

Design and materials selection

First experiment

Name: -Infrared Spectroscopy

Aim: - Material characterization using FTIR spectroscopy

Infrared (IR) spectroscopy is a popular method for characterizing polymers. This technique is based on the vibrations of the atoms of a molecule. An infrared spectrum is obtained by passing infrared radiation through a sample and determining which fraction of the incident radiation is absorbed at a particular energy. The energy, at which any peak in an absorption spectrum appears, corresponds to the frequency of vibration of a part of the sample molecule. Most infrared spectroscopy is carried out by using Fourier-transform infrared (FTIR) spectrometers. This method is based on the interference of radiation between two beams to yield an interferogram, i.e. a signal produced as a function of the change of path-length between the two beams. The two domains of distance and frequency are inter-convertible by the mathematical method of Fourier transformation. The basic components of an FTIR spectrometer are shown schematically in Figure (2-16). The radiation emerging from the source is passed through an interferometer to the sample before reaching a detector. Upon amplification of the signal, in which high-frequency contributions have been eliminated by a filter, the data are converted to a digital form by using an analog-to-digital converter and then transferred to the computer for Fourier transformation to take place.

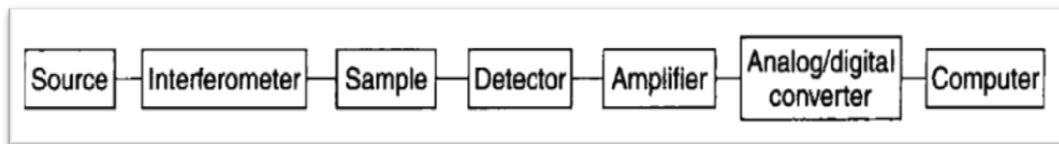


Figure (2-16): Schematic of a typical Fourier-transform infrared (FTIR) spectrometer [60].

The output from an infrared instrument is referred to as a spectrum. Inverse wavelength units (cm^{-1}) are used on the x-axis - this is known as the wavenumber scale. The y-axis may be represented by % transmittance, with 100% at the top of the spectrum. It is commonplace to have the choice of absorbance or transmittance as a measure of band intensity. The transmittance is traditionally used for spectral interpretation, while absorbance is used for quantitative work. The infrared spectrum can be divided into three regions, namely the far-infrared ($< 400 \text{ cm}^{-1}$), the mid-infrared ($400\text{-}4000 \text{ cm}^{-1}$) and the near-infrared ($4000\text{-}13000 \text{ cm}^{-1}$). Most infrared applications employ the mid-infrared region, although the near- and far-infrared regions can also provide specific information about materials. The near-infrared region consists largely of overtones or combination bands of fundamental modes appearing in the mid-infrared region. The far-infrared region can provide information regarding lattice vibrations. Spectrum interpretation is simplified by the fact that the bands that appear can be assigned to particular parts of the molecule, thus producing what are known as group frequencies [60]. The mid-infrared spectrum may be divided into the following four regions:

- X-H stretching region ($4000\text{-}2500 \text{ cm}^{-1}$)
- triple-bond region ($2500\text{-}2000 \text{ cm}^{-1}$)
- double-bond region ($2000\text{-}1500 \text{ cm}^{-1}$)
- fingerprint region ($1500\text{-}600 \text{ cm}^{-1}$)

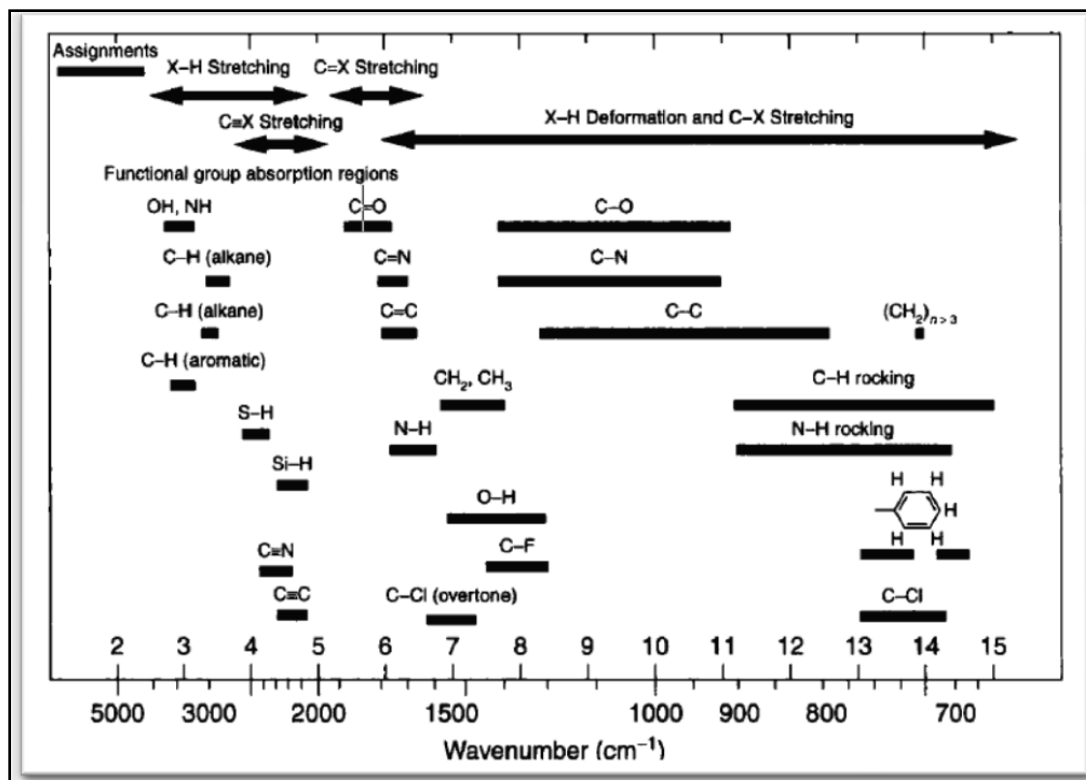


Figure (2-17): A typical correlation table for the infrared modes of polymers [60]