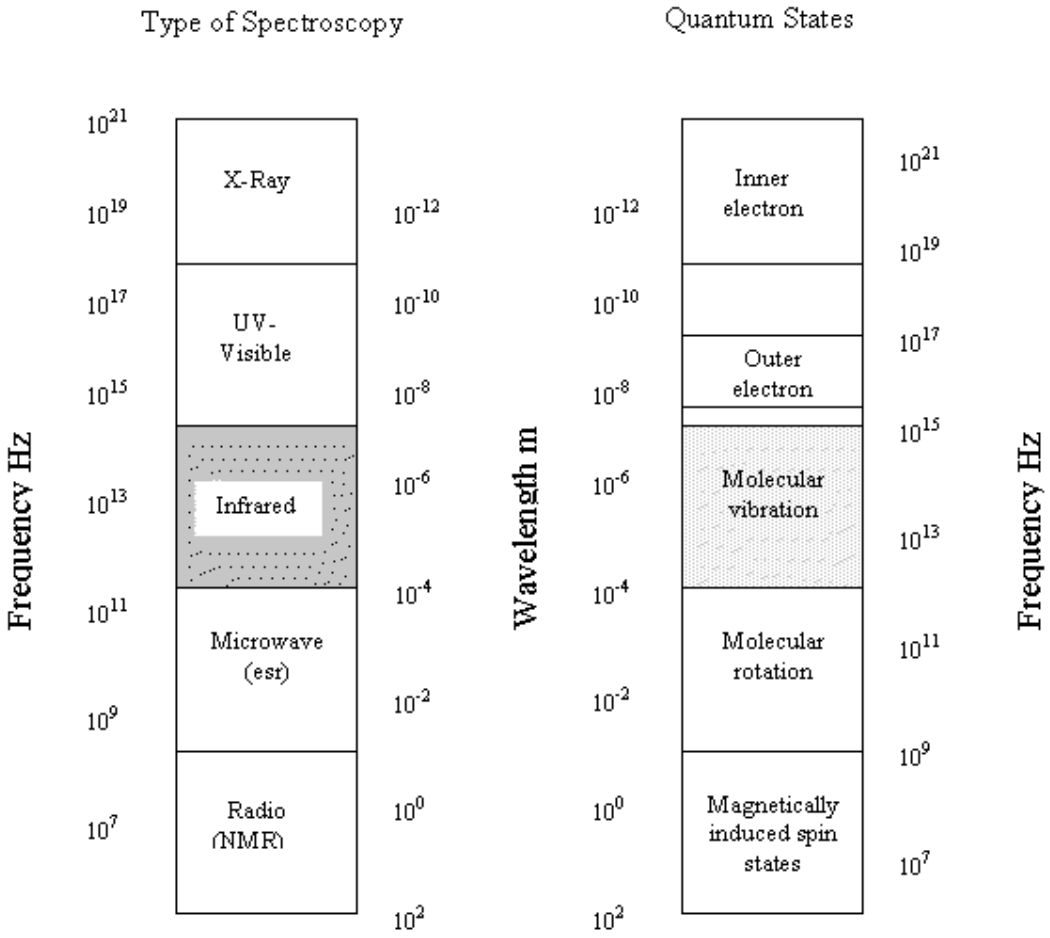
vitális
instruments and processing systems

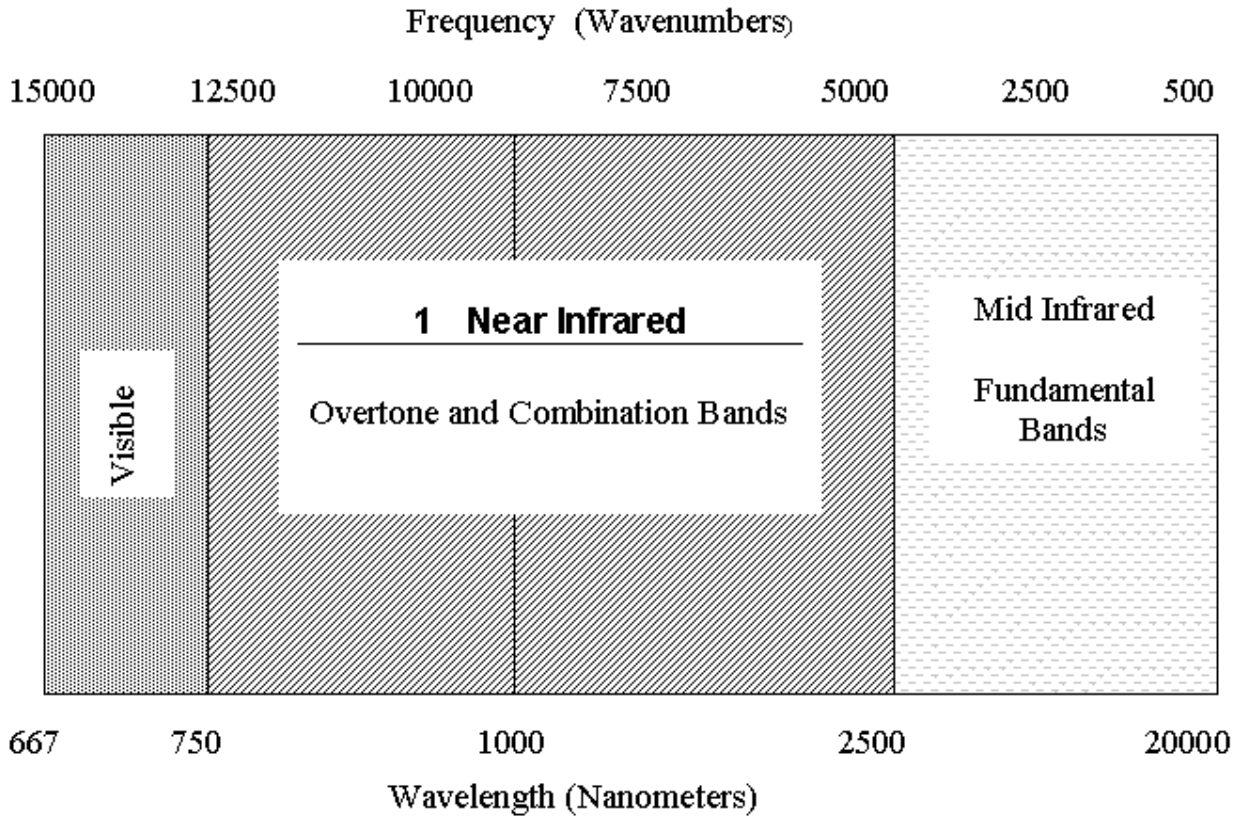
Technology Description

What is NIR?

Near Infrared (NIR) radiation lies in the spectral region between 750-2500 nm in the electromagnetic (EM) spectrum, ie. between the visible and mid-infrared (IR).

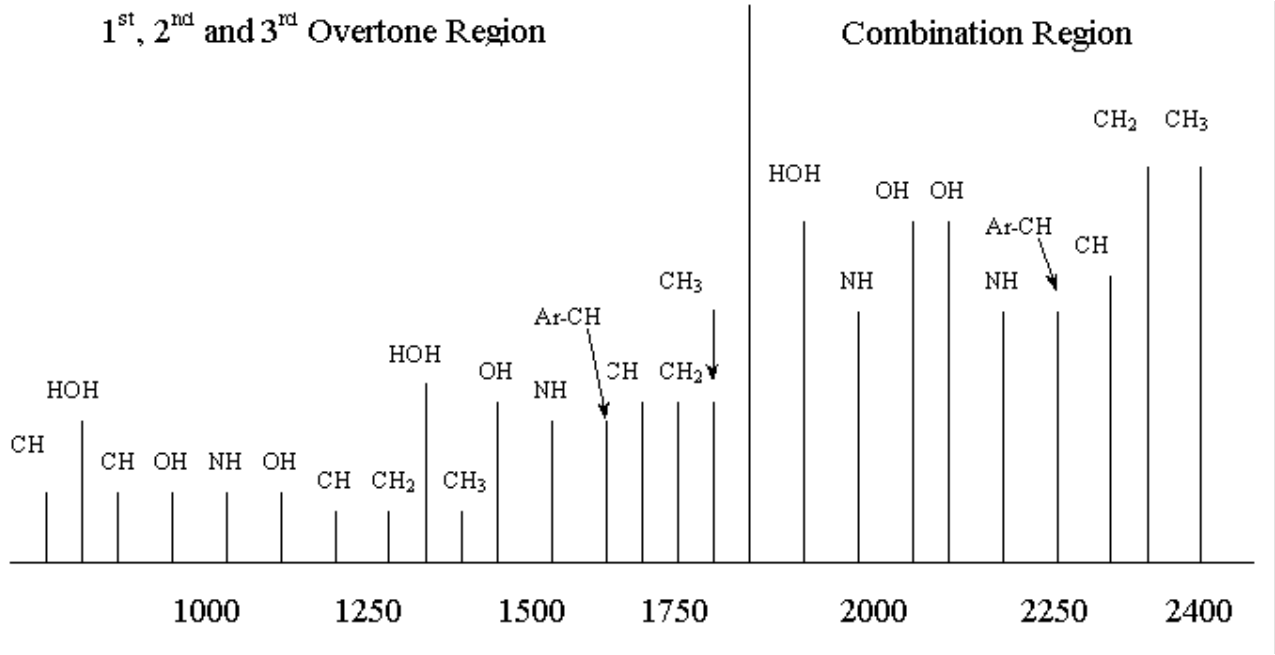


Parts of the electromagnetic spectrum used for spectroscopy.
In general, IR spectroscopy is concerned with the absorption of radiation resulting in molecular stretching, bending and rotations.



Two Regions of the NIR

The NIR region of the EM spectrum is concerned with overtone and combination bands associated with the mid-IR (fundamental) frequencies.



- The Cropscan 2000G scans the range between 720-1100 nm
- The NIT and FOP analyser scans between 500-1100 nm

Spectral Information

Understanding NIR spectral information serves 2 purposes:

1. Allows prediction of where a particular chemical species should absorb.
2. Provides an assessment of the ability of NIR to perform an application.

C-H Absorptions

The carboxy-group (CH) is fundamental to compounds such as aliphatics and aromatics.

N-H Absorptions

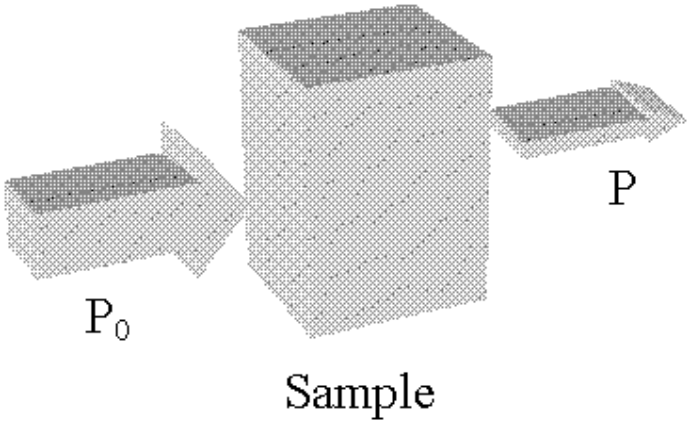
The measurement of the N-H vibrations makes quantitative measurement of proteins by NIR possible.

O-H Absorption

The hydroxy-group (OH) is fundamental to compounds such as alcohols and water.

Fundamental Principles of Spectroscopy

Absorption of Light



The incident radiation P_o passes through a layer of an absorbing species of pathlength *b* and concentration *c*. As a consequence of absorption, the power of the incident light beam is attenuated from P_o to P.

Transmittance is defined by:

$$\%T = \frac{P}{P_o} \times 100$$

Absorbance is defined by:

$$A = -\log_{10} T = \log \frac{P_o}{P}$$

Absorbance and Transmittance are both wavelength dependent quantities, therefore to obtain a spectrum, absorbance must be measured at each particular wavelength the instrument scans.

The Relationship Between Absorbance and Concentration.

The Beer-Lambert Law

$$A = \varepsilon bc = \log \frac{P_o}{P}$$

Where: A = absorbance
e = absorptivity
b = pathlength
c = concentration

Absorptivity e (sometimes referred to as the molar extinction coefficient) related to the probability that a transition (either electronic or vibrational) will occur.

The Beer-Lambert law is used extensively in the calibration and determination of unknown species in solution using UV-Vis spectroscopy.

Modes of Sampling

Three modes of sampling will be discussed

1. Transmission
2. Diffuse Reflectance
3. Interactance

Transmission

Refer to diagram for single beam instrument. The Cropscan 2000G is a transmission instrument

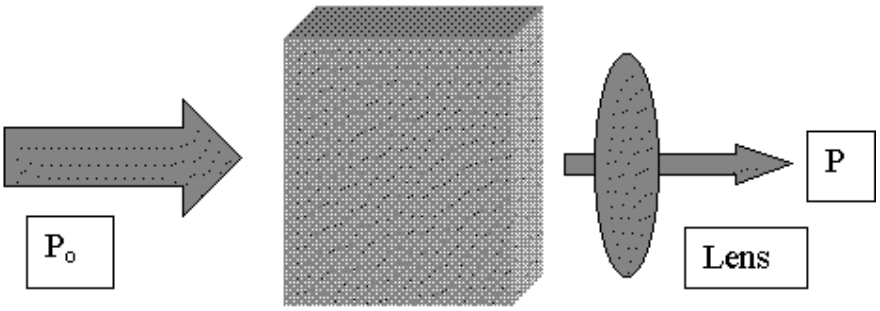
- 100% scan measured directly from lamp.
- Light beam passes through sample.
- Usually requires minimal sample preparation.
- Available as single or double beam configurations

Two types of transmission measurement should be considered:

- Pure Transmission
- Transflectance

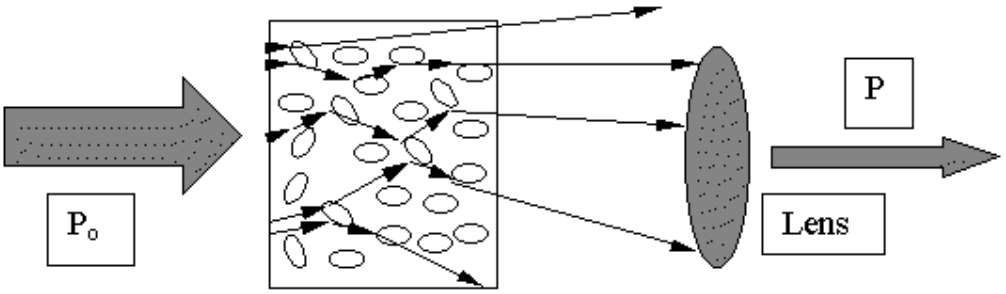
Pure Transmission

This type applies to homogenous samples, such as liquids, where minimal scatter of the incident radiation occurs and that measured at the detector is pure absorbance by the sample.



- Spectra obtained are usually reproducible and result in good calibration data (depending on the accuracy of the reference method and whether the property being measured can be related to its spectra)

Transflectance



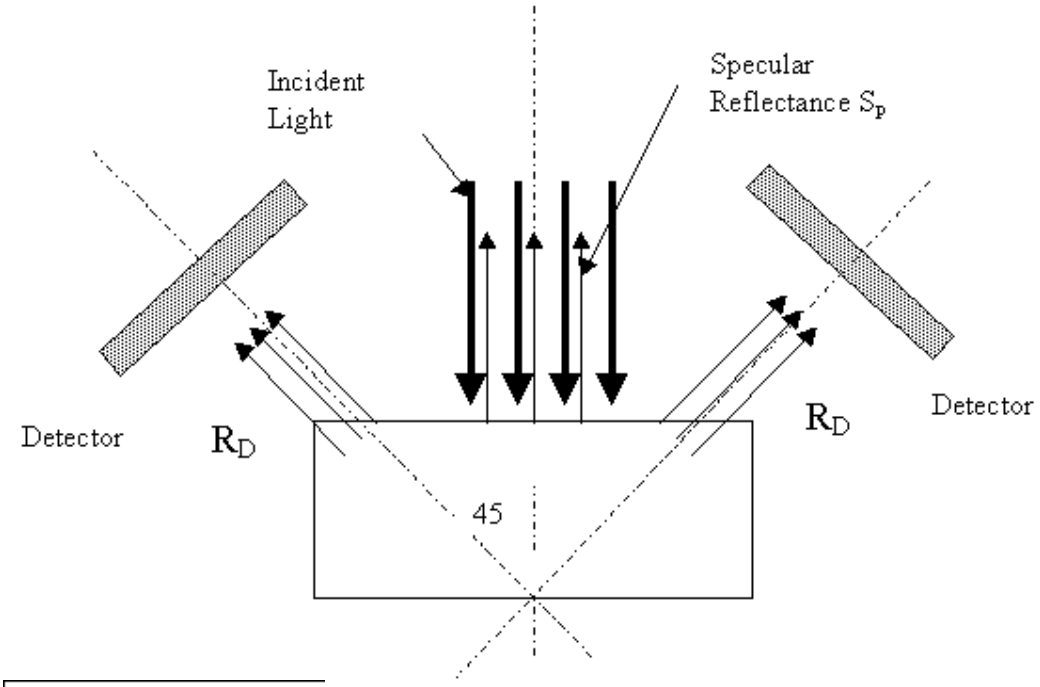
- This type of scattering occurs when the sample packing cannot be accurately reproduced.
- Sample must be scanned several times and an average of the packings it taken as the final result
- Absorbance spectra are not purely sample characteristic absorptions, they also contain a bulk absorption component related to sample packing density.
- Although sample absorbances may be as high as 4.5abs, the spectral base to peak height is still usually within 1abs.
- The above principals apply to liquid samples containing microparticulate matter, which can exaggerate scattering effect even more than whole grains.

Modes of Sampling (cont.)

Diffuse Reflectance

This is the mode of operation used by the Fibre Optic Probe (FOP) Analyser.

Principle of Diffuse Reflectance



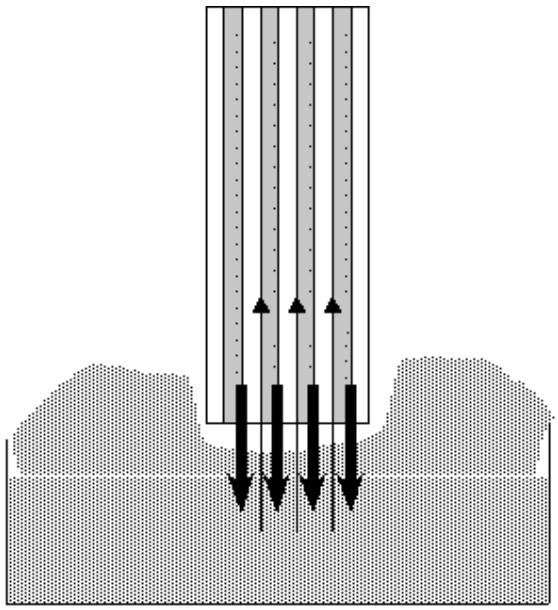
$$\text{Reflectance} = S_p + R_D$$

$$A = \log\frac{100}{s} = \log\frac{1}{R}$$

- Requires reflectance standard to obtain 100% spectrum.
- Material must be homogenised or ground to a constant particle size for reproducible measurements.
- US bureau of standards report that optimal light detected at 45° to source.
- Reflected light is a combination of Specular reflectance S_p and Diffuse reflectance R_D.
- Must contain more diffuse reflectance information than specular to be useful.

Modes of Sampling (cont.)

Interactance



- Aim of interactance is to try and push as much light into the sample and measure the light that is reflected.
- Used for difficult to measure samples and non-homogeneous slurries.

Why Use NIR?

- Relatively cheap materials allow for the construction of portable instruments for agricultural and industrial purposes.
- Sampling cells can be made from glass, compared to mid-IR which requires sodium chloride or potassium bromide (expensive preparation devices and rigorous sample preparations).
- Relatively little sample preparation.
- Because of low molar absorptivity and high-energy throughput in this region, pathlengths of up to 30mm may be used.
- Lamp sources are commercially available.
- The use of stationary gratings allows the production of robust portable instruments.
- Primarily used for the detection of C-H, N-H and O-H (ie. for the quantitative determination of oils, protein and moisture).
- High scatter coefficient allows for excellent diffuse reflectance spectra of solids.

Compatible with fibre optic cables for portable QC analyses.