

# FT-IR in QA/QC Laboratories and on Manufacturing Floors

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## Introduction

The growth in popularity and acceptance of Fourier transform infrared (FT-IR) spectrometers for use in quality assurance (QA) laboratories and on manufacturing floors is one of the major developments affecting industrial environments in recent years. FT-IR spectroscopy offers almost unlimited analytical opportunities in many areas of production and quality control. It covers a wide range of chemical applications, especially in the analysis of organic compounds. In addition to its more classical role in qualitative analysis, its use in quantitative determinations has grown due to the improvements in signal-to-noise performance coupled with the development of advanced statistical analysis algorithms. Thanks to its compact design and ruggedness, the instrumentation can be located in the analytical laboratory or near the production line. Low cost, speed, and ease of analysis make FT-IR a method of choice for many industrial applications.

Nicolet™ FT-IR spectrometers offer many advantages over other analysis techniques. The most important include a drastic reduction of the time needed for data acquisition, component specificity, and sensitivity. Other benefits include the internal wavelength calibration, which ensures the precision of the analysis. With constant improvement in computing power, modern spectroscopy software, and advanced chemometric methodology, FT-IR is becoming ever more prevalent in addressing a wide variety of commercial applications. From simple identifications using library comparisons to sophisticated quantitative analysis, method development, spectrometer operation, and data manipulation are both simple and powerful.

Developments in FT-IR instrumentation and dramatic changes in sample handling techniques resulted in an extensive range of new accessories that simplify and, in many cases, eliminate tedious sample preparation. Many of these sampling techniques feature constant optical path-length, regardless of the sample volume or thickness, making reproducible quantitative analysis simple and elegant.

Thermo manufactures a wide range of Nicolet FT-IR spectrometers, offering products that address the needs of quality control (QC) and quality assurance (QA) laboratories. Nicolet FT-IR spectrometers offer the full advantages of FT-IR technology combined with the simplicity of push-button operation. Rugged instrument construction and design allow reliable, uninterrupted operation in many industrial laboratory environments. Depending on the sampling interface, the spectrometers can be used for gas, liquid, or solid sample evaluations.

The spectrometers can be configured to run specific methods developed for individual applications. This makes them ideal as dedicated, easy-to-use QA/QC laboratory analyzers. They can be programmed to include custom methods that allow full flexibility of data collection, analysis, and interpretation of results with a single keystroke. This configuration permits operation by non-technical personnel. It also ensures consistent, high-quality analytical results with the highest accuracy and precision.

This note illustrates several examples of dedicated applications that have been developed on Nicolet FT-IR spectrometers.

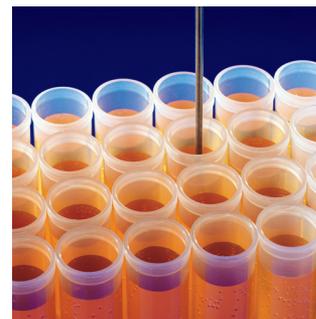


Figure 1: FT-IR is ideal for dedicated QA/QC laboratory analysis

## Analysis of Oxygenated Extenders in Gasoline

The use of organic extenders in gasoline for octane rating improvement and emission control is increasing. Owing to their unique spectral features, oxygenated extenders are easily detected and quantified in gasoline.

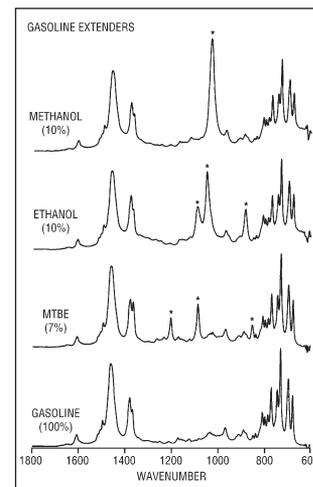


Figure 2: Methanol (10%), Ethanol (10%), and MTBE (7%) in gasoline spectra. Major extender peaks marked with (\*).

## Key Words

- FT-IR
- Production Monitoring
- Quality Assurance
- Quality Control

## Toluene Diisocyanate in Pre-polymer Mixtures

Toluene diisocyanate (TDI) is used in various resin blends in the manufacture of polymeric foams. The TDI concentration in the pre-polymer mixture affects the quality of the final product. Attenuated total reflectance (ATR) FT-IR spectroscopy can be used to quantitatively determine the TDI concentration in resin blends prior to polymerization to ensure product quality. Once the calibrated method is developed, analysis can be performed with a single keystroke.

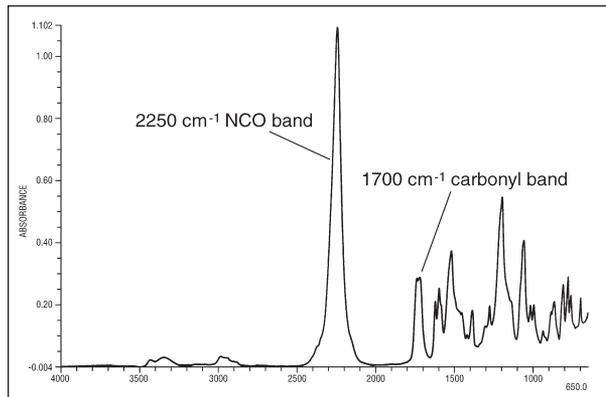


Figure 3: Toluene diisocyanate pre-polymer spectrum obtained on a horizontal ATR accessory. Bands used for quantitative determination are indicated

## Monitoring of Fluorination Level of Polyethylene

Chemically reinforced polyethylene is used in many industrial applications. Fluorination of the polyethylene surface is one of the processes for improving its performance. The fluorination level can be conveniently monitored using a Nicolet FT-IR spectrometer, offering price and performance advantages over currently used neutron activation analysis (NAA) and electron scatter analysis (ESCA).

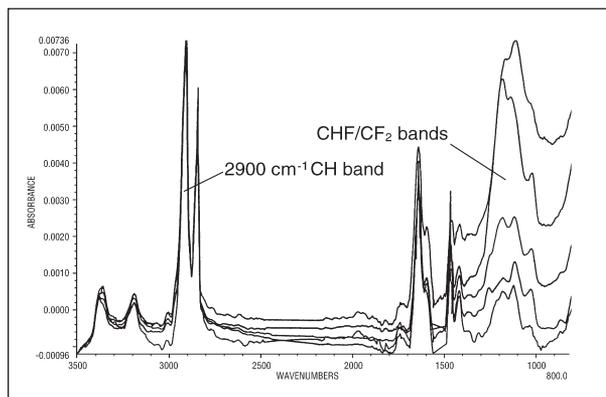


Figure 4: Series of calibration spectra obtained for fluorinated polyethylene samples. Bands used for determination of fluorination levels are indicated

## Corn Syrup

Rapid measurement of dextrose equivalent (DE) and dry substance (DS) at intermediate steps of corn syrup processing allows for better control of syrup production. The parameters are calibrated against the reference method using Partial Least Squares quantitative analysis software, providing a powerful yet rapid monitoring process for product quality.

## Lubricating Oil Blend

Lubricating oils are blended from a number of different components, including base oil, additives, pour point depressants, and viscosity enhancers. FT-IR can be used to measure the levels of these components in the finished product.

## Lubricating Oil Condition Monitoring

FT-IR analysis of used lubricating fluids followed by subtraction of the appropriate new oil reference is an effective tool for monitoring changes in the lubricant. These changes are the result of oxidation processes or contamination from other parts of the mechanical system.

## Hydroxyl Number in Glycols

Knowledge of the hydroxyl group content of glycols is important for predicting the functional characteristics of the products. The hydroxyl value relates to molecular weight, viscosity, extent of reaction, and other parameters important to and dependent on the final application. Assessment of this value can be quickly and easily done using FT-IR.

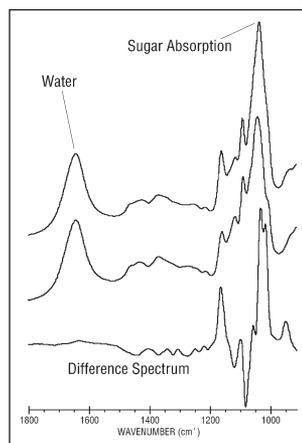


Figure 5: Spectra of corn syrup production lot samples having different DE and DS levels with the spectral subtraction result below

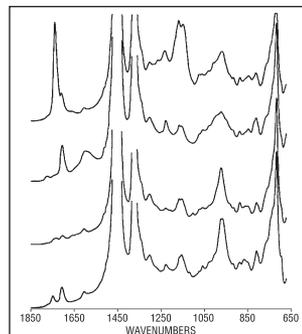


Figure 6: Overlay spectra of commercial lubricating oils showing differences in base oils and additives

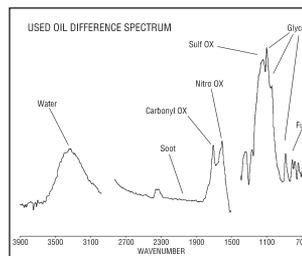


Figure 7: Typical used engine oil difference spectrum with components of interest labeled

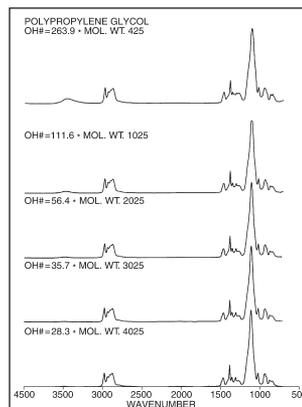


Figure 8: Spectra of polypropylene glycol samples with different hydroxyl values

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