FTIR Spectroscopy

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Spectroscopic phenomena
Interaction of electromagnetic radiation with matter

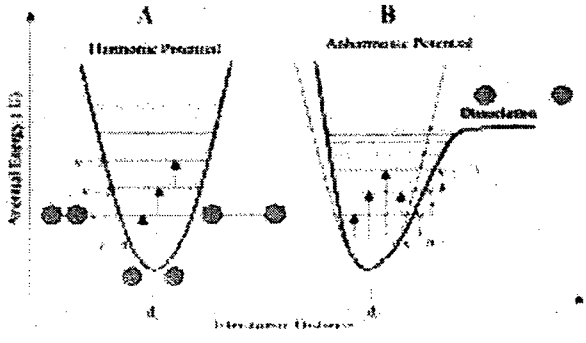
The sum of the contributing energy terms :

$$E_{total} = E_{electronic} + E_{vibrational} + E_{rotational} + E_{translational}$$

Infrared Spectra: formed as a consequence of the absorption of electromagnetic radiation at frequencies that correlate to the vibration of specific sets of chemical bonds from within a molecule.
Vibrational frequency is given by

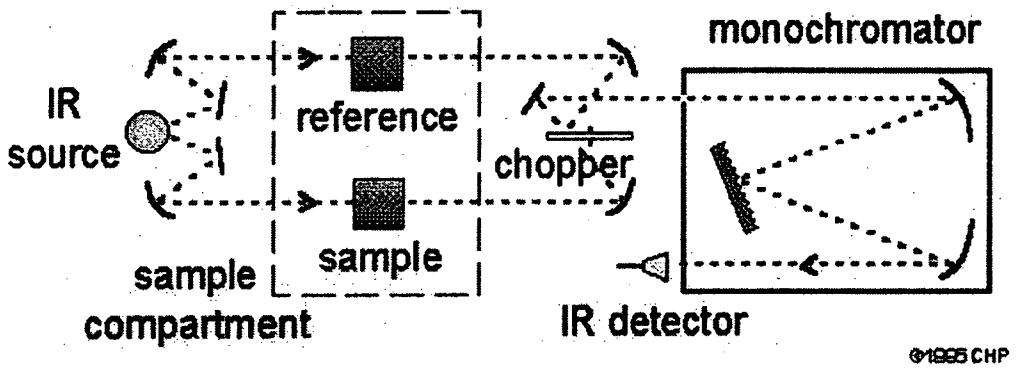
$$\nu = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

Where, ν fundamental vibration frequency, k force constant, and μ reduced mass.

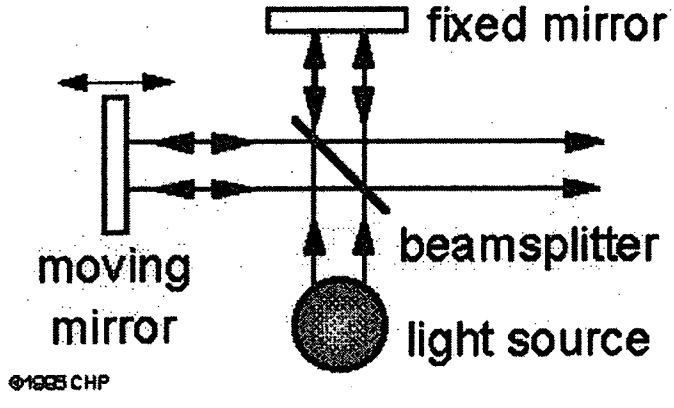


Infrared spectroscopy can result in a positive **identification** (qualitati ve analysis) of every different kind of material. In addition, the size of the peaks in the spectrum is a direct indication of the **amount** of material present. With modern software algorithms, infrared is an excellent tool for quantitative analysis.

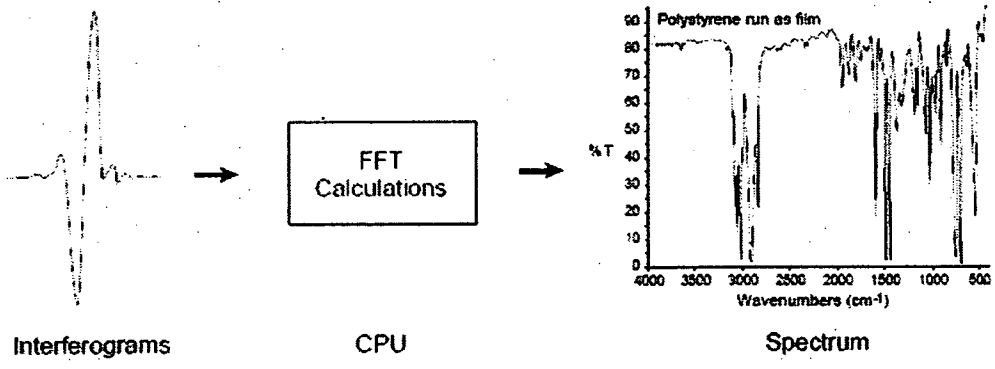
Early days infrared instruments were of the **dispersive** type. These instruments separated the individual frequencies of energy emitted from the infrared source. This was accomplished by the use of a prism or grating. An infrared prism works exactly the same as a visible prism which separates visible light into its colors (frequencies). A grating is a more modern dispersive element which better separates the frequencies of infrared energy.



Fourier transform infrared spectroscopy is preferred over dispersive or filter methods of infrared spectral analysis for several reasons:
This does not contains complicated optics; major part is very simple unit consisting of two mirrors called interferometer



This does not measure the spectrum (frequency vs absorbance) directly. First measure a time domain signal called interferogram and converted to a spatial one by FT calculation.



Some of the major advantages of FT-IR over the dispersive technique include:

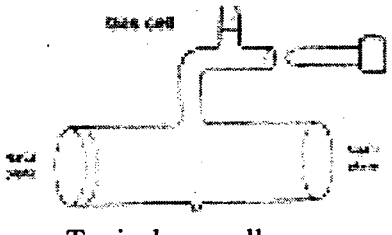
- **Speed:** Because all of the frequencies are measured simultaneously, most measurements by FT-IR are made in a matter of seconds rather than several minutes. This is sometimes referred to as the **Felgett Advantage**.
- **Sensitivity:** Sensitivity is dramatically improved with FT-IR for many reasons. The detectors employed are much more sensitive, the optical throughput is much higher (referred to as the **Jacquinot Advantage**) which results in much lower noise levels, and the fast scans enable the coaddition of several scans in order to reduce the random measurement noise to any desired level (referred to as **signal averaging**).
- **Mechanical Simplicity:** The moving mirror in the interferometer is the only continuously moving part in the instrument. Thus, there is very little possibility of mechanical breakdown.
- **Internally Calibrated:** These instruments employ a HeNe laser as an internal wavelength calibration standard (referred to as the **Connes Advantage**). These instruments are self-calibrating and never need to be calibrated by the user.

These advantages, along with several others, make measurements made by FT-IR extremely accurate and reproducible. Thus, it is a very reliable technique for **positive identification** of virtually any sample. The sensitivity benefits enable identification of even the smallest of contaminants. This makes FT-IR an invaluable tool for **quality control** or quality assurance applications whether it be batch-to-batch comparisons to quality standards or analysis of an unknown contaminant. In addition, the sensitivity and accuracy of FT-IR detectors, along with a wide variety of software algorithms, have dramatically increased the practical use of infrared for **quantitative analysis**. Quantitative methods can be easily developed and calibrated and can be incorporated into simple procedures for routine analysis. Thus, the Fourier Transform Infrared (FT-IR) technique has brought significant practical advantages to infrared spectroscopy. It has made possible the development of many new sampling techniques which were designed to tackle challenging problems which were impossible by older technology. It has made the use of infrared analysis virtually limitless.

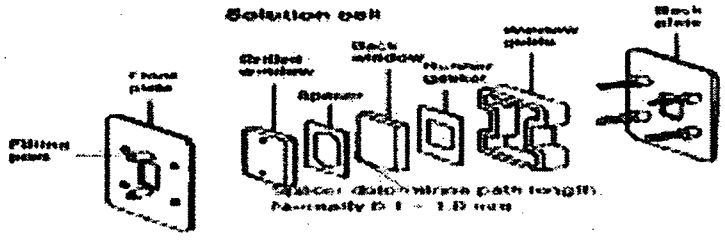
Modes of FTIR Spectroscopy

Transmission : gas, liquid samples, thin films and pellets
ATR: liquids, solids(powders)
DRIFT : powder samples

Special types of cells are used for the measurements in different modes



Typical gas cell

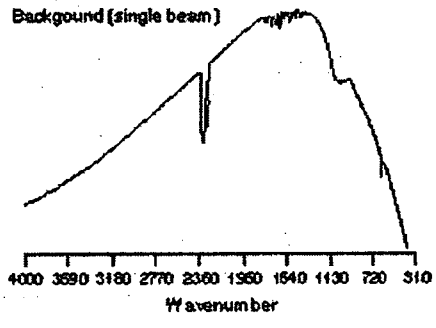


Liquid cell

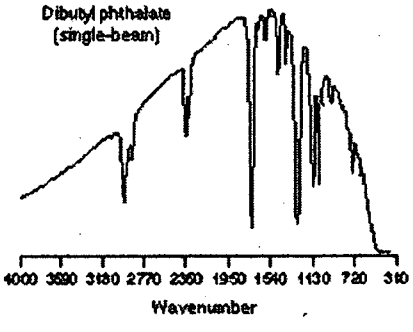
Thin KBr pellets are used in transmission mode to measure spectra of powder samples.

How to perform a measurement:

First background (air) spectrum is measured



Then sample spectrum



Finally, the output spectrum looks