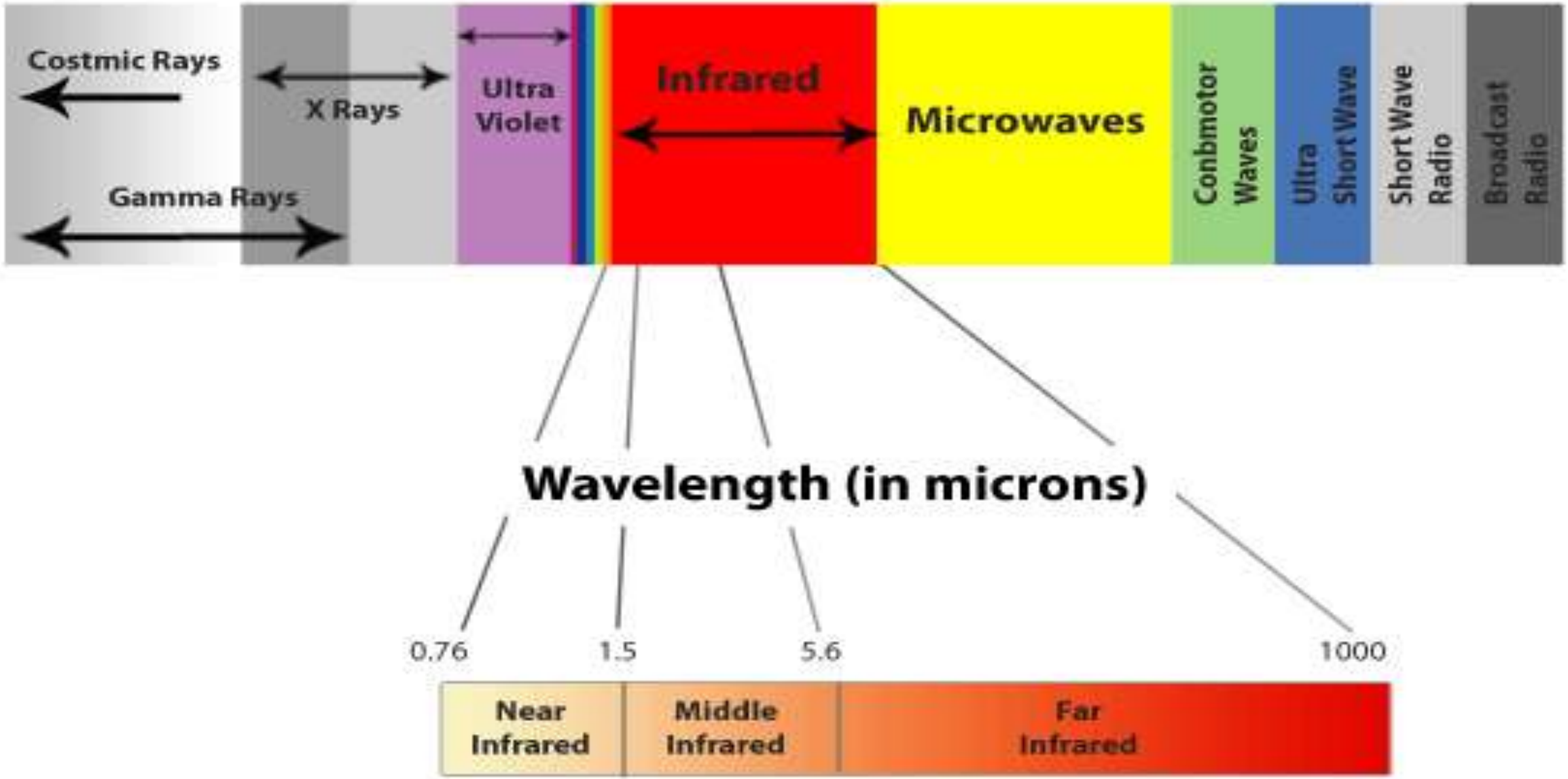
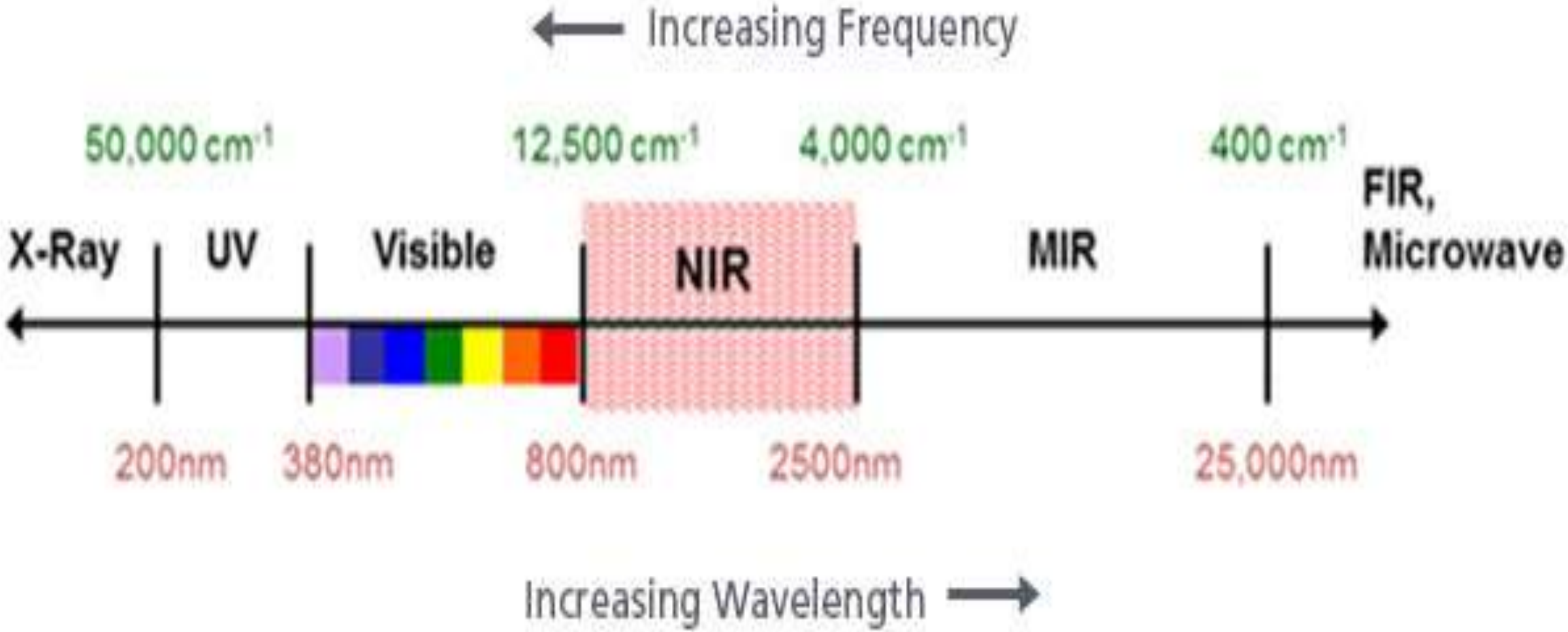
IR Spectrophotometry (Technique)

IR Spectroscope (Instrument)

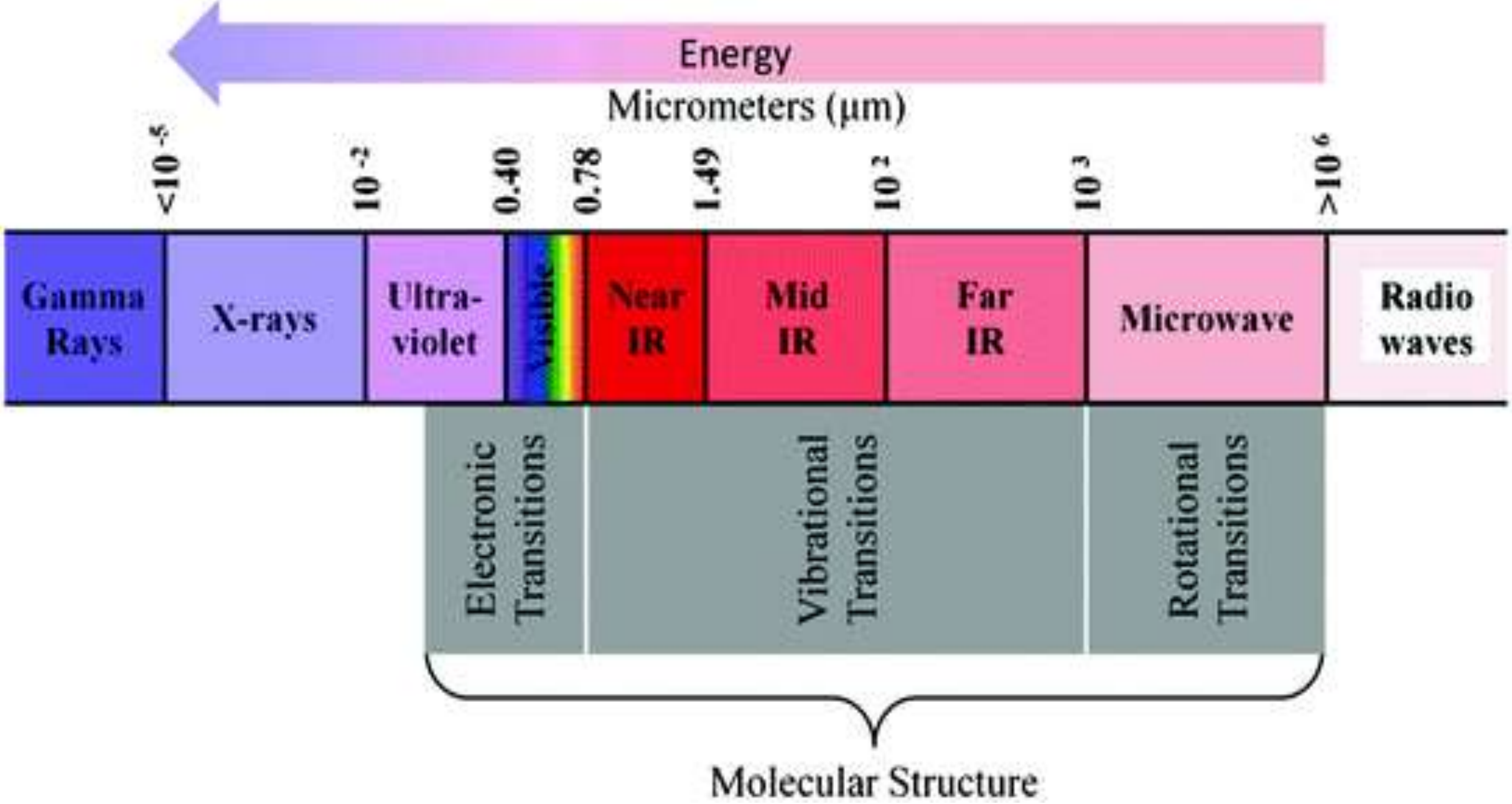
Introduction

- Infrared (IR) spectrophotometry or vibrational spectroscopy is an analytical technique that takes advantage of the vibrational transitions of a molecule
- It is one of the most common and widely used techniques employed mainly by inorganic and organic chemists due to its usefulness in determining structures of compounds and identifying them
- The method or technique of infrared spectrophotometry is conducted with an instrument called an infrared spectrophotometer to produce an infrared spectrum


Costmic Rays
X Rays
Ultra Violet
Infrared
Microwaves
Conbmotor Waves
Ultra Short Wave
Short Wave Radio
Broadcast Radio
Gamma Rays
Wavelength (in microns)
0.76
1.5
5.6
1000
Near Infrared
Middle Infrared
Far Infrared



Frequency = 1 / wavelength


Energy
Micrometers (μm)
<10 -5
10 -2
0.40
0.78
1.49
10 1
10 3
>10 6
Gamma Rays
X-rays
Ultra-violet
Visible
Near IR
Mid IR
Far IR
Microwave
Radio waves
Electronic Transitions
Vibrational Transitions
Rotational Transitions
Molecular Structure

Principle

- Infrared Spectrophotometry is the analysis of infrared light interacting with a molecule
- The portion of the infrared region most useful for analysis of organic compounds have a wavelength range from 2,500 to 16,000 nm (250 μm to 1600 μm)
- Photon energies associated with this part of the infrared are not large enough to excite electrons, but may induce vibrational excitation of covalently bonded atoms and groups
- Infrared spectrophotometers is similar in principle to other spectrometer, permit to obtain absorption spectra of compounds that are a unique reflection of their molecular structure
- It measures the vibrations of atoms, and based on this it is possible to determine the functional groups

- **Stronger bonds and light atoms will vibrate at a high stretching frequency (wavenumber)**
- **It is known that in addition to the facile rotation of groups about single bonds, molecules experience a wide variety of vibrational motions, characteristic of their component atoms**
- **Consequently, virtually all organic compounds will absorb infrared radiation that corresponds in energy to these vibrations**
- **Molecules absorb specific frequencies of light that are characteristic of the corresponding structure of the molecules**

Instrumentation

The main parts of IR spectrometer are as follows:

- **Radiation source**
- **Monochromators**
- **Sample cells and sampling of substances**
- **Detectors**
- **Recorder**

1. Sources of IR radiations

- Nernst glower
- Incandescent lamp
- Mercury arc
- Tungsten lamp
- Glober source
- Nichrome wire

2. Sample cell and Sampling substances

- IR spectroscopy has been used for the characterization of solid, liquid or gas samples
- It carries both sample cell along with reference cell

3. Monochromators

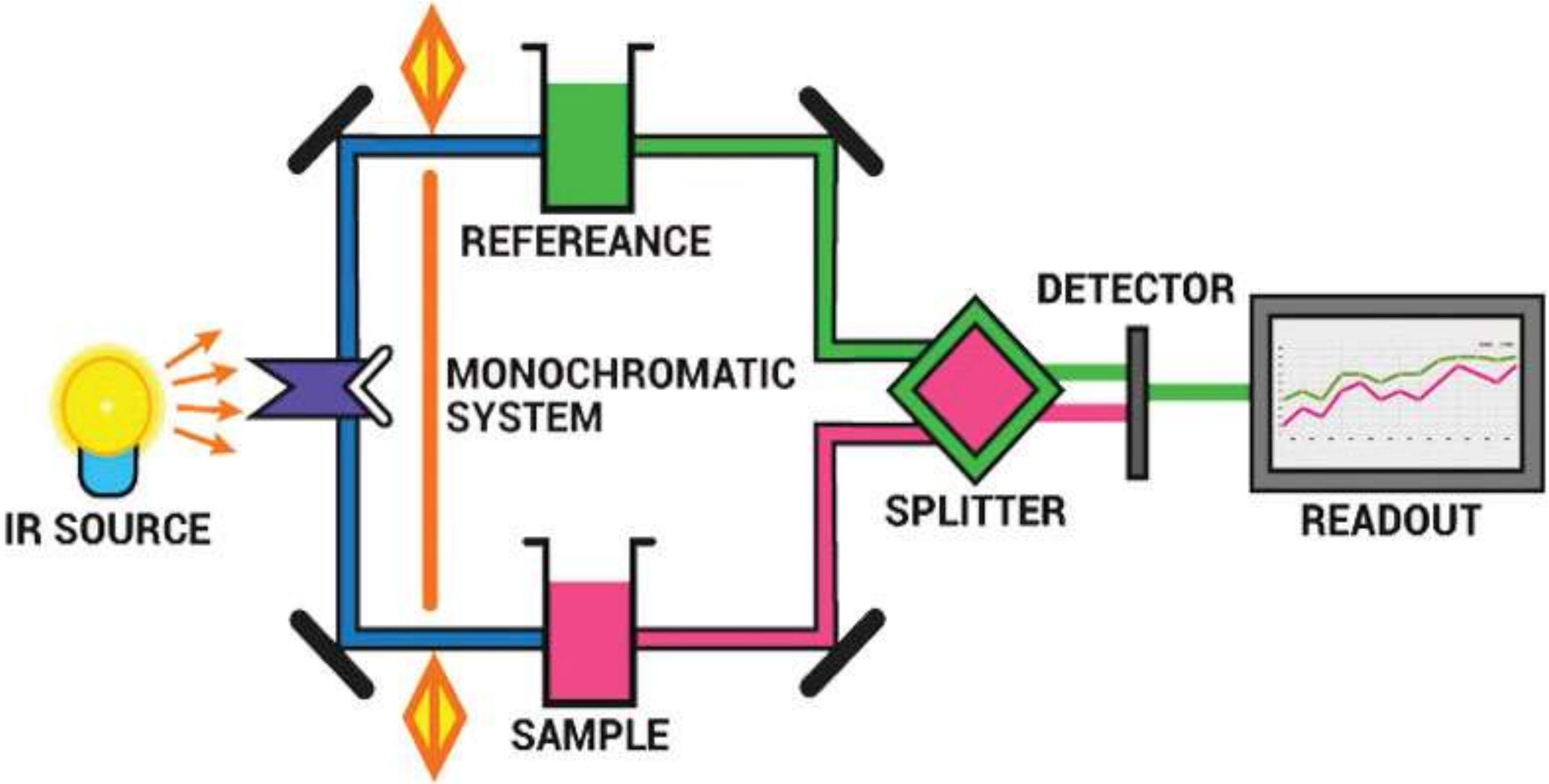
- Various types of monochromators are prism, gratings and filters
- Prisms are made of Potassium bromide, Sodium chloride or Caesium iodide
- Filters are made up of Lithium Fluoride and Diffraction gratings are made up of alkali halides

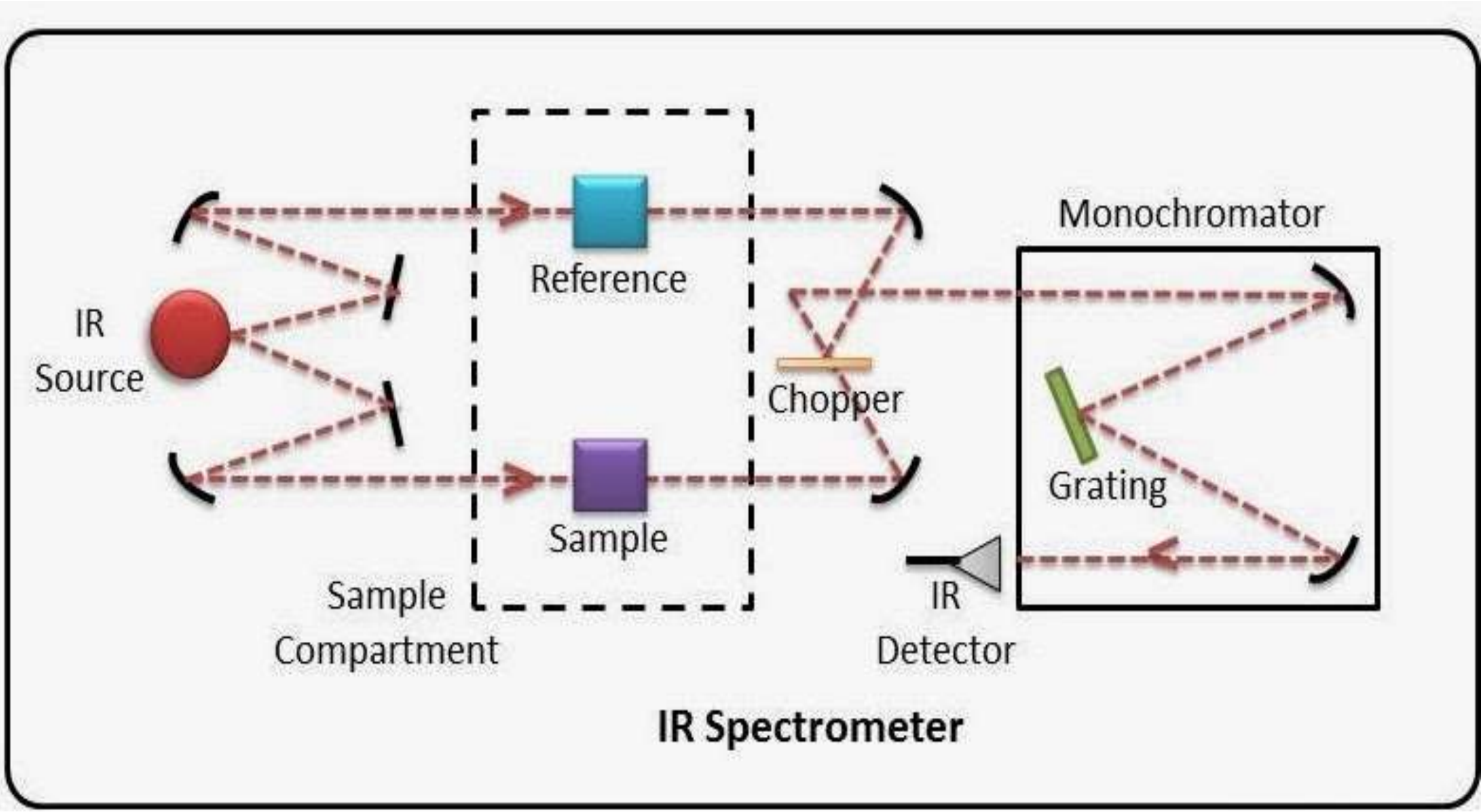
4. Detectors

- Detectors are used to measure the intensity of unabsorbed infrared radiation
- Detectors like thermocouples, Bolometers, thermisters, Golay cell, and pyro-electric detectors are used

5. Recorders

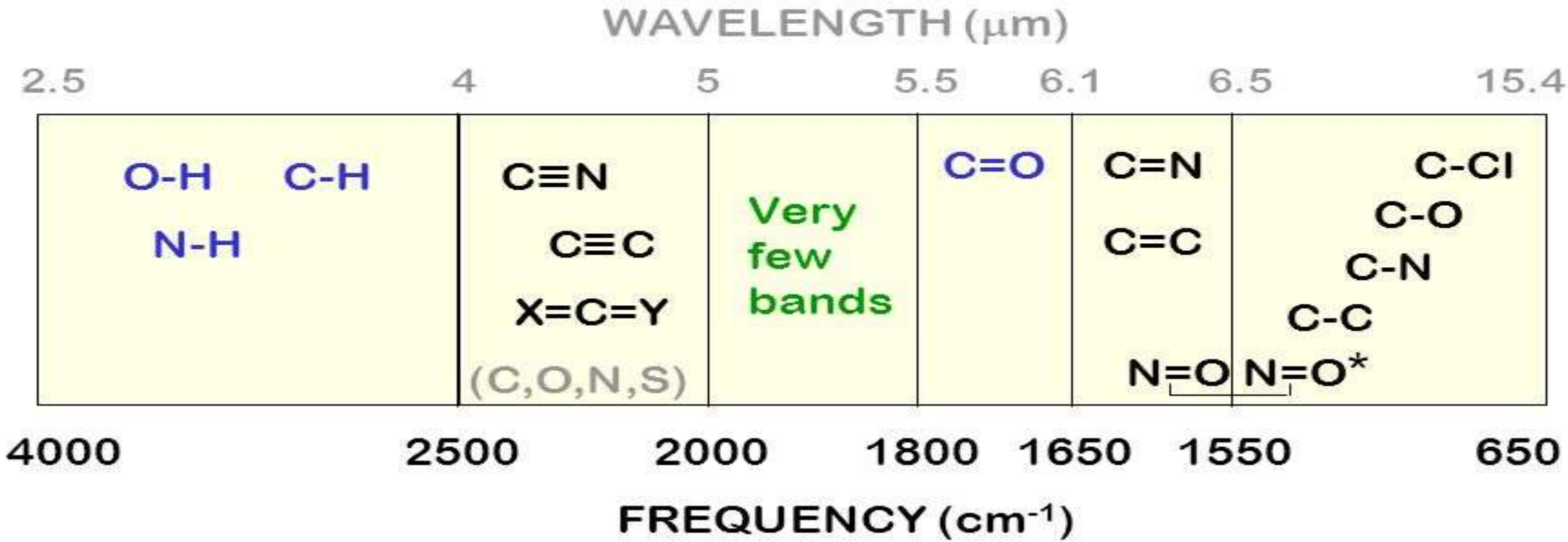
- Recorders are used to record the IR spectrum


REFEREANCE
MONOCHROMATIC SYSTEM
IR SOURCE
SAMPLE
DETECTOR
SPLITTER
READOUT

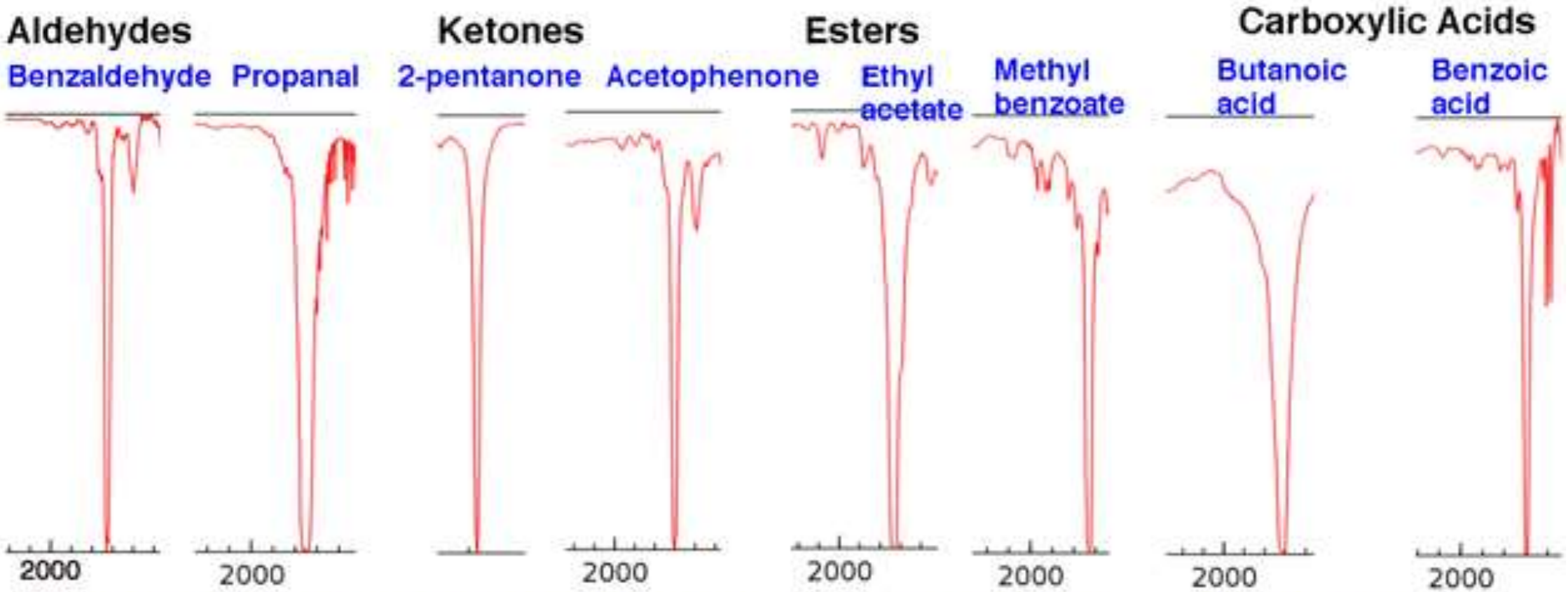


IR Spectrometer

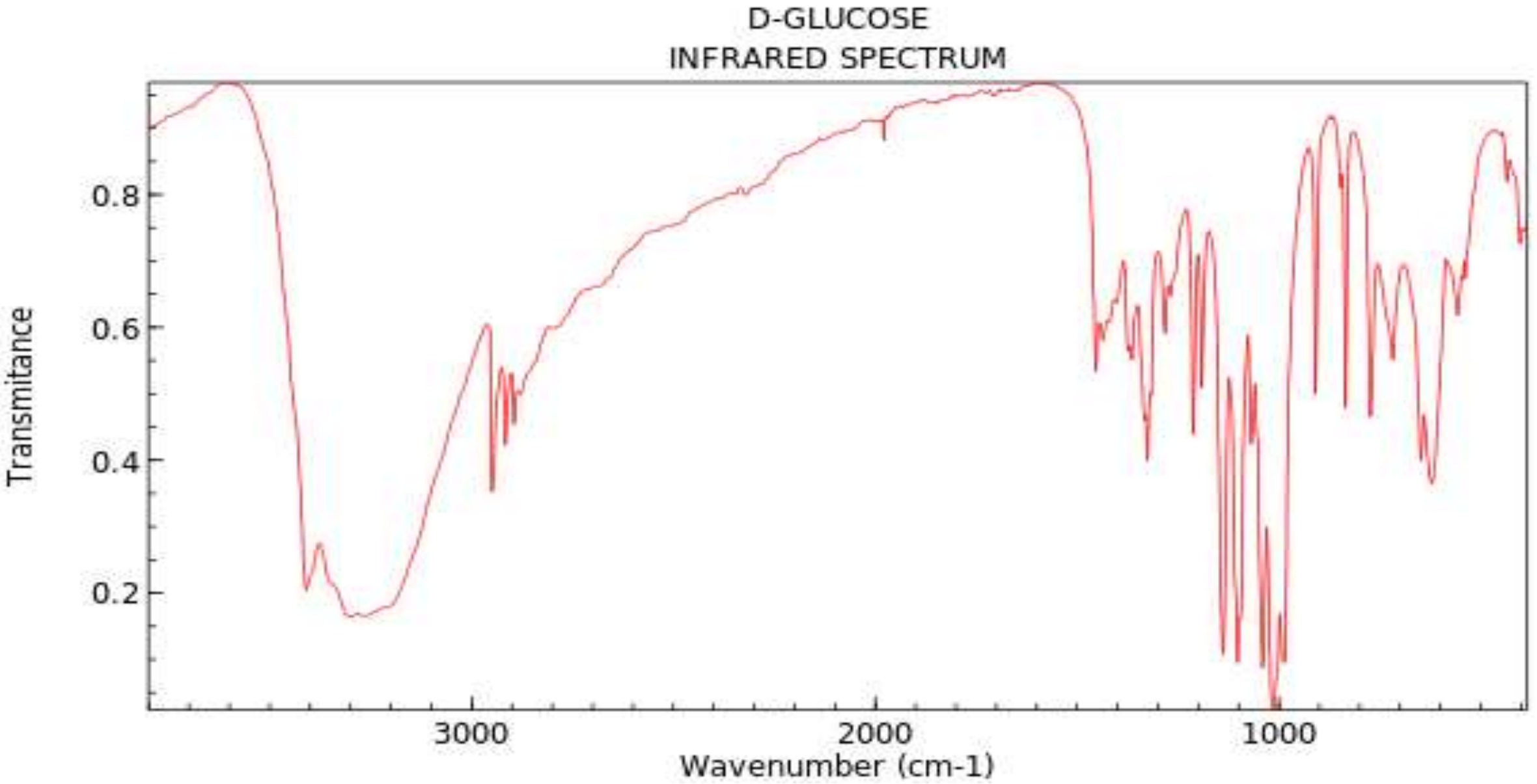
Typical Infrared Absorption Regions



A collection of “swords” - the C=O stretch around 1700 cm



Almost always the strongest peak on the spectrum


D-GLUCOSE
INFRARED SPECTRUM
Transmitance
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)

Applications of Infrared (IR) Spectroscopy

- Protein characterization
- Nanoscale semiconductor analysis
- Space exploration
- Analysis of gaseous, liquid or solid samples
- Identification of compounds
- Quantitative analysis
- Information regarding functional groups of molecules and constitution of molecules can be deduced from IR spectrum
- To know about interaction among molecules