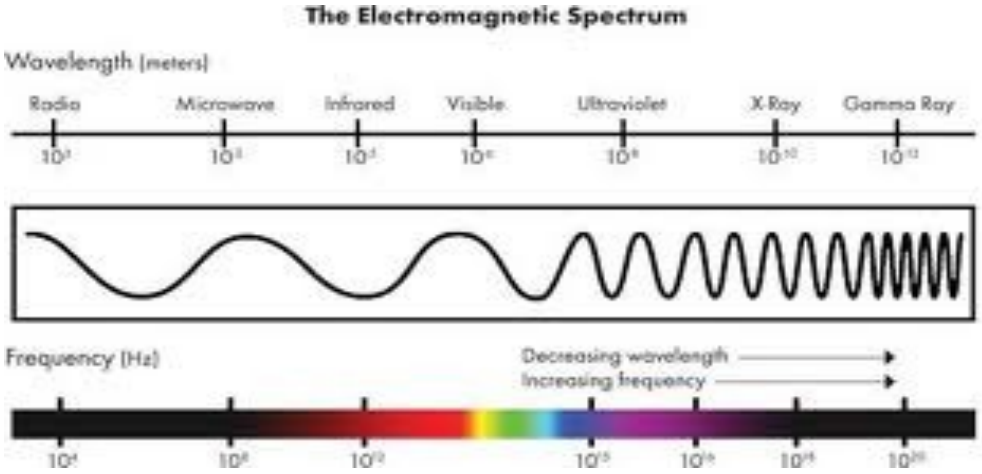
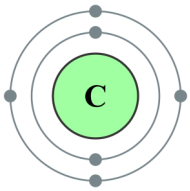
Near Infrared Spectroscopy

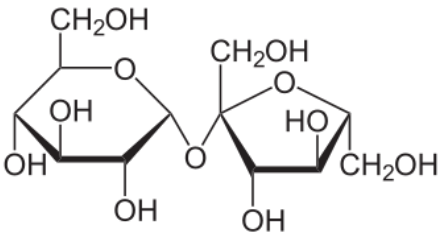
The electromagnetic spectrum from 400nm to 10000nm covers the Visible, NIR and Mid IR spectral regions. When light energy interacts with a material, energy is absorbed at specific frequencies associated with the atomic and molecular structure of the material.



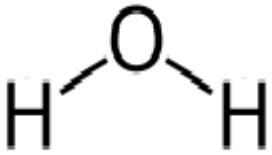
In the Visible region, ie, 400 to 680nm, energy is absorbed when electrons jump from a lower to a higher energy state or orbit. In this region, chromaphores such as metal chelates, ionic salts and some organic coloured compounds absorb visible light. Likewise Atomic Absorption Spectroscopy also uses this phenomenon to measure metals species as they burn in a flame.



In the Mid Infrared region, i.e. 2500 to 10000nm, energy is absorbed by molecules at resonant frequencies for each type of vibrational motion, eg, stretching, bending, wagging, twisting etc. In the Mid IR region, all chemical bonds in organic molecules exhibit strong absorption bands. Typically the Mid IR region is suitable for characterizing C-C, C-O, C-N, C-H, O-H, N-H, N-O and many other chemical bonds. Sample preparation such as dissolving in a solvent, preparing a nujol mull, drawing film etc, is required in order to get sufficient light through a sample. Mid IR spectroscopy is generally used for non-water bearing materials such petrochemicals, plastics, polymers and chemicals. Mid IR spectroscopy is used mainly for qualitative analysis rather than quantitative analysis.

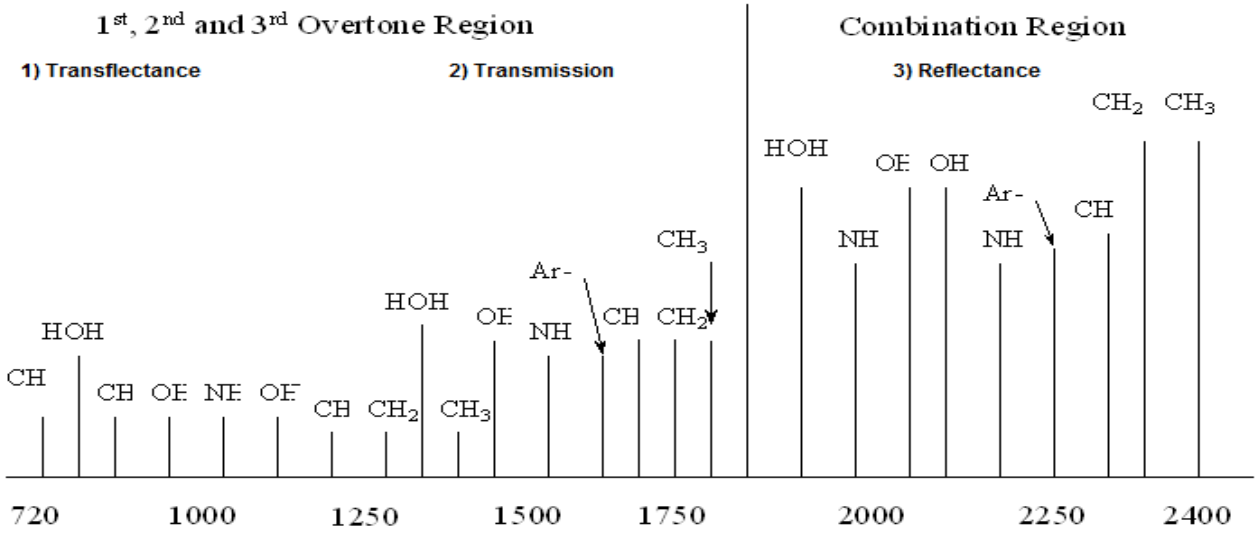


The NIR spectral region, i.e., 720 to 2500nm, is the Overtone and Combination region of the Mid IR region. NIR spectra contain absorbance bands mainly due to three chemical bonds, i.e., C-H (fats, oil, hydrocarbons), O-H (water, alcohol) and N-H (protein, amines, admides). Other chemical bonds may exhibit overtone bands in the NIR region, however they are generally too weak to be considered for use in analysis of complex mixtures such as foods, agricultural product, pharmaceuticals, toiletries, cosmetics, textiles etc. NIR spectra do not have the resolution of the Mid IR spectra however NIR spectra can generally be collected off or through materials without sample preparation. As well the NIR spectral region is suitable for measuring high and low water content materials. Whereas Mid IR is mainly a qualitative technique, NIR is mainly a quantitative technique. NIR provides a very rapid means of measuring multiple components in foods, agricultural products, pharmaceuticals, cosmetics, toiletries, textiles and virtually any organic material or compound.



Three NIR Regions

Figure 1. shows the NIR region from 720 to 2500nm. There are three sections of the NIR spectral region, 1) Transflectance, 2) Transmission and 3) Reflectance.



- Transflectance: 720 to 1100nm. This section is most suited to transflectance through a thick sample, such as, seeds, slurries, liquids and pastes. The absorption bands are due to 3rd overtones of the fundamental stretching vibrational motions in the Mid IR region.

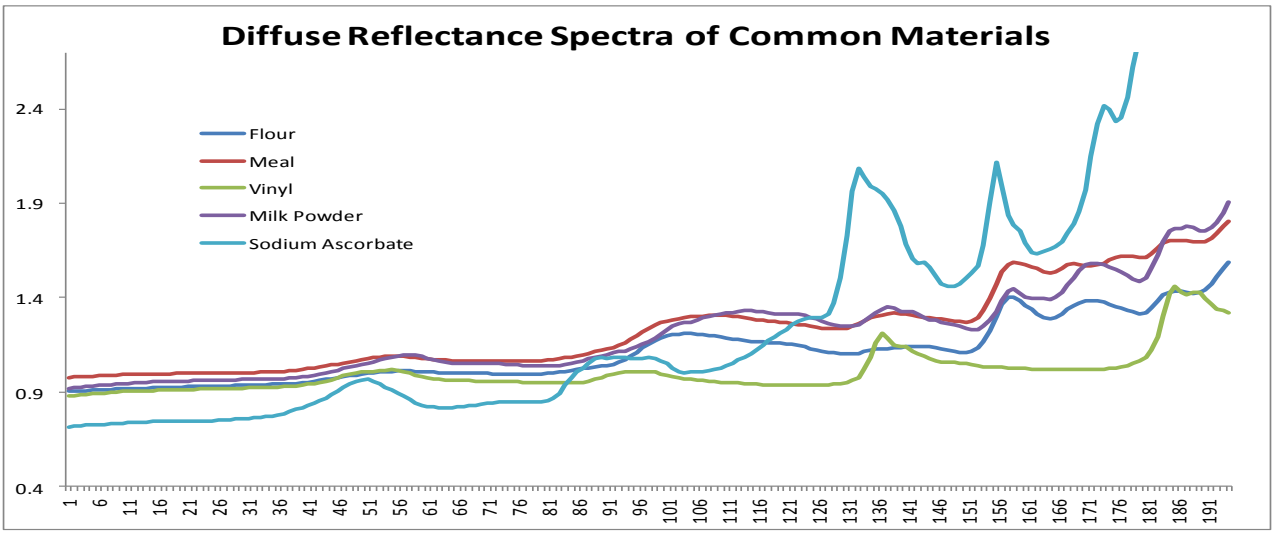
- Transmission: 1200 to 1850nm. This section can be used for transmission through liquids and films, as well as for diffuse reflectance measurements off samples with high water contents. The absorption bands are due to the 1st and 2nd overtones of the fundamental stretching vibrational motions in the Mid IR region.

- Reflectance: 1850 to 2500nm. This section is predominantly used for making diffuse reflectance measurements off ground or solid materials. The absorption bands are due to combination bands, i.e., combinations of C-H stretch and bend vibrational bonds.

The Transflectance region is of particular interest in the analysis of foods because it is suitable for measuring high moisture and high fat content products including meat, dairy products, jams and conserves, dough and batters. The major advantage of working in this region is that longer pathlength sample cells can be used to collect the NIT spectra. Typically a 10-20 mm pathlength can be used. This makes sampling easier and allows viscous and non-homogeneous samples to be scanned without further sample processing.

The Reflectance region, 1900-2500nm, should be used for measuring powdered materials or solids because the spectral bands are better resolved and the % of energy reaching the detector is highest in this region.

Figure 2. shows the diffuse reflectance spectra of flour, meal, vinyl powder, milk powder and ascorbic acid. Note that the spectra gradually increases towards the top end of the spectra region and that the spectral bands are sharper and better separated than in the 1200-1800nm region. This shows why the 1900-2500nm region is preferred for performing diffuse reflectance scans.



Wavelength Range vs Detectors

Figure 3, shows the spectral response for several detectors used in the Visible, NIR and Mid IR regions. The most sensitive detector is the Silicon Photodiode however it is only useful between 350 and 1100nm. The Indium Gallium Arsenide Photodiode detectors come in several options. The normal InGaAs detector covers 900 to 1700nm. By doping the InGaAs material then the wavelength range can be shifted to cover 1200 to 2600nm. The sensitivity of InGaAs detectors is comparable to Silicon. Another detector used in the NIR region is Lead Sulphide, PbS. This type of detector is a thermopile, which has an output that is related to the change in conductance due to children. The sensitivity of PbS is 10^{9} where as the Si and InGaAs photodiodes are 10^{11}-10^{12}. Deuterium Triglyceride DTGS is another thermopile that has a very wide spectral range but very low sensitivity.

NIR

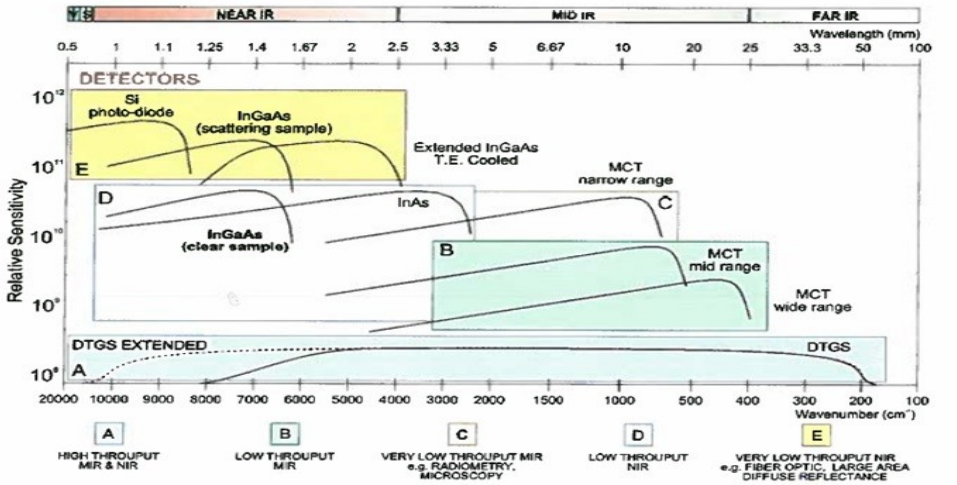
- **TEC InGaAs 2.6 um**
- **TEC InAs**

Mid/NIR

- **DTGS-ZnSe**
- **DTGS-BK7**

Mid

- **LiTaO3**



Detectors are either single detectors or array detectors. There are several array detector that can be used in the NIR region, however at present these array detectors are limited to a top wavelength of 1700nm. As such dispersive NIR spectrometers that use array detectors only cover the wavelength range 900 to 1700nm or less. Since these instruments are setup for diffuse reflectance measurements, then by only scanning to 1700nm means that methods developed will be sub optimal. Note that all research studies in the past 40 years in the NIR region include the most valuable spectral region, 1900-2500nm.