Advanced Spectroscopy

Chemistry - MSc
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Lecture 1

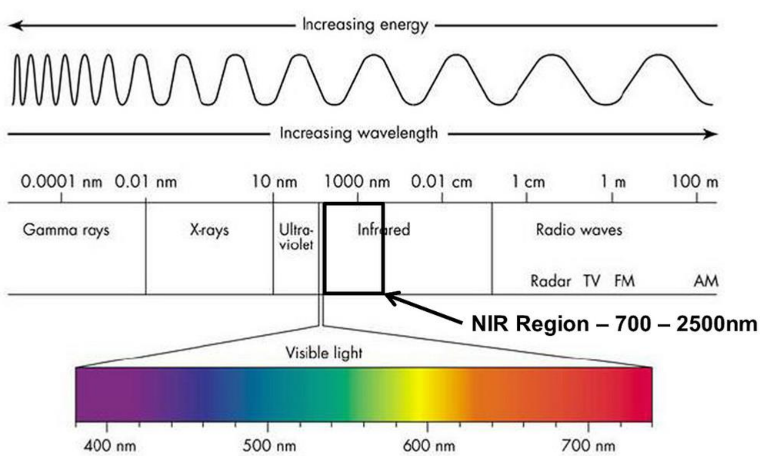
Introduction

- Spectroscopy is the interaction of radiant energy with matter.
- The basic principle of spectroscopy can be explained as:
  - When a compound is subjected to the energy of an electromagnetic radiation, some of the radiation energy will be absorbed and the rest is transmitted.
  - Different compounds behave differently under a given radiation.
  - A spectrum is obtained as a result of this process
  - Combining information obtained from spectra of different techniques provide valuable clues about the identity/quantity of compounds of interest

IR Spectroscopy

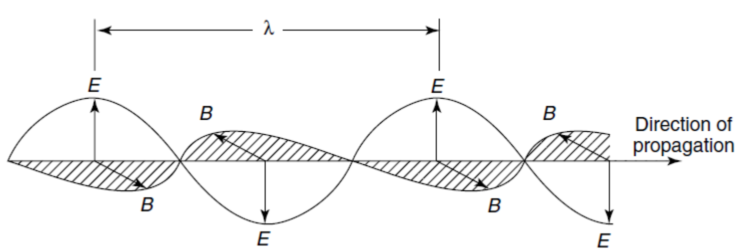
- Infrared spectroscopy is an important analytical technique having the advantage of the possibility of measuring any sample in any state (liquids, solutions, pastes, powders, films, fibres, gases and surfaces) can all be examined given the correct choice of sampling technique.
- As a consequence of improved instrumentation, a variety of new sensitive techniques have now been developed in order to examine formerly intractable samples.

- Infrared radiation is part of the electromagnetic radiation



- IR is used in the identification of organic compounds by utilizing the different vibrational movement associated with the bonds present in a compound
- IR radiation ranges from 0.7 – 200 µm between the visible and microwave regions.
- The region utilized in structural analysis ranges between 2.5 – 16 µm. The shorter and longer wavelengths are known as the (near- and far-IR regions)
- IR is also expressed in wave numbers (1/λ) in cm^{-1} units corresponding to (4000-625 cm^{-1})

Symbols and units in IR spectroscopy



C : the speed of light = $2.997\ 925 \times 10^8\ ms^{-1}$.

λ : the distance between adjacent peaks (wavelength)

ν : *frequency* (the number of cycles per second)

Therefore,

$$c = \lambda\nu$$

Units of wavelength:

$$1\ \text{Å} = 10^{-10}\ \text{m} \qquad 1\ \text{nm} = 10^{-9}\ \text{m} \qquad 1\ \mu\text{m} = 10^{-6}\ \text{m}$$

- Another unit used in IR spectroscopy is the *wavenumber*, $\bar{\nu}$, in cm^{-1}. This is the number of waves in a length of one centimeter and is given by the following relationship:

$$\bar{\nu} = 1/\lambda = \nu/c$$

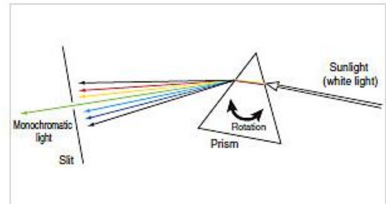
This unit has the advantage of being linear with energy.

$$E = h\nu = hc/\lambda$$

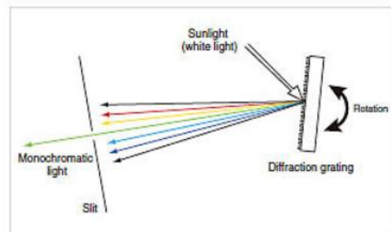
Where, h (plank constant) = $6.626 \times 10^{-34}\ m^2\ kg\ /\ s$

IR instrument

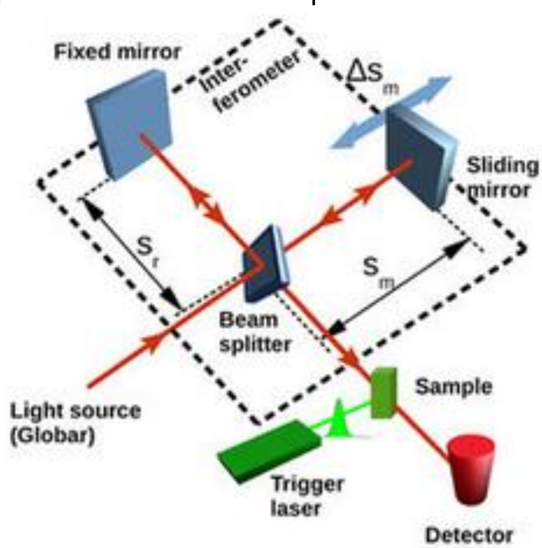
- Infrared spectrometers have been commercially available since the 1940s. At that time, the instruments relied on prisms to act as dispersive elements



- In mid 1950s, diffraction gratings had been introduced into dispersive machines



The most significant advances in infrared spectroscopy, however, was a result of the introduction of Fourier-transform spectrometers. This type of instrument employs an interferometer and exploits the mathematical process of Fourier-transformation



Globar is silicon carbide rod 20-50 mm and width 5-10 mm it is heated to temperatures of 1000 to 1650°C in the near infrared range. They produce wavelength range from 1 to 50 µm.
A Globar source is then combined with an interference filter to produce radiation having wavelengths of 4 to 15 µm.