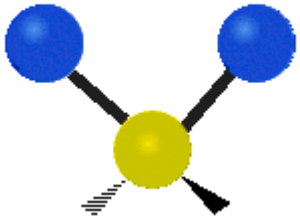
The bending vibrations are often subdivided into ***scissoring, rocking, wagging, and twisting***.



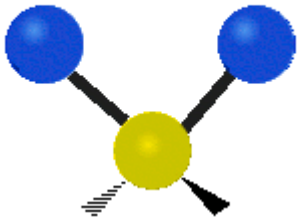
Symmetrical stretching



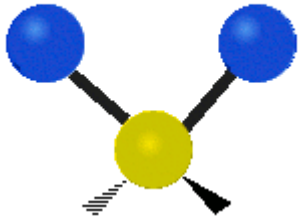
Scissoring



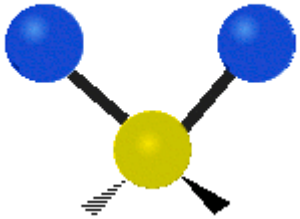
Rocking



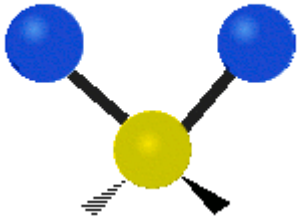
Antisymmetrical stretching



Wagging

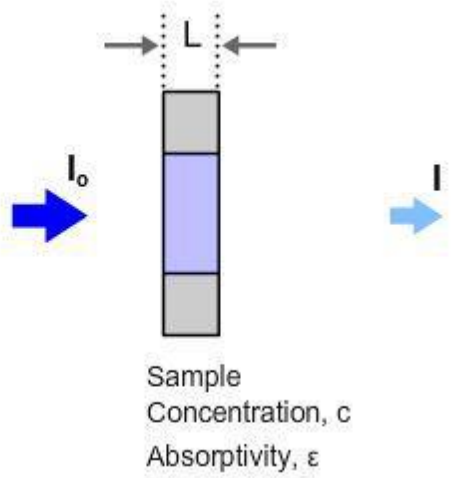


Twisting



IR Absorption

The amount of infrared radiation absorbed or transmitted by the sample, at any given wavelength, can be measured.



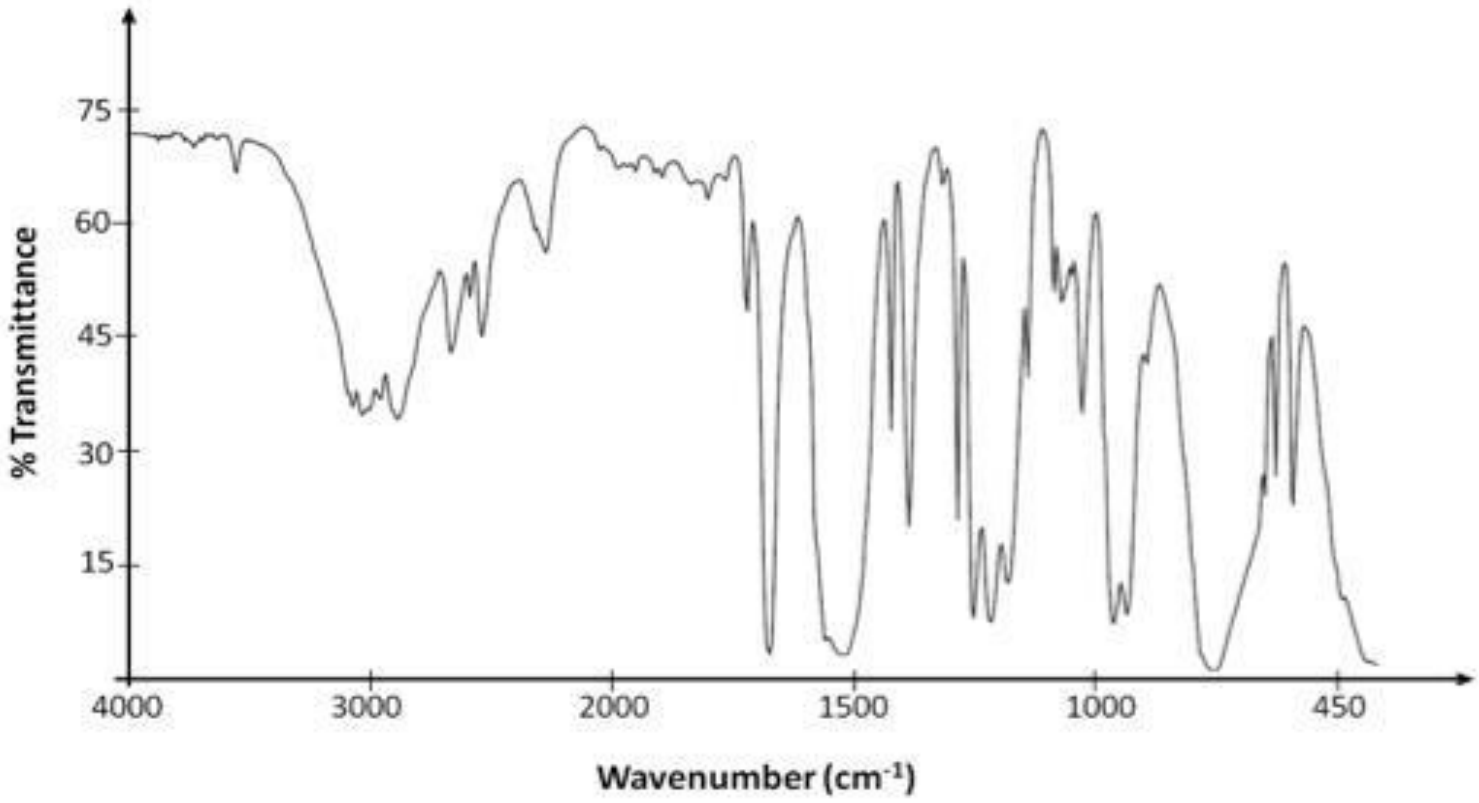
Absorption of infrared radiation of radiant power I_0. The radiation leaving the sample has radiant power I.

The transmittance is :

$$\%T = \frac{I}{I_o} \; x \; 100$$

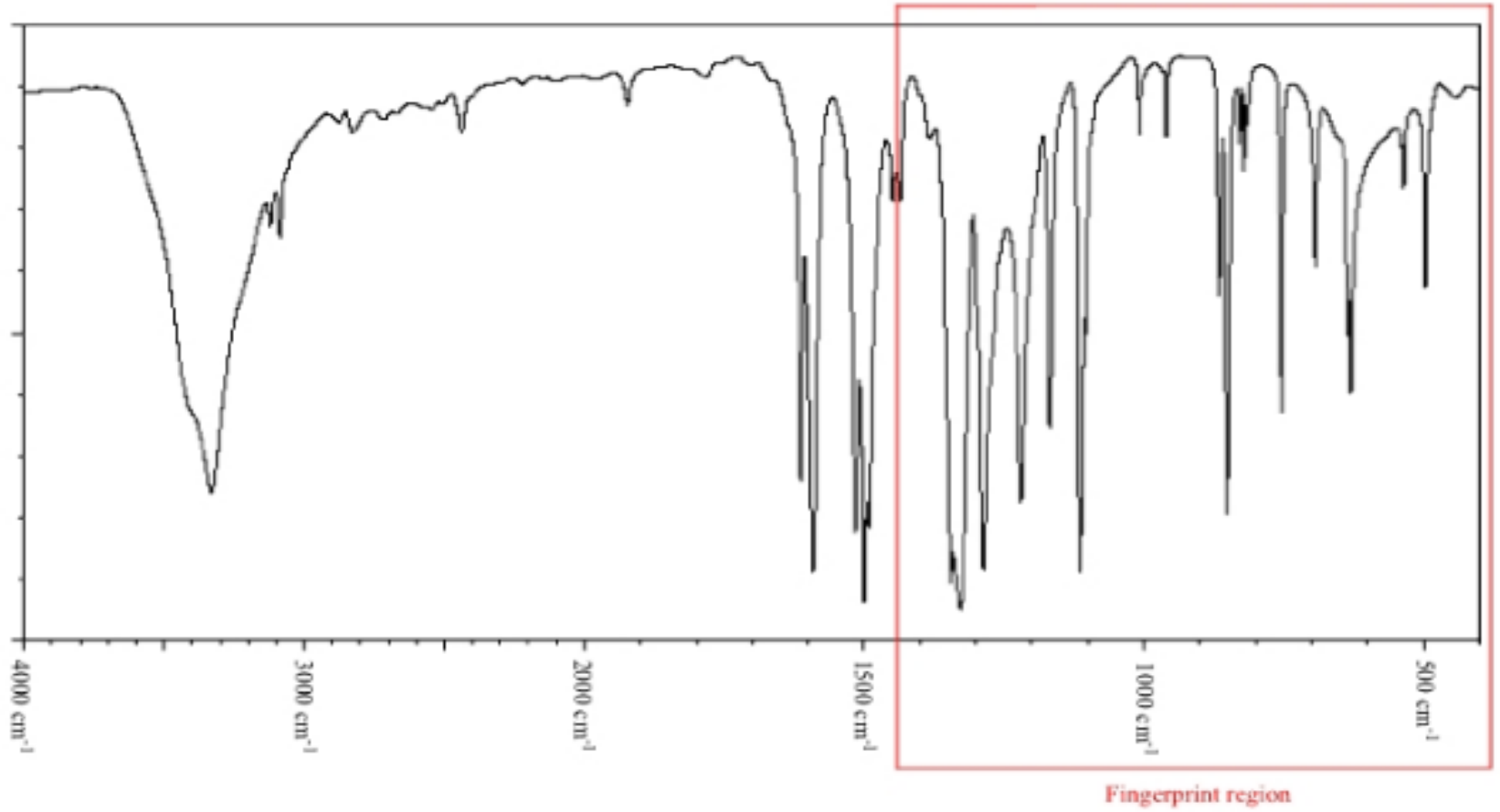
The IR Spectrum

Infrared spectra have been represented as percent of transmittance versus either the wavenumber or wavelength.



Typical IR spectrum has 2 regions:

- functional group region from 4000 cm^{-1} to 1450 cm^{-1}
- fingerprint region from 1450 cm^{-1} to 500 cm^{-1}.

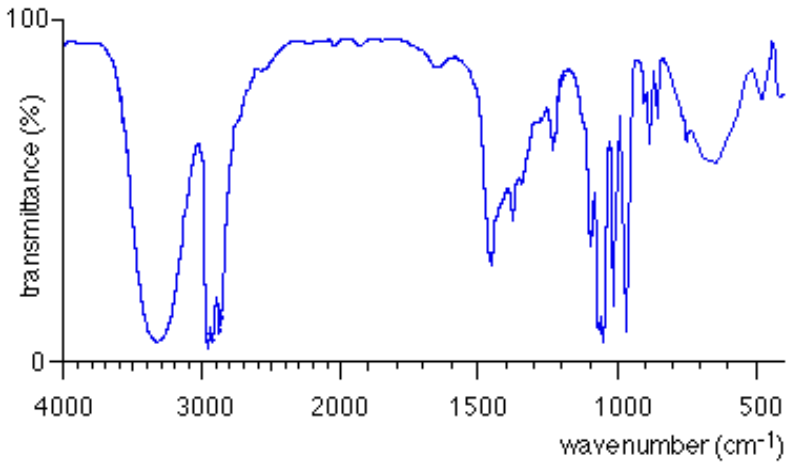


- The functional group region contains relatively few peaks. They are associated with the stretching vibrations of functional groups.

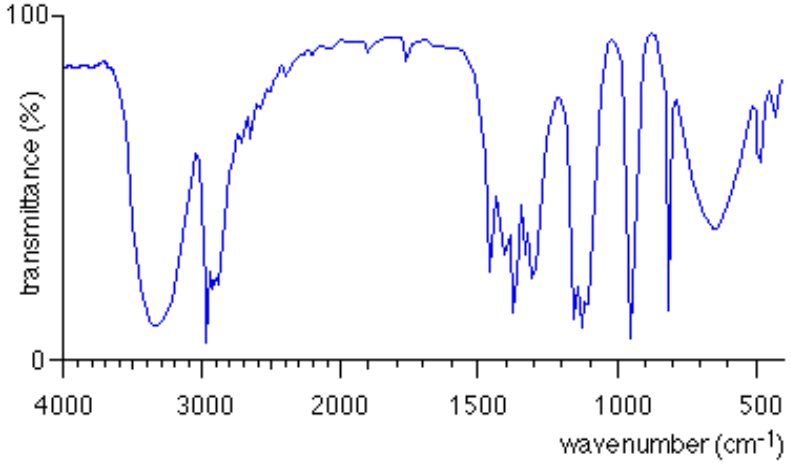
- In the fingerprint region, the spectra usually consist of bending vibrations within the molecule. The fingerprint region is important because each different compound produces its own unique pattern of peaks (like a fingerprint) in this region.

Compare the IR spectra of propan-1-ol and propan-2-ol.

infra-red spectrum of propan-1-ol, $CH_3CH_2CH_2OH$



infra-red spectrum of propan-2-ol, CH_3CHCH_3 (OH)



Fourier Transform Infrared Spectrometer (FTIR)

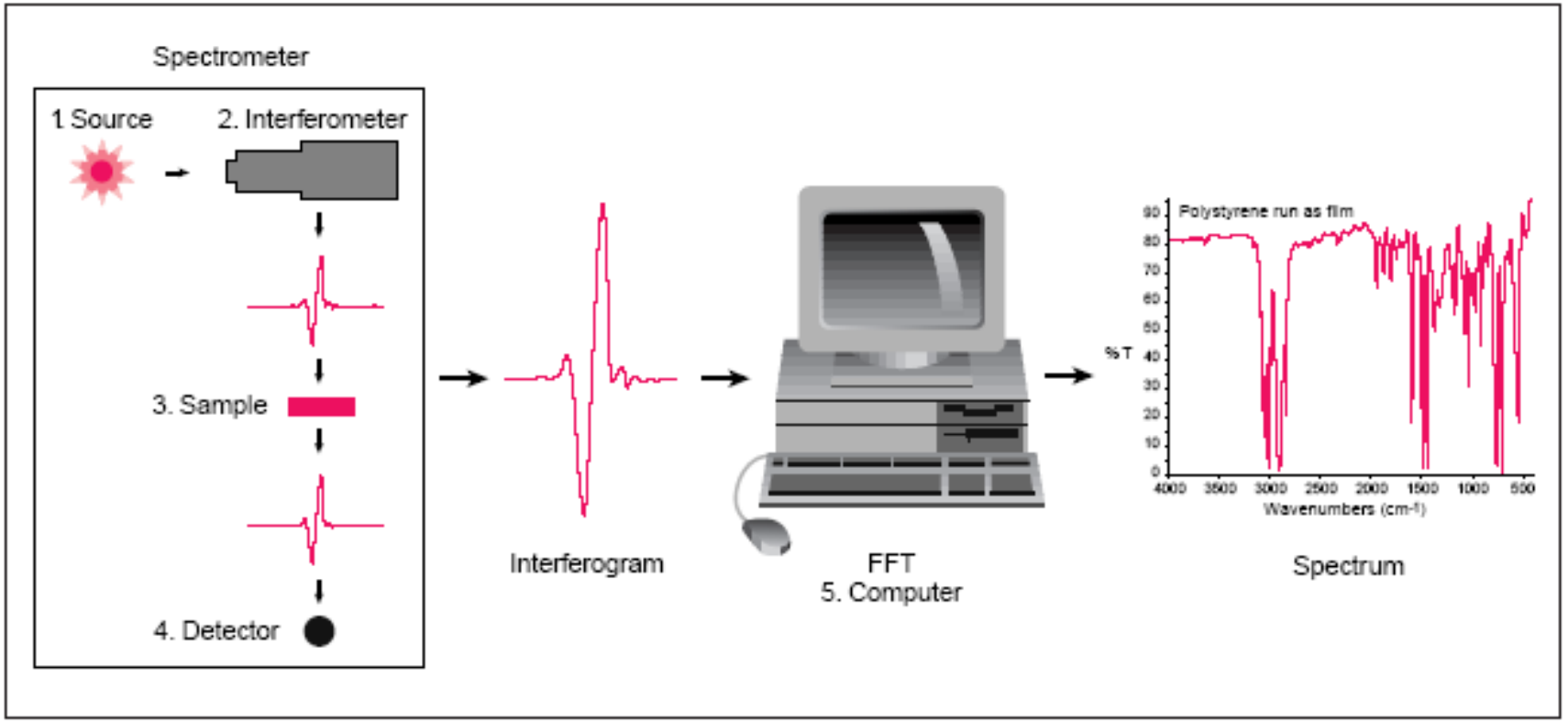
FTIR spectrometer works by taking a small quantity of sample and introducing it to the infrared cell, where it is subjected to an infrared light source, which is scanned from 4000 cm-1 to around 600 cm-1.

The intensity of light transmitted through the sample is measured at each wavenumber allowing the amount of light absorbed by the sample to be determined as the difference between the intensity of light before and after the sample cell. This is known as the infrared spectrum of the sample.

How FTIR works?

FTIR instruments use Fourier transform techniques with a Michelson interferometer.

FTIR first collecting an interferogram of a sample signal using an interferometer, then performs a Fourier Transform on the interferogram to obtain the spectrum.



IR source

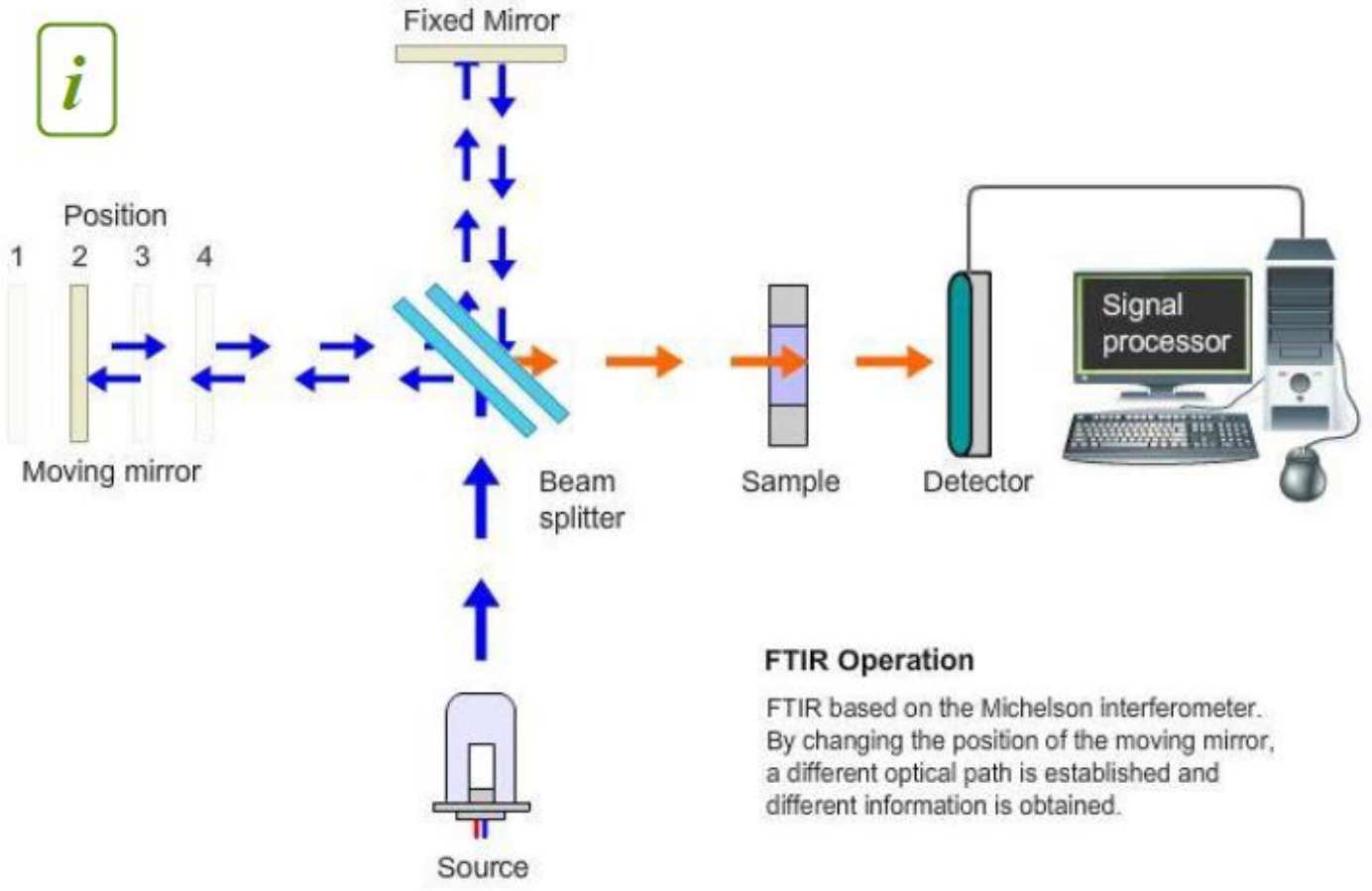
IR radiation is emitted from a glowing black body source. IR radiation passes through an aperture which controls the amount of radiation that reaches the sample, and therefore, the detector.

Common IR sources are:

1. Silicon carbide rods known as a Globar. An electric current is passed through the rod which becomes very hot (1300 K) and emits large amounts of IR radiation.
2. Nichrome and Kanthanl wire coils
3. Nernst Glowers manufactured from a mixture of refractory oxides

Interferometer

The first interferometer was invented by Albert Abraham Michelson, who received a Nobel Prize for his work in 1907. By changing the position of the moving mirror, a different optical path is established and different information is obtained.



The two beams are reflected from their respective mirrors and recombine at the beam splitter. The signal that exits the interferometer is the result of these two beams interfering with each other, and is called an interferogram.

Sample

Beam enters the sample compartment where it is transmitted through or reflected off of the surface of the sample

The Detector

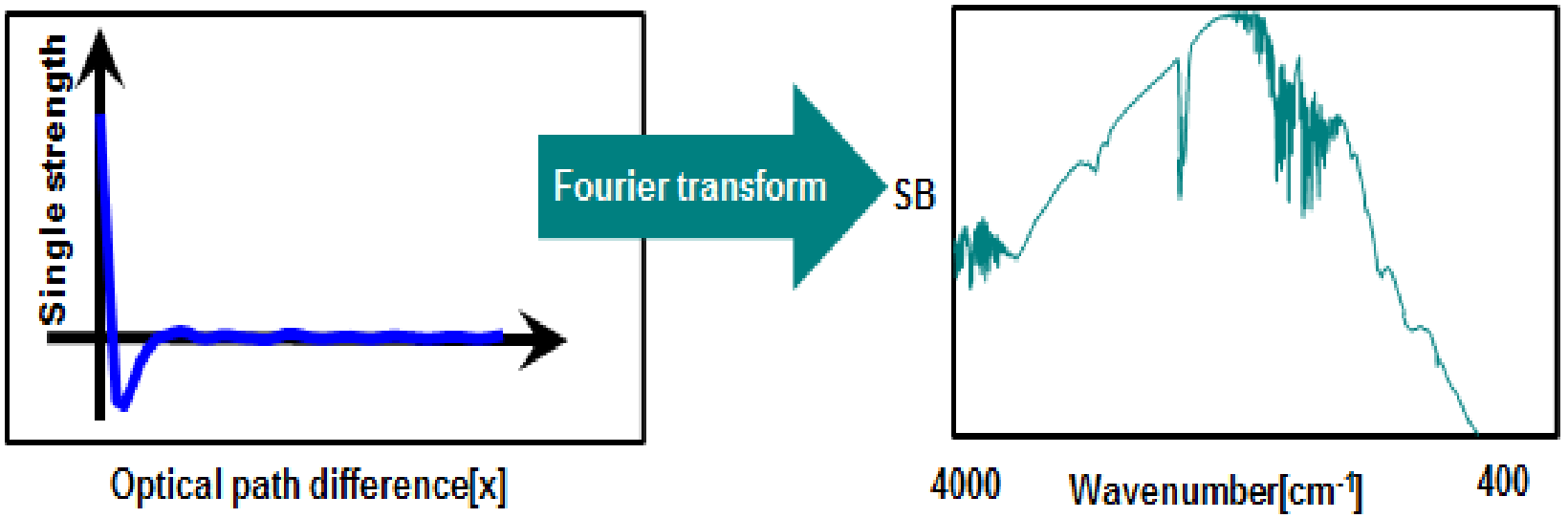
The beam finally passes to the detector for final measurement.

There are two classes of infrared detectors; thermal and photonic detectors. Thermal detectors use the IR radiation as heat; whereas, quantum mechanical (photonic) detectors use the IR radiation as light which results in a more sensitive detector.

The Computer

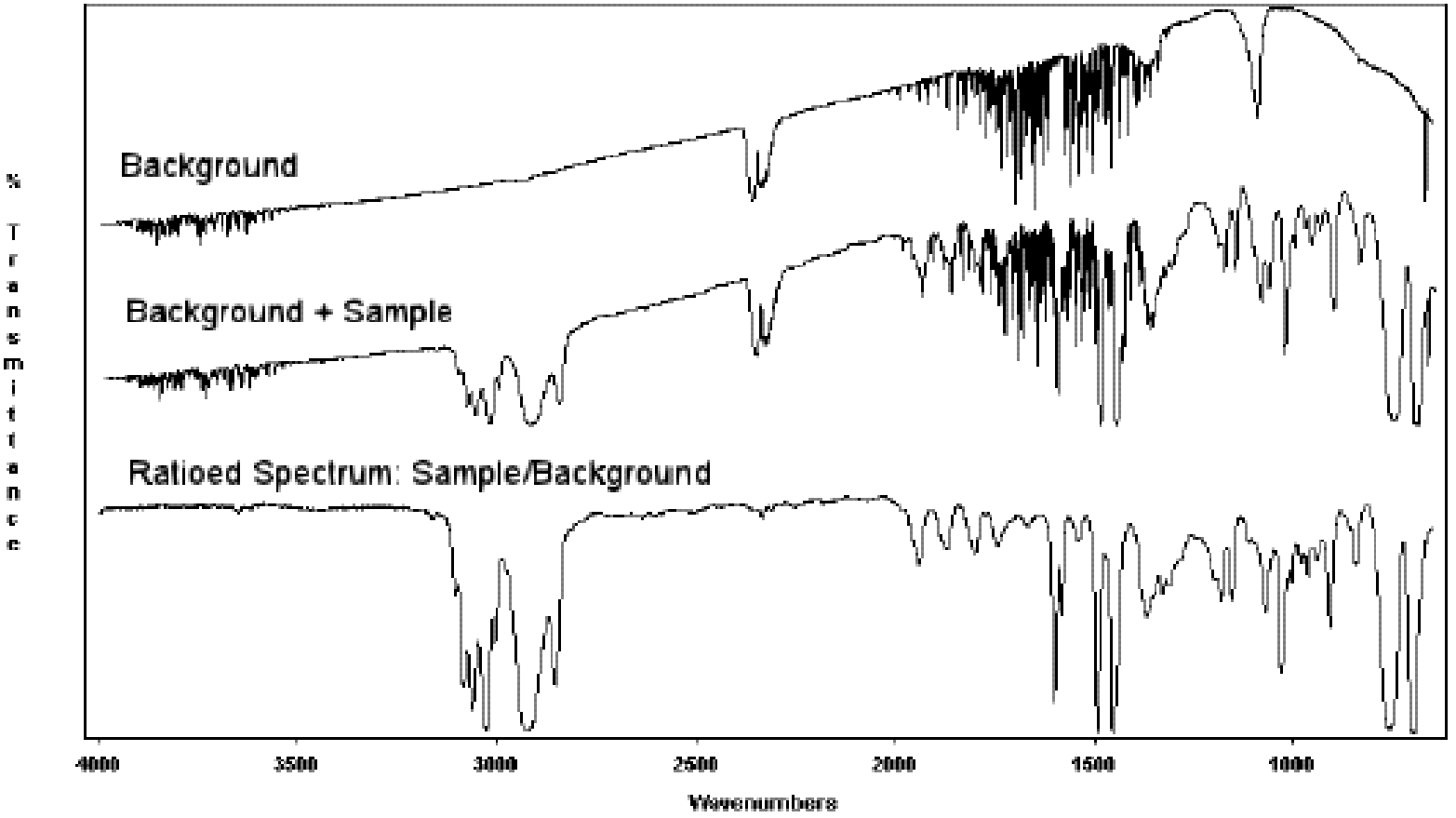
The measured signal is digitized and sent to the computer where the Fourier transformation takes place. The final infrared spectrum is obtained.

Fourier Transform



Time axis by FFT ➡ Wavenumber

Background spectrum is a measurement with no sample in the beam. This can be compared to the measurement with the sample in the beam to determine the “percent transmittance.”



Spectra Collected in IR Spectroscopy (Polystyrene)

FTIR Advantages

Speed: All IR frequencies are measured simultaneously, resulting in measurements being taken in seconds rather than minutes. This is often referred to as the Felgett Advantage.

Sensitivity: The detectors utilized are highly sensitive which results in lower signal to noise ratios. This is known as the Jacquinot Advantage.

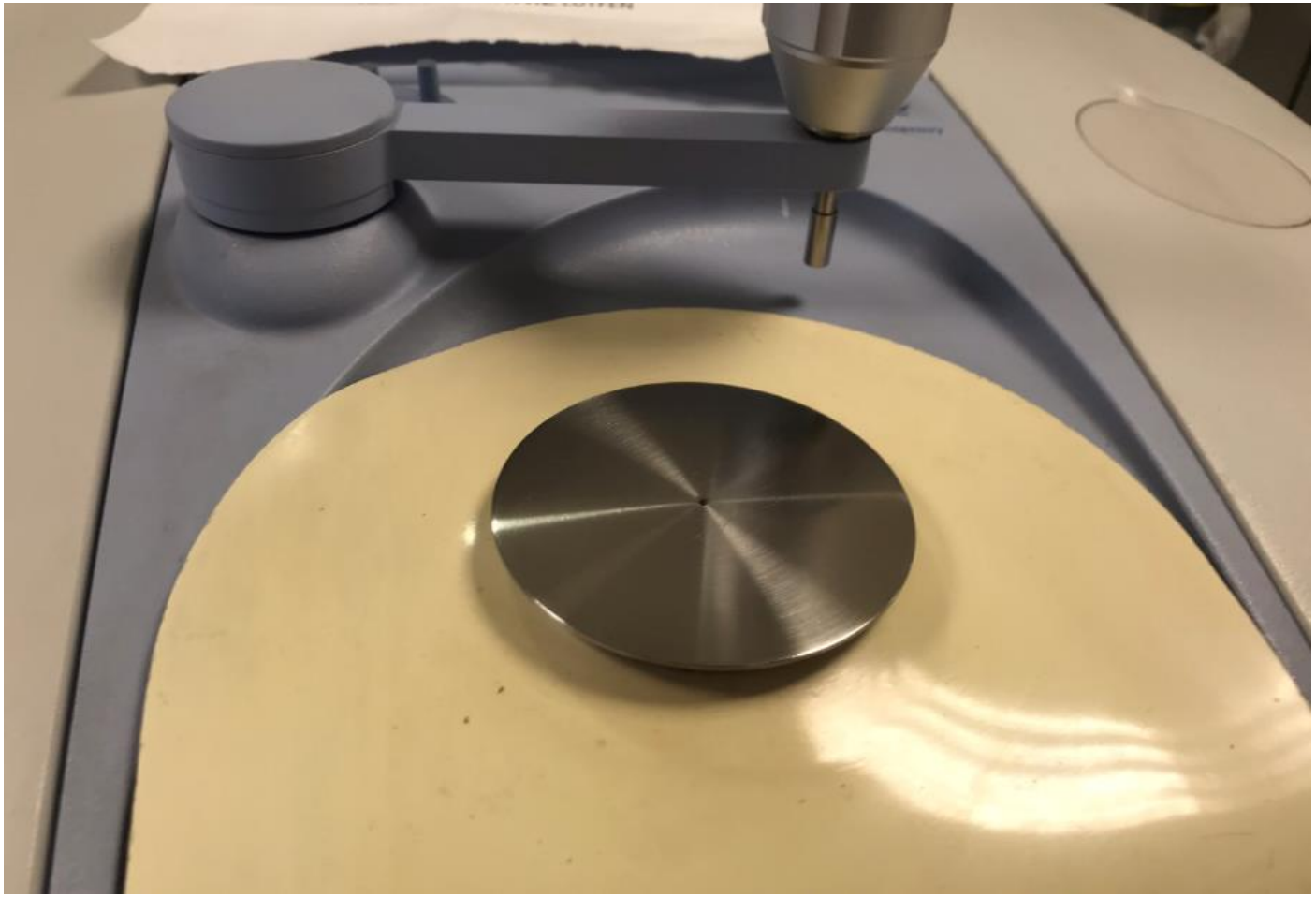
Simplicity: The only moving part in an FTIR instrument is the mirror in the interferometer; therefore, there is very little need for mechanical maintenance.

Internal calibration: The internal laser is used to self-calibrate the moving mirror in the FTIR instrument. This is denoted as the Connes Advantage.

Experiment
Determination of FTIR Spectrum of Oil

Watch Video

IMG_8339 giriş1.mp4



Watch Video

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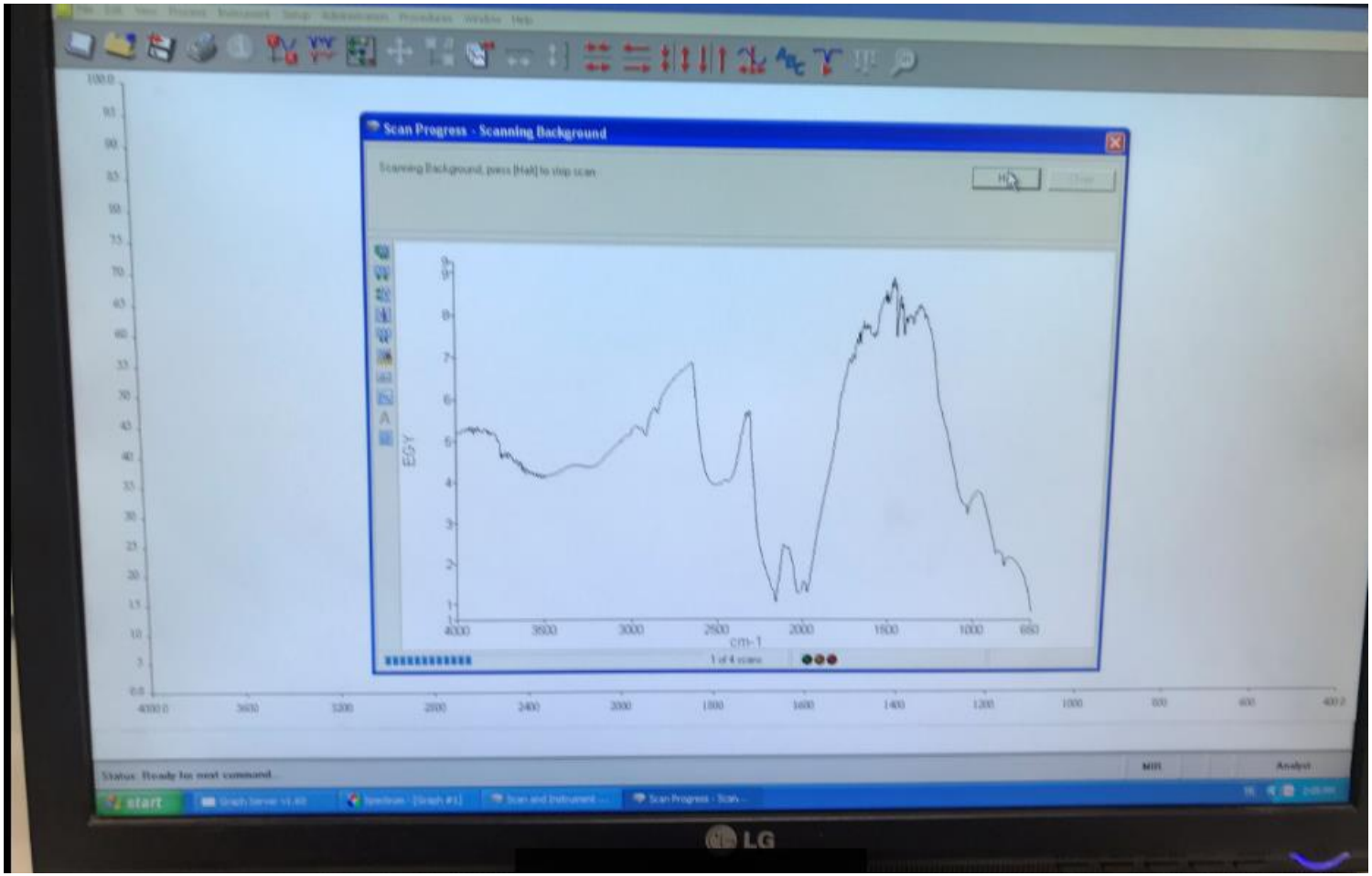

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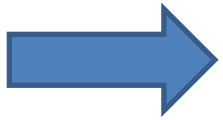

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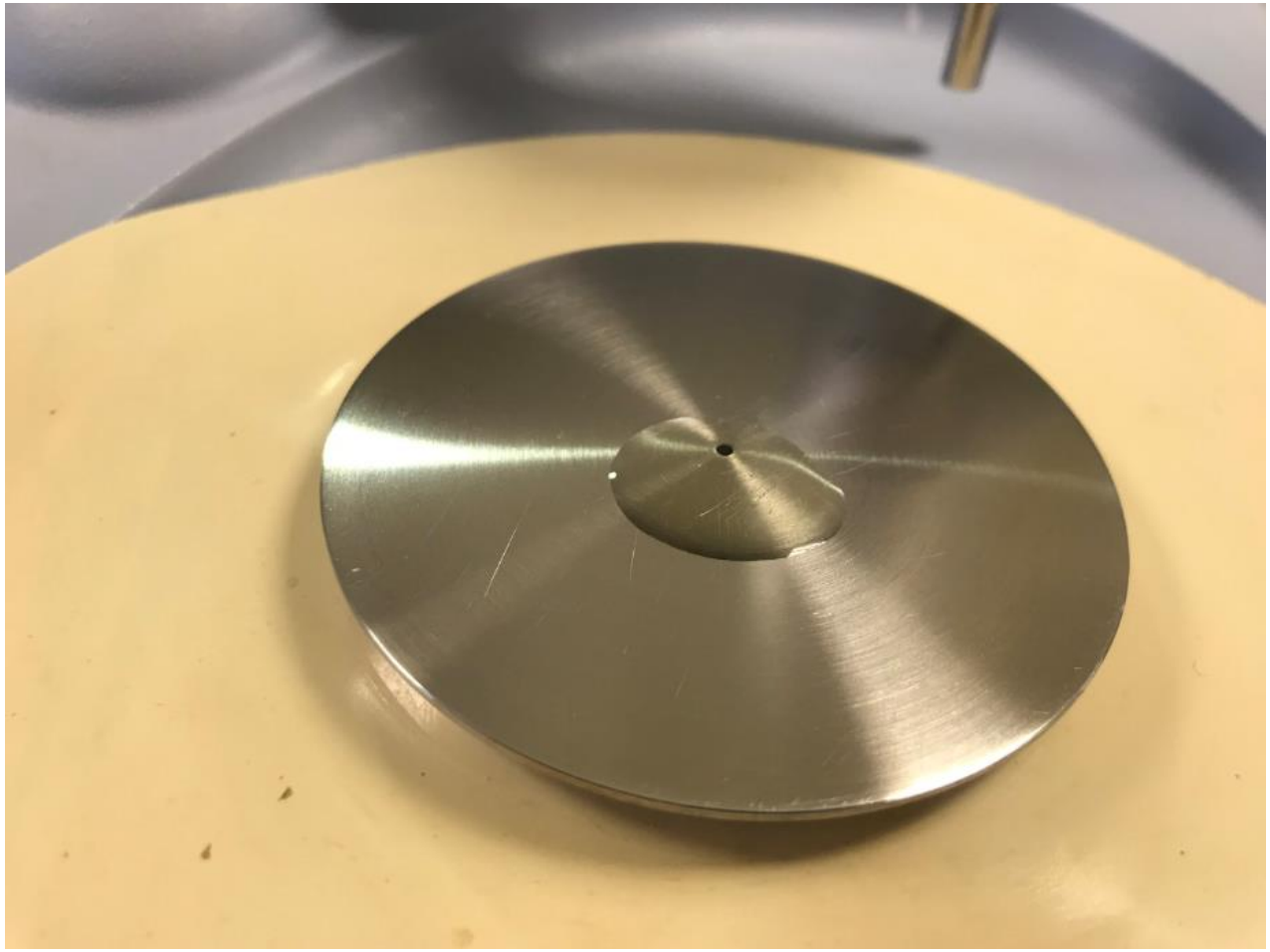

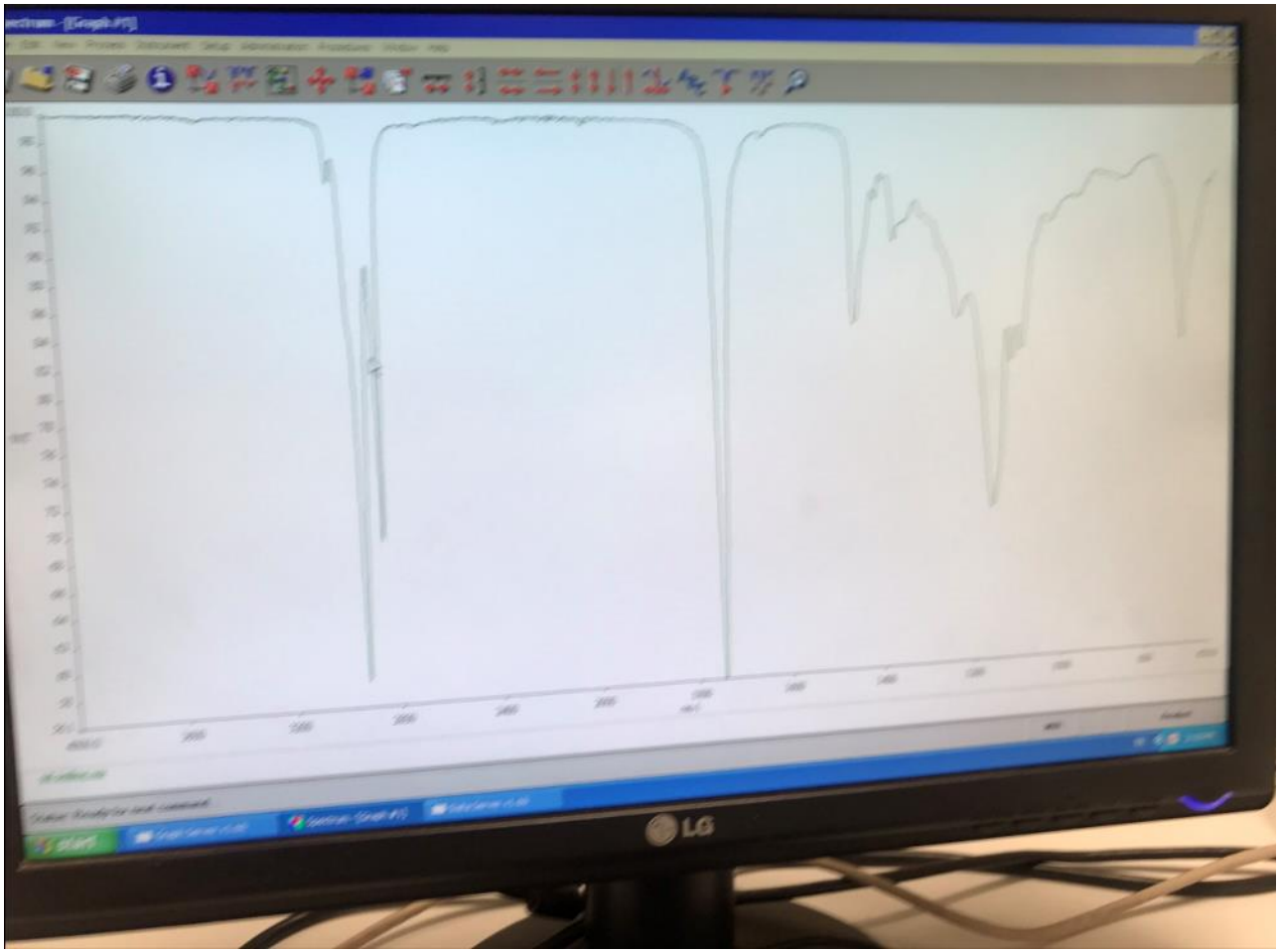
LG

Tips for Your Reports

1. Find the wavenumbers of:
    - Carbonyl group
    - Water
    - Cis-unsaturated fatty acids
    - Trans-unsaturated fatty acids
2. Define each of these components in each oil sample if present
3. Compare oil samples with respect to these components

YOUR DATAS (FTIR SPECTRUMS) ARE ON MY WEBSİTE:
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