FOURIER TRANSFORM INFRARED SPECTROSCOPY

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OUTLINE

- History of IR Radiation and FTIR
- General Information about IR Spectroscopy
- Types of IR Spectrometers
- Sample Preparation
- Instrumentation
- Applications of FTIR

Goals of presentation;

To give general information

- about differences between IR spectrometers
- about FTIR theory

History of IR and FTIR spectroscopy

- Chemical IR spectroscopy was emerged as a science in 1800 by Sir William Herschel
- Firstly most IR instrumentation was based on prism or grating monochromators
- Michelson invented interferometer in 1881

- In 1949 Peter Fellgett obtained the first IR spectrum by using FTIR spectrometer
- In 1960s commercial FTIR spectrometers appeared
- In 1966 Cooley-Tukey developed an algorithm, which quickly does a Fourier transform

What is Spectroscopy?

Spectroscopy deals with interactions between matter and energy

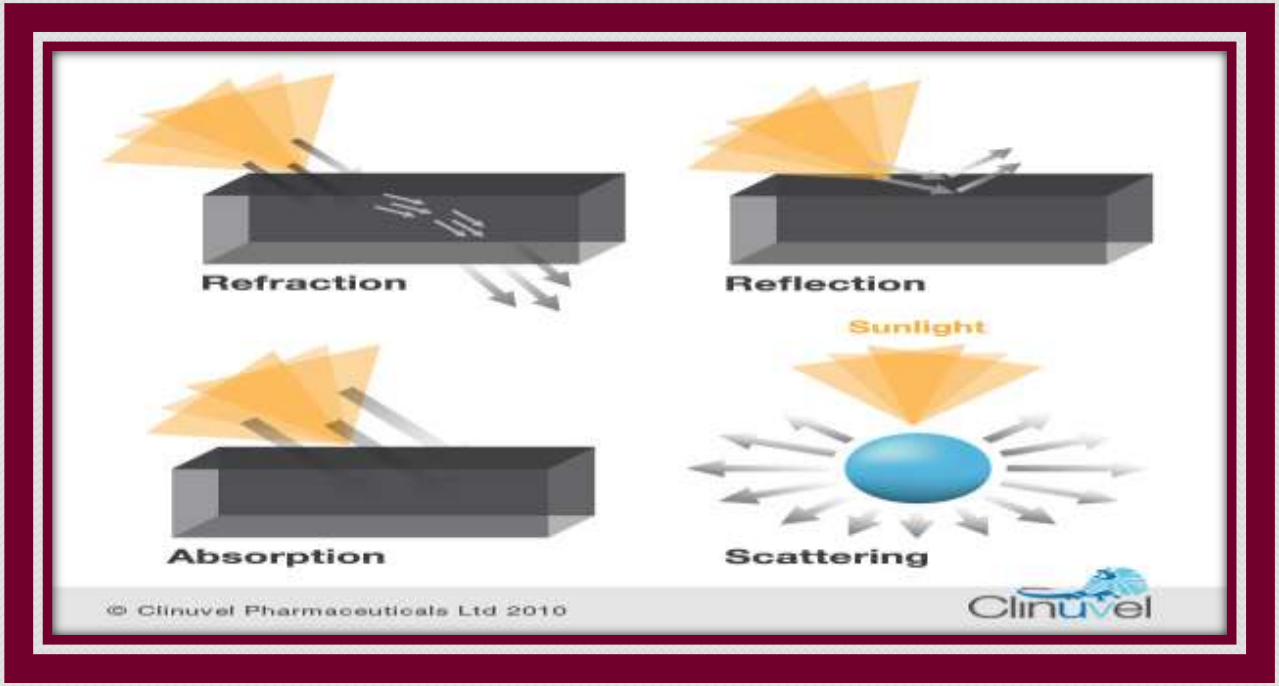


Figure 1 : interaction between matter and energy

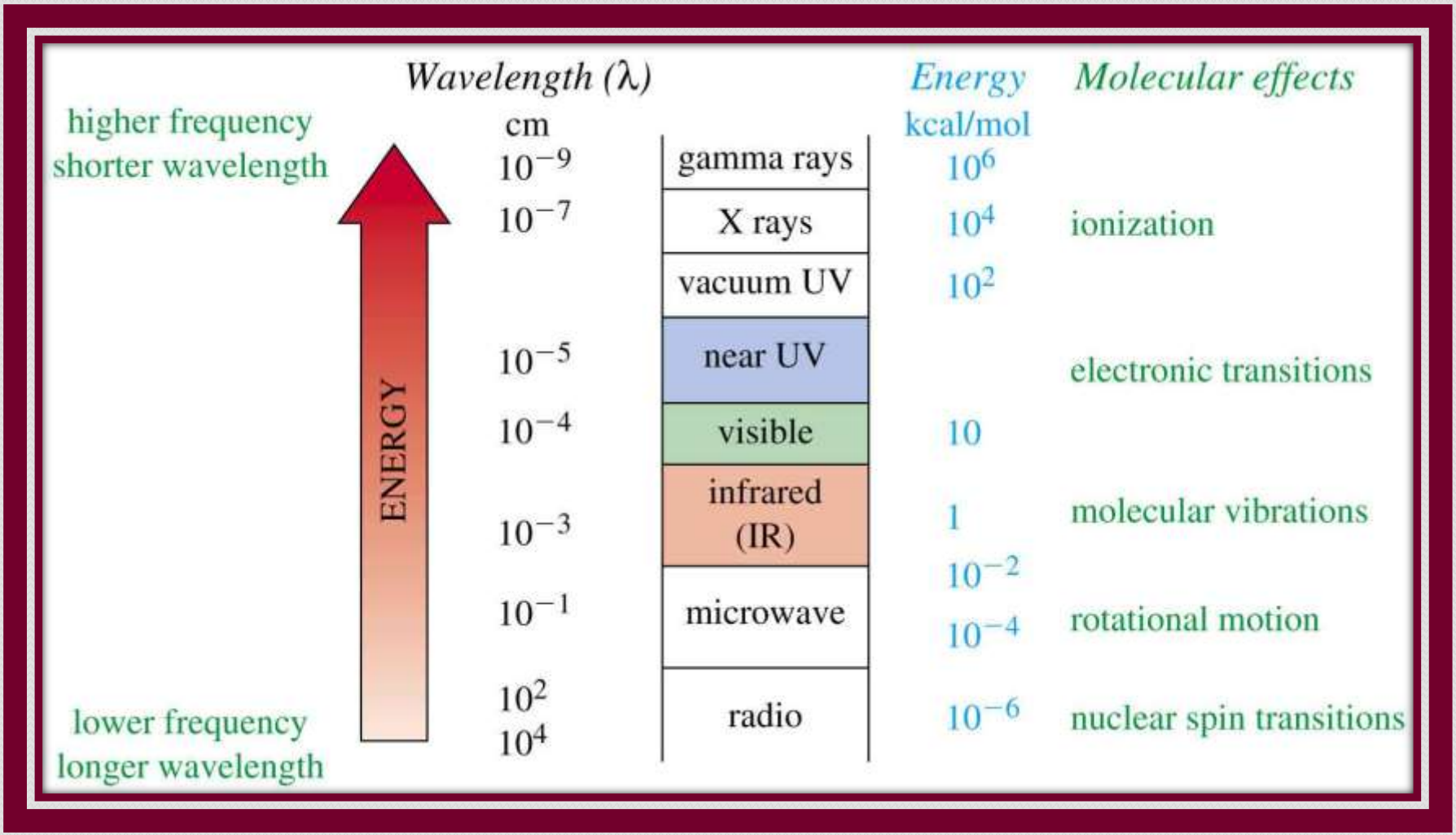


Figure 2 : electromagnetic spectrum

Motion of atoms and molecules ⟶ IR radiation

higher temperature

↓

motion

↓

more IR radiation emission

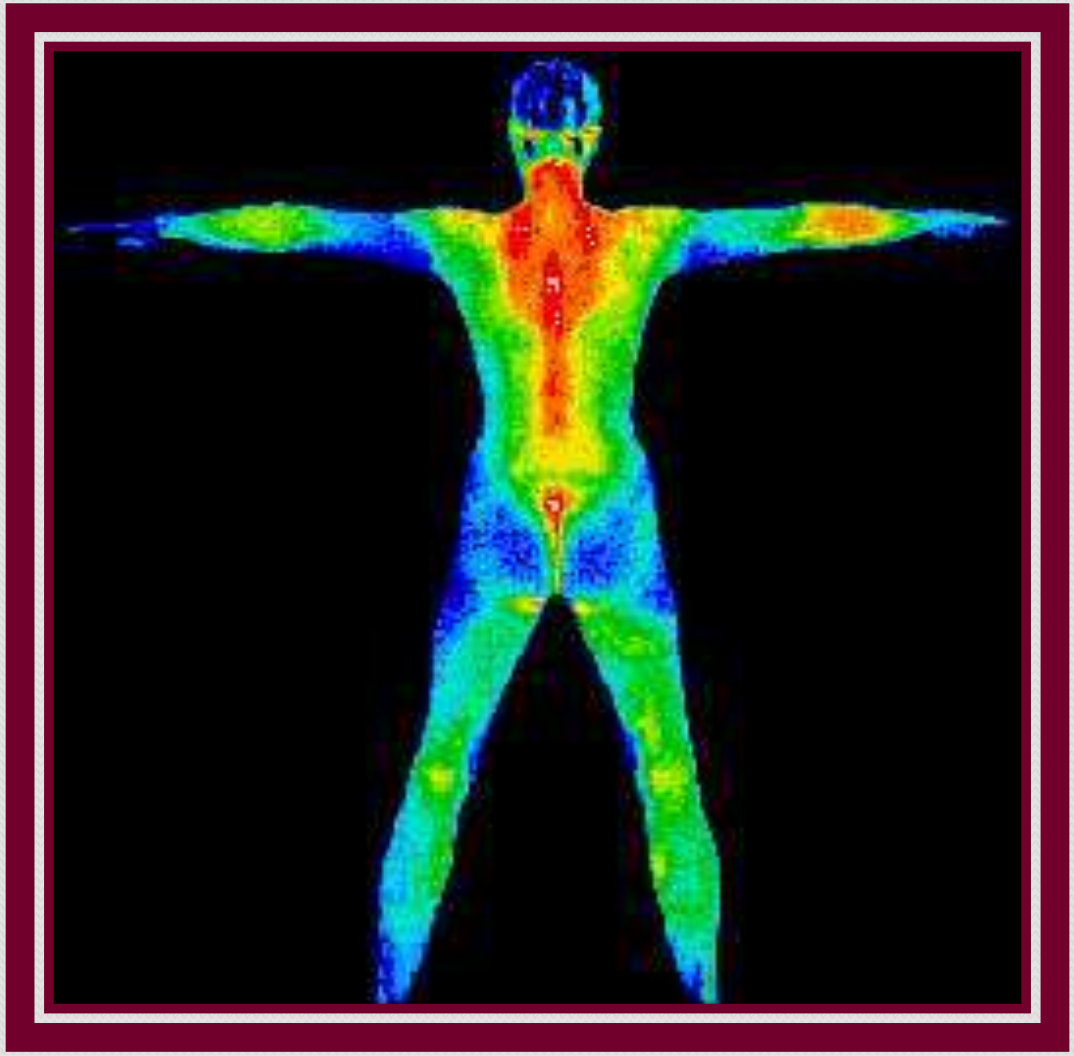
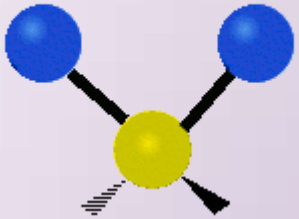
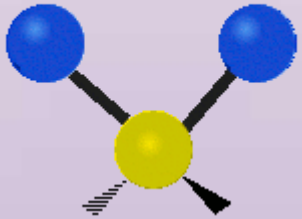
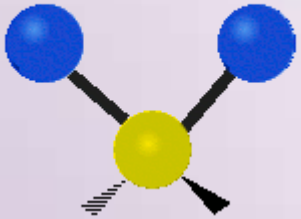
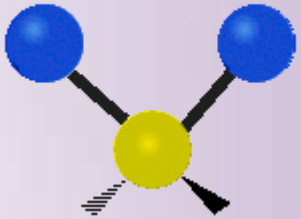
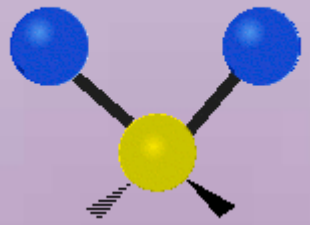
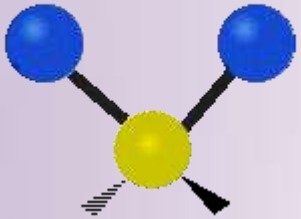


Figure 3 : human body at normal body temperature

Vibrations of Molecules

Symmetrical stretching	Antisymmetrical stretching	Scissoring
		
Rocking	Wagging	Twisting
		

Absorption of IR Radiation

- Net change in molecules' dipol moment
- Equıvalence in frequencies

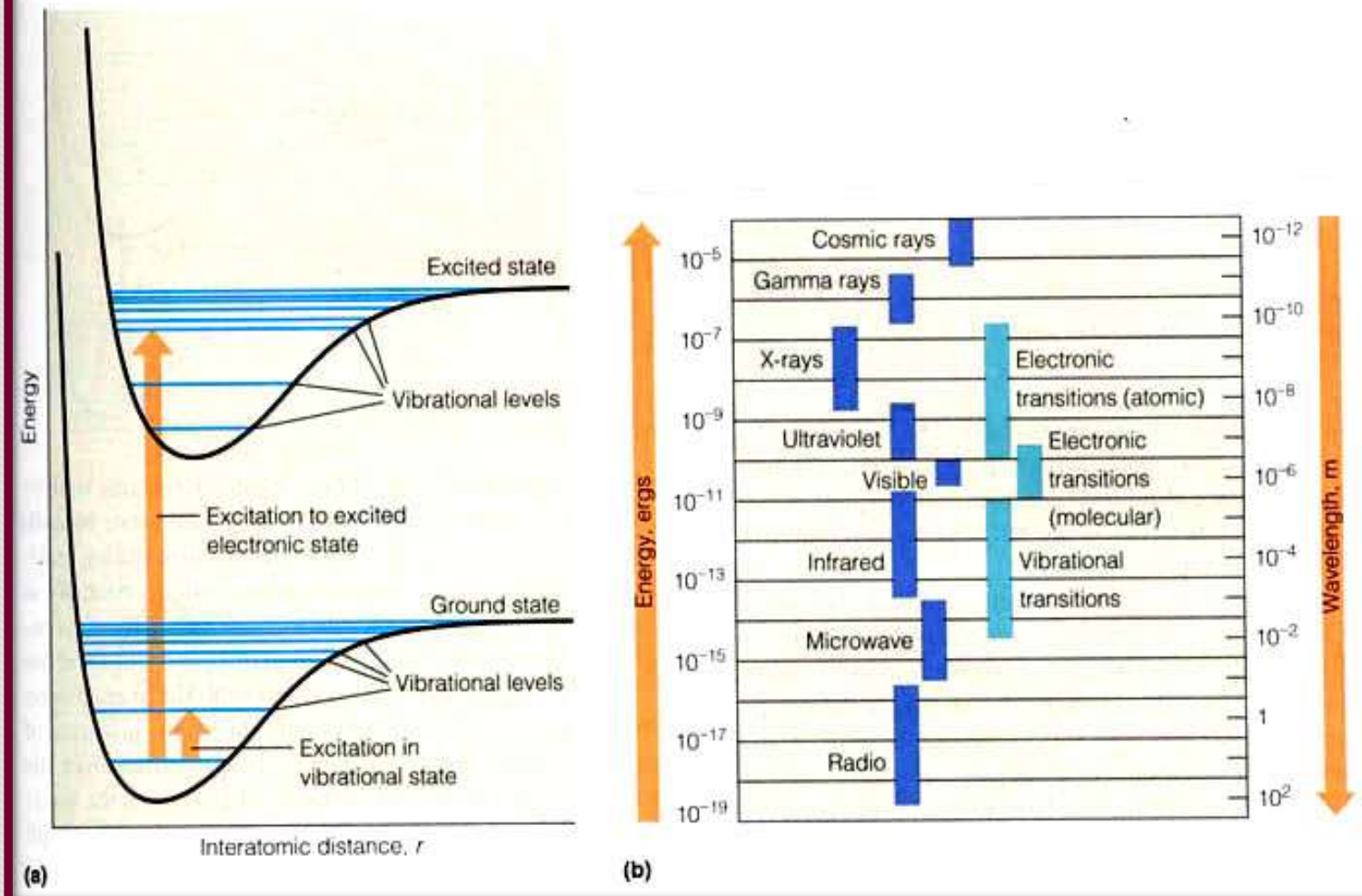


Figure 4 : vibration energy levels of molecules

The spectrum tells us;

The infrared spectrum for a molecule is a graphical display

The spectrum has two regions:

- The *fingerprint* region 600-1200 cm^{-1}
- *Functional group* region 1200-3600 cm^{-1}

- determining structures of compounds
- identifying compounds

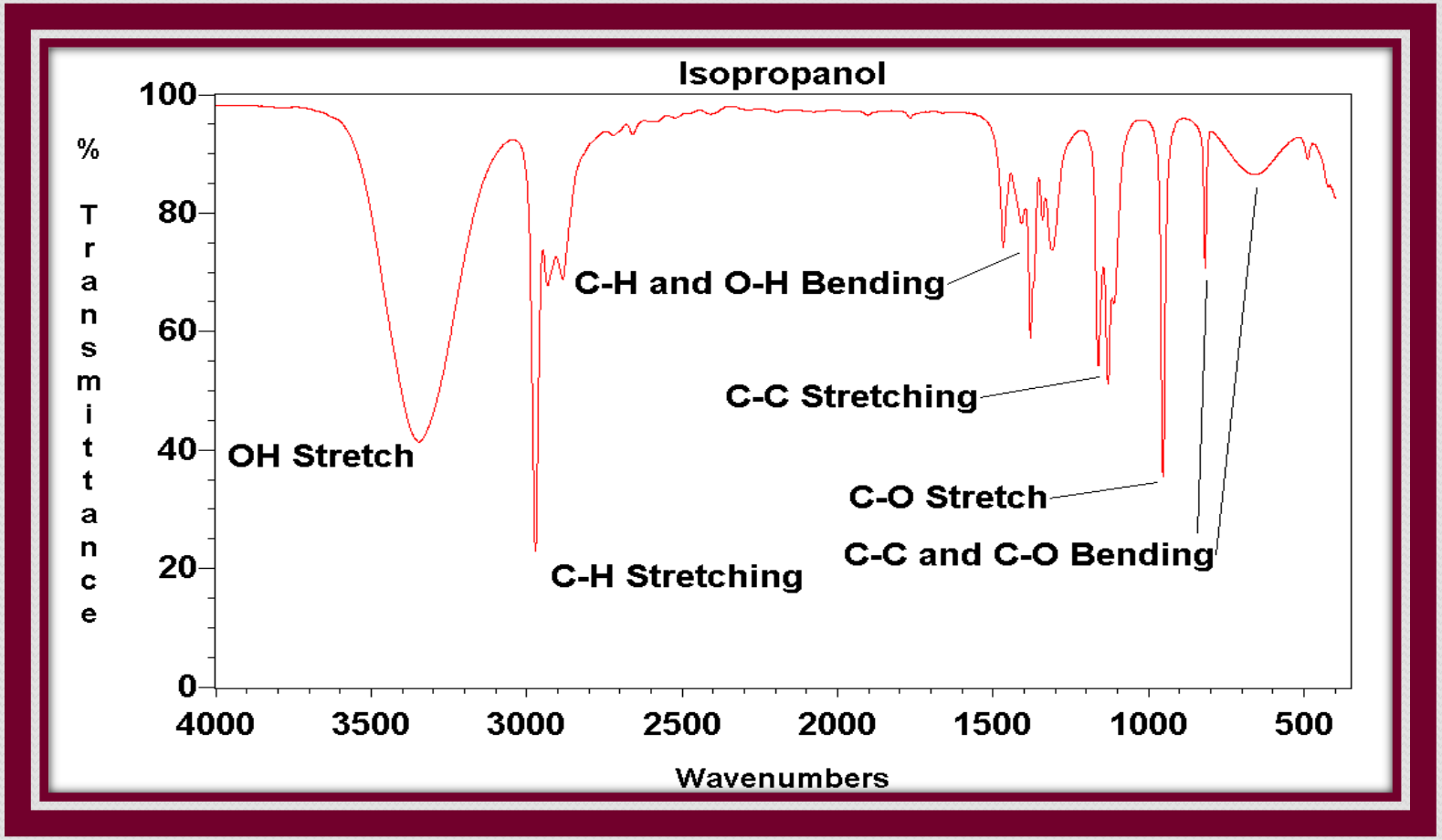


Figure 5 : infrared spectrum of isopropanol

Two types of instrumentations are used to obtain IR spectrum;

- Dispersive Type
- Fourier Transform Infrared (FTIR)

Dispersive Type Spectrometer

- Having a filter or grating monochromator

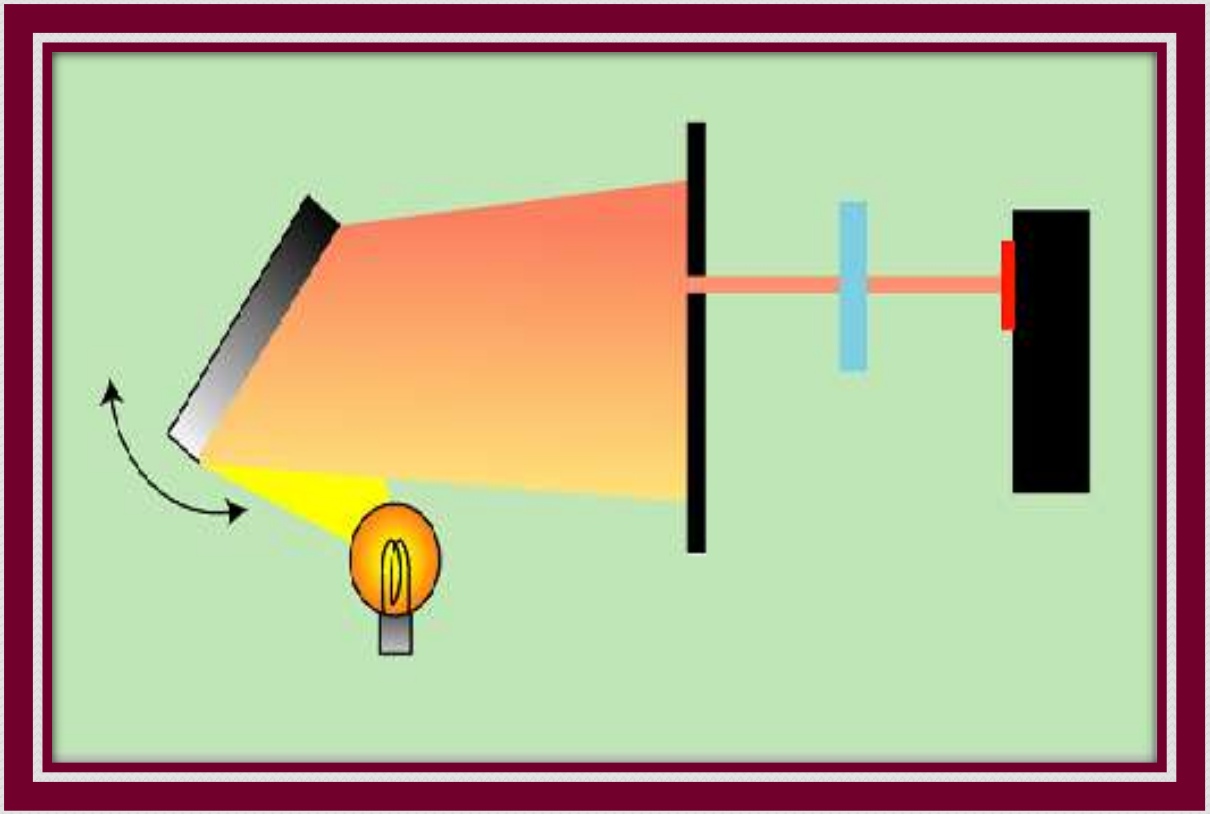


Figure 6 : dispersive type spectrometer instrumentation

Fourier Transform Infrared Spectrometer

- collecting an interferogram
- simultaneously measuring
- acquiring and digitizing the interferogram
- outputing the spectrum

Why FT-IR spectroscopy?

- Non-destructive technique
- Good precision
- No external calibration
- High speed
- Signal-Noise ratio
- Mechanically simple

What information can FT-IR provide?

- Identify unknown material
- Determine quality or consistency of sample
- Determine amount of components in mixture

Sample Preparation

- Gaseous samples

Long pathlength to compensate for the diluteness

- Liquid samples

Can be sandwiched between two plates of a salt

- sodium chloride
- potassium bromide
- calcium fluoride

- Solids
  - KBr pellet
  - Nujol mull
  - Dissolving in organic solvent(CCl_4)

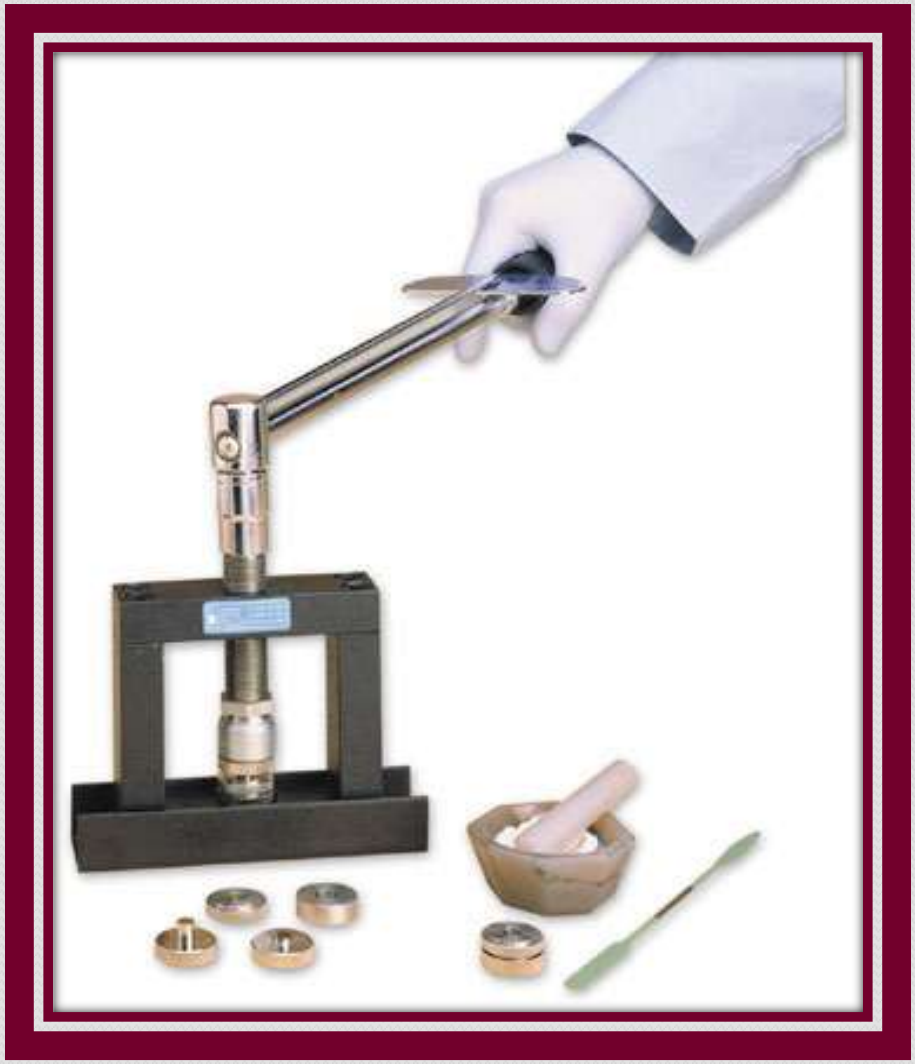


Figure 7 : preparation KBr pellet

INSTRUMENTATION

1.Radiation Sources

Black-body radiation

- Nernst filament (ZrO and some other rare earth oxides)
- Globar (Si-C)
- Ni-Cr wire
- Heated ceramic
- Mercury lamp

2.The Interferometer

- spectral encoding
- resulting interferogram signal obtains

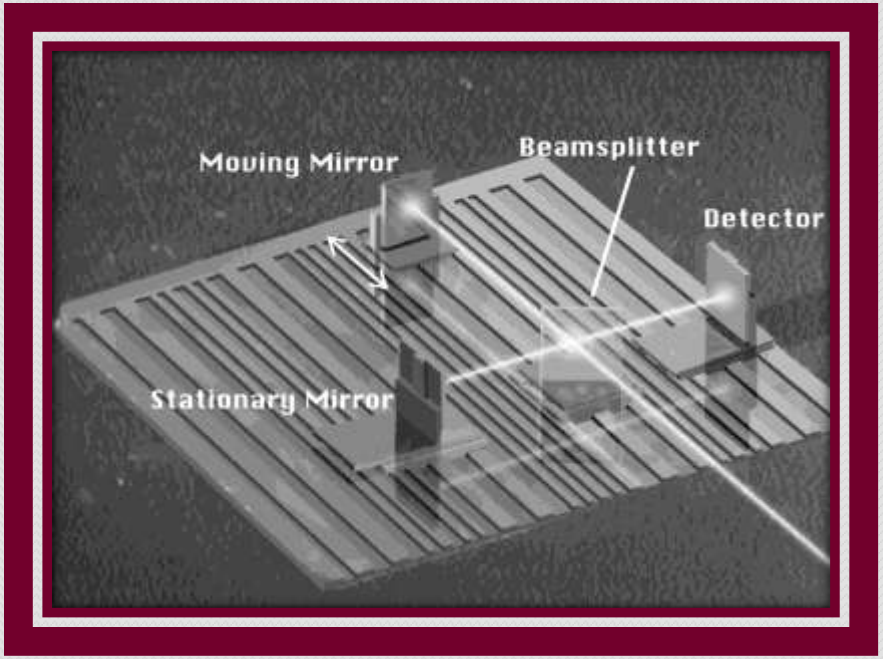


Figure 8 : an interferometer

How does it work?

1. Dividing the radiation into two beams
2. One of them goes to fixed mirror
3. Other one goes to movable mirror
4. Recombining
5. Sending to detector

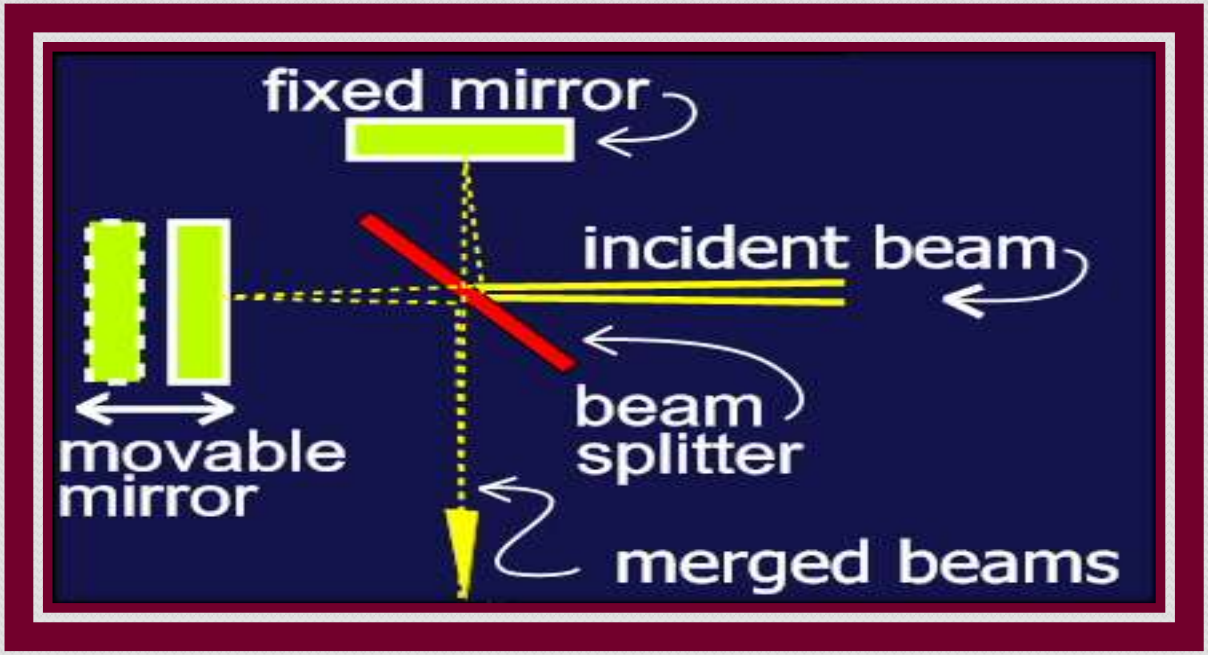


Figure 9:
ligth travel in
interferometer

- $\delta=0$ or $\delta= n\lambda \longrightarrow$ constructive interference
- $\delta=\lambda/2$ or $\delta = (n + 1)\lambda/2 \longrightarrow$ destructive interferences

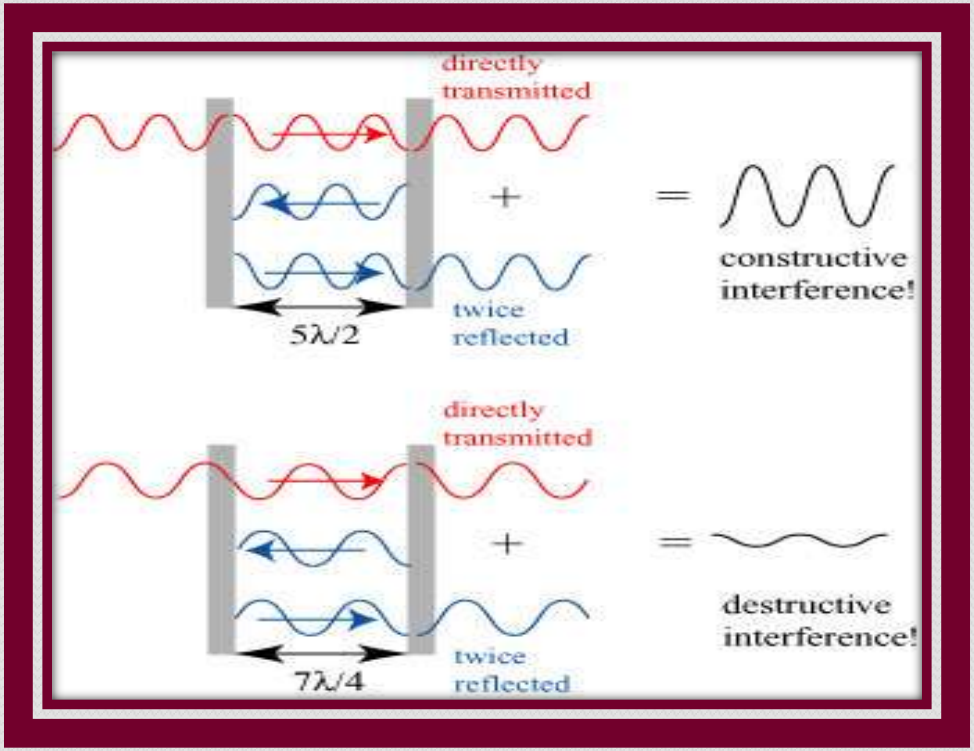


Figure 9 : constructive-destructive interfrence of waves

Interferogram: Name of the signal which has time domain and occurs as a result of constructive interferences.

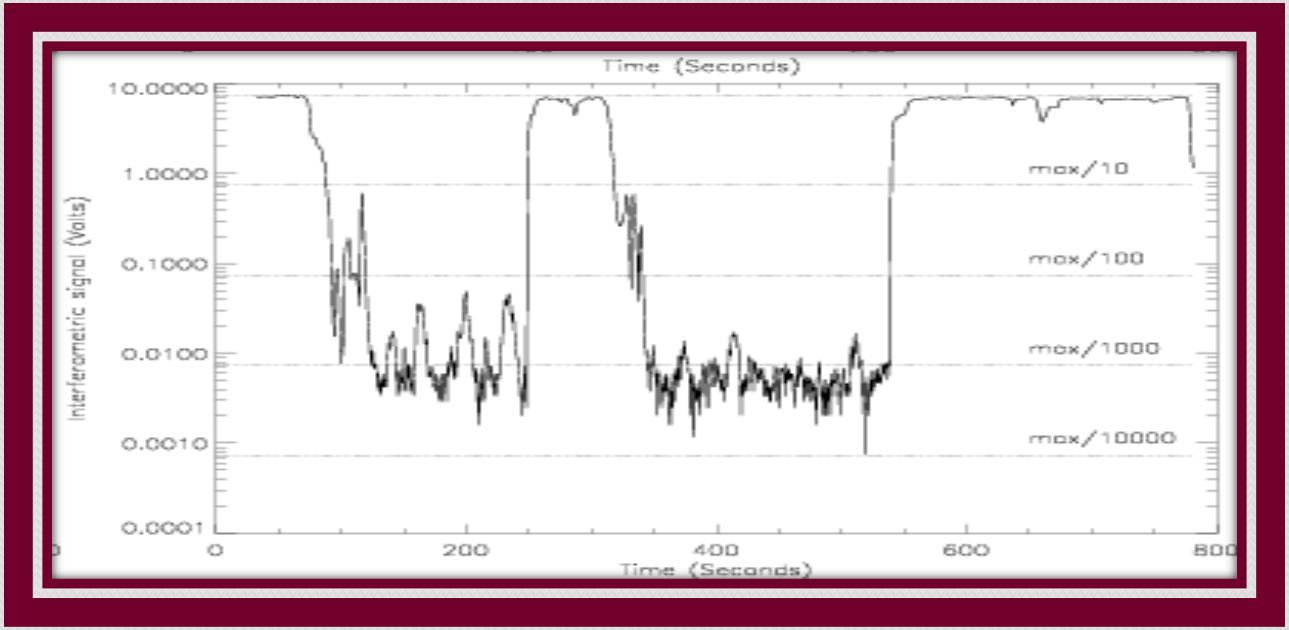


Figure 11 : an interferogram example

A Fourier transform converts the time domain to the frequency domain with absorption as a function of frequency.

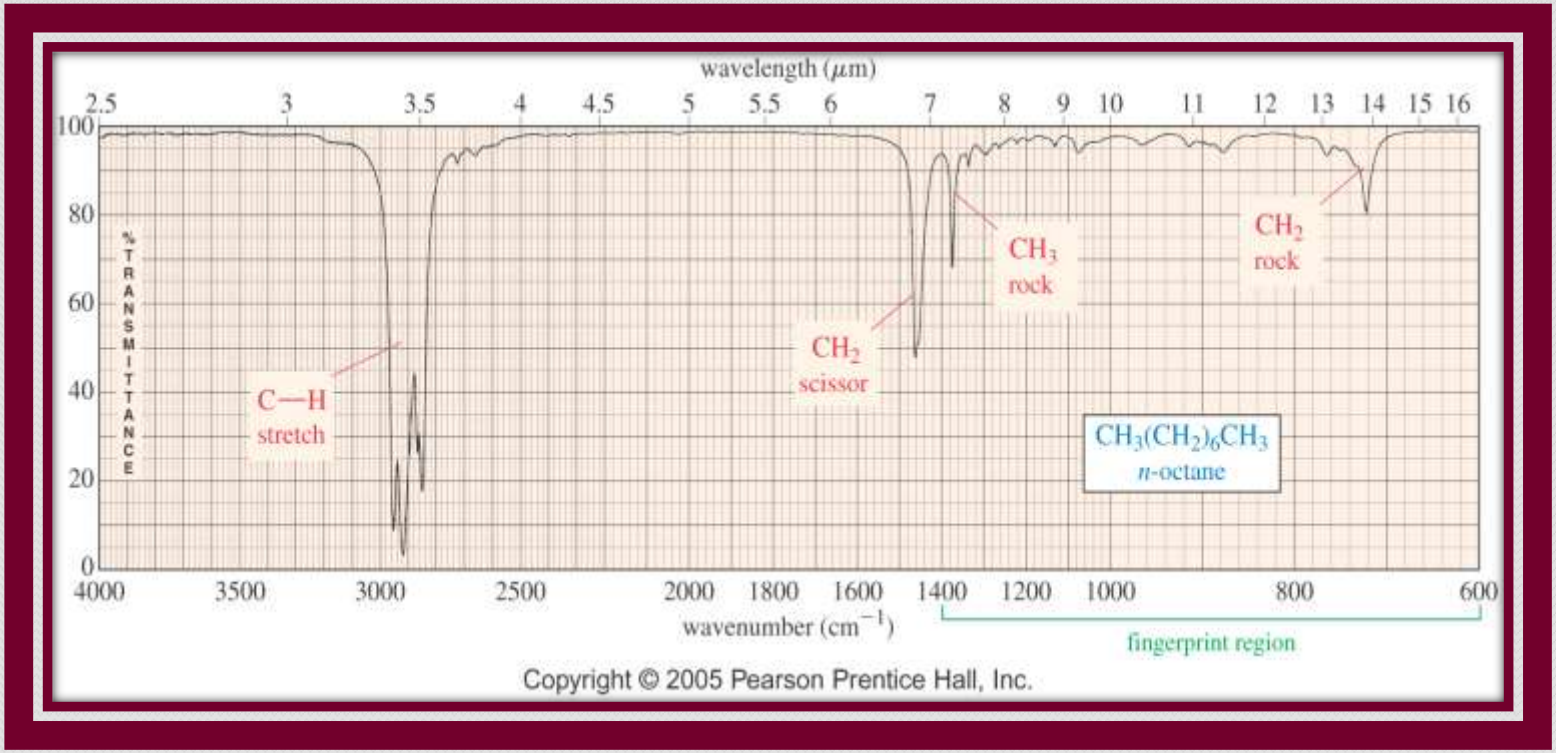


Figure 12: example of spectrum that is converted by fourier transform

3.Detectors

The beam finally passes to the detector

❖ Thermal detectors

- Thermocouples
- Bolometer

❖Photoconducting detectors

- most sensitive detectors.

❖Pyroelectric detectors

- much faster response time
- insulator material
- Triglycine sulphate

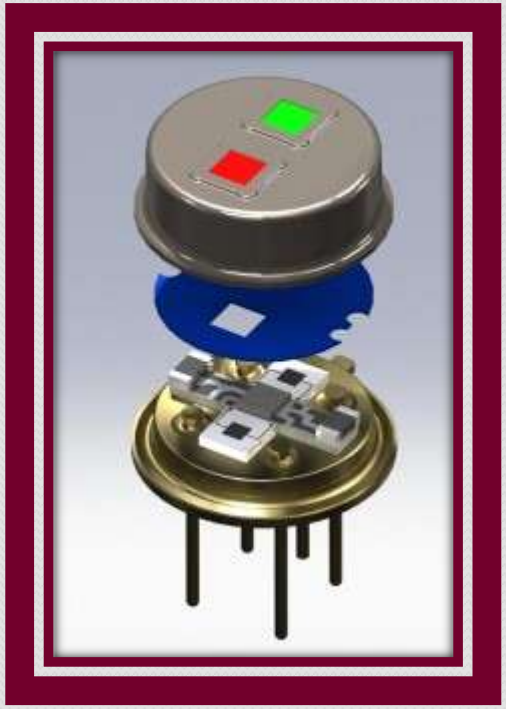


Figure 13:
pyroelectricc detector

4.The Computer

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

Figure 14 : FTIR spectrometer

The Sample Analysis Process

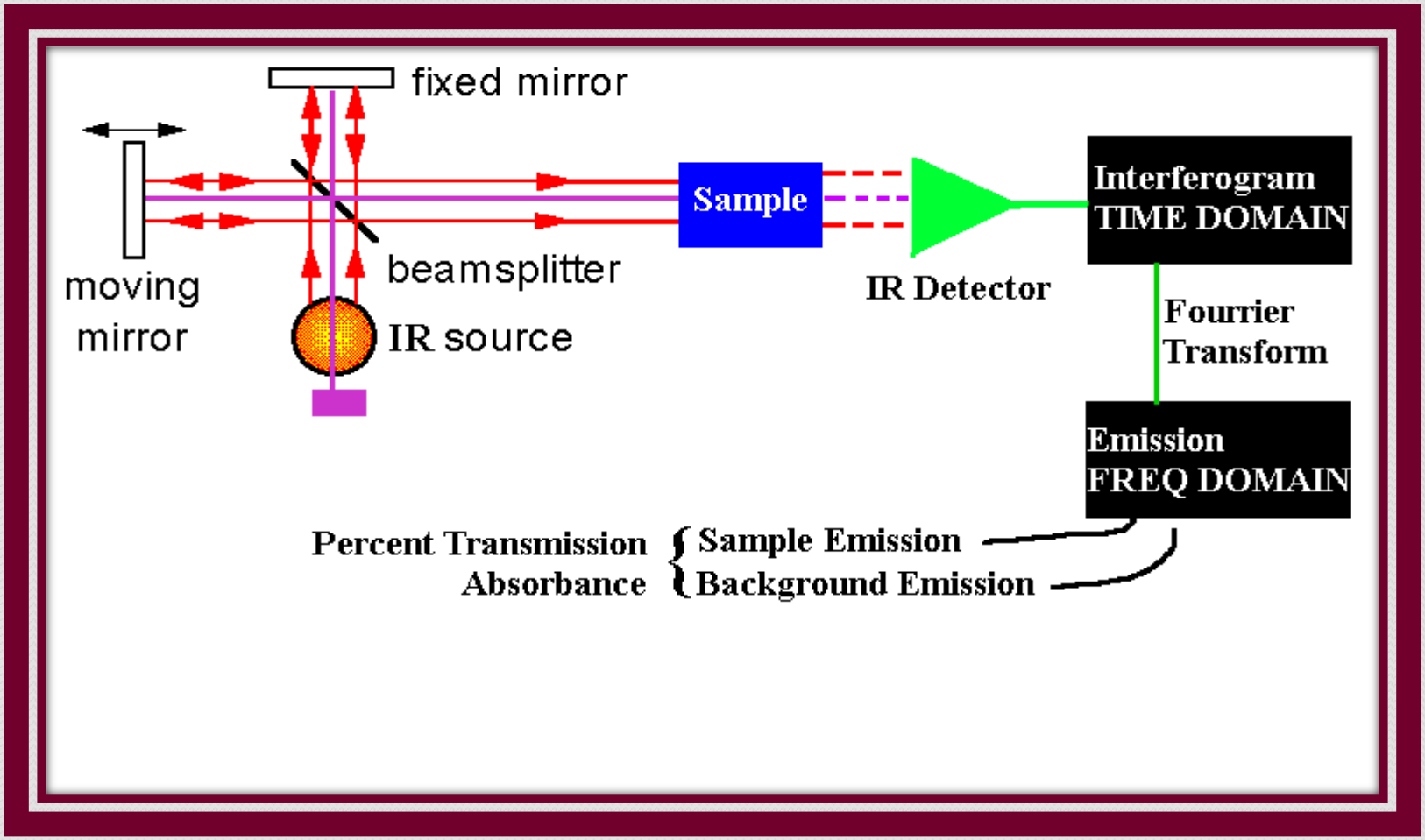


Figure 15 : FTIR spectrometeranalysis process

Applications of FT-IR

- Pharmaceutical research
- Forensic investigations
- Polymer analysis
- Lubricant formulation and fuel additives
- Foods research
- Quality assurance and control
- Environmental and water quality analysis methods
- Biochemical and biomedical research

coatings and surfactants

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Thank You for Listening