MATERIALS IDENTIFICATION

Fourier Transform Near Infrared Spectroscopy (FT-NIR)
(Fast, Accurate, Reliable, and Non-destructive)

The FT-NIR Technology, in the last decade, has emerged as a fast, accurate and non-destructive analytical tool for quality control, identification of materials and R&D. The NIR technology has found many diverse applications in industries such as petrochemicals, polymer/plastics, pharmaceutical, agricultural, medical, and food. This Technical Note attempts to describe the FT-NIR technology in simple terms and present its unique capabilities in the instantaneous and non-destructive identification of different materials. We hope that the readers will be able to see the simplicity and speed with which the FT-NIR technology can help in the identification of materials, enhance quality control or help in R&D applications. The FT-NIR technology requires no or minimal sample preparation depending on the test sample.

What is NIR?

- In spectroscopic terms, NIR means the measurement of the wavelength and intensities of the absorption of near infrared light by a sample. The absorption or reflectance spectrum is directly proportional to the chemical composition of the material.
- In simple terms, a near infrared light is pointed at a sample using a fibre optic probe and the reflected signal is processed for absorption or reflectance characteristics. In other words, we take a chemical fingerprint of a material using infrared light at a specific point in time.
- In economical terms, near infrared means fast, accurate, reliable, cost-effective and non-destructive measurements for identification of materials, quality assurance and research and development.

Scanning: The scanning process is as simple as pointing the fibre optic probe to the sample (soft contact) and pressing the trigger to start scanning.

Scanning time: Normally, each measurement takes about 5 seconds and in most cases three to five measurements are taken for spectral averaging and identification purposes.

Identification Process: The outcome of the scanning process is an absorption spectrum. The near infrared light absorption range is between 800 nm to 2500 nm (12,500 cm^{-1} to 4,000 cm^{-1} wave number). The NIR absorption is due to overtones and combination bands of functional group vibrations in the mid-infrared region. The strong signals include C-H, O-H, C=O, N-H, -COOH, and aromatic C-H groups. A typical absorption spectrum for polyethylene and polystyrene are shown in the attached chart. It is generally difficult to assign an absorption band in the near infrared region to a specific functional group due to overlapping of several combinations and overtones. Now, with the advancements in computing power and instrumentation in the last decade combined with chemometrics (multivariate analysis methods) we are able to analyze complex systems. For example, using the software analysis tools one can convert the absorption spectrum to its 2^{nd} derivative equivalent and use the spectral differences for a fast, accurate, non-destructive and reliable identification of materials. A typical 2^{nd} derivative spectrum for vitamin E samples is shown and as can be seen the peak intensities change with the change in the vitamin E concentration in each sample.

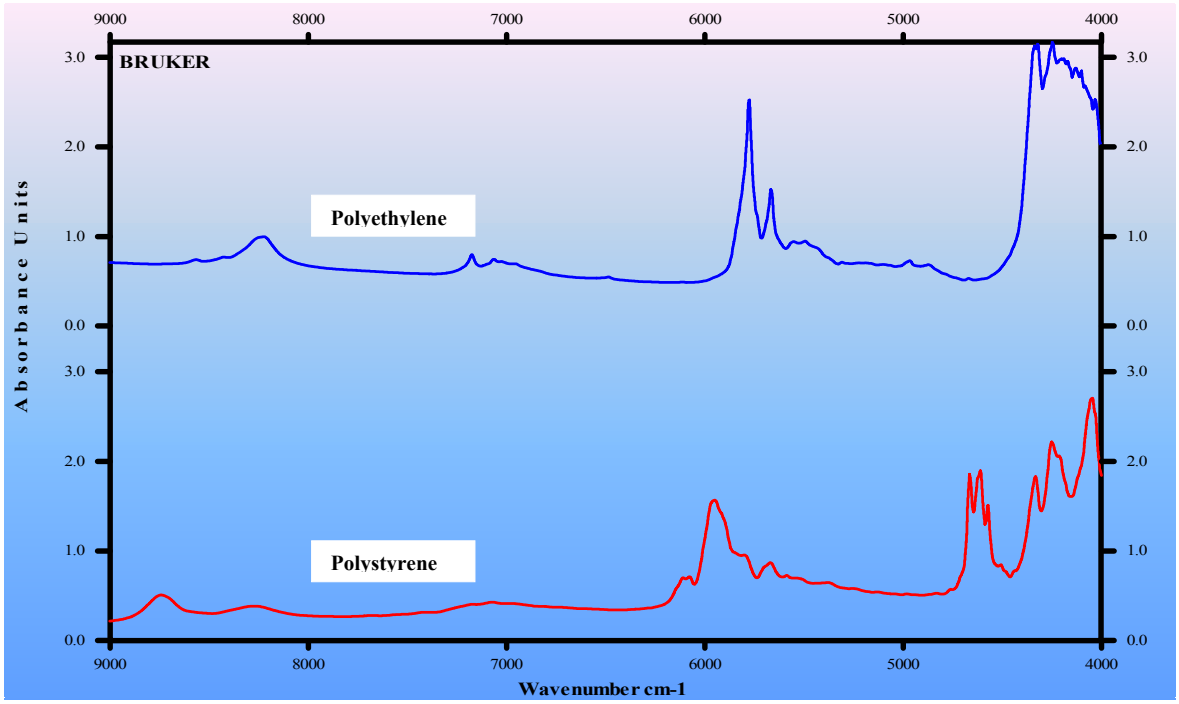
Multivariate analysis is applied in the identification of materials. Like many other spectroscopic techniques, the FT-NIR method is a comparative technology, so, once a reference spectral model is developed, identification of a test sample can be achieved within seconds! Identification of a test sample (Fingerprint) is comprised of scanning and comparison of spectrum or the average spectrum with all or a particular reference spectrum in the spectral reference model. The outcome of this comparison is a spectral distance 'D' also known as 'Hit Quality'. The smaller the 'D' value the closer the match to the reference sample within an acceptable threshold value. There are three different outcomes:

1. Identical, the test sample is identical to the reference sample.
2. Not identical, means that no reference spectrum could be found to match the test sample.
3. It can be confused with <N> samples, in this case more than one reference in the spectral reference model was found to be identical to the test sample.

The identification results are then shown in an Identity Test Report.

For more information on ***NIR Technologies Inc.*** visit our web site www.nirtechnologies.com **or contact us** ***Tel: (905) 469-6767; Fax: (905) 469-0881; e-mail*** research@nirtechnologies.com

Absorption Spectra for Polyethylene and Polystyrene



2nd Derivative Spectra of Vitamin E Samples in Different Concentrations