Technical Note: 51504

Multiplying Productivity: The Nicolet iZ10 Module

Mike Bradley, Ph.D., Thermo Fisher Scientific, Madison, WI, USA

Key Words

- Auxiliary Experiment Module
- Micro-well Plate
- NIR Integrating Sphere
- Thermal Gravimetric Analysis

Introduction

The Thermo Scientific Nicolet™ iS™10 FT-IR spectrometer sets new standards for performance in compact laboratory FT-IR, especially through performance verification and ease of use. The greatest power of the Nicolet iS10 is the philosophy built into it from the beginning – the system is more than just a spectrometer: it provides solutions with confidence to your analysis problems. This sweeping statement is supported by the tremendous range of laboratory productivity and validation tools available for the Nicolet iS10.

Analytical laboratories rely on multiple techniques to answer questions about samples. Basic sampling, such as compositional verification, gives way to contaminant identification or product deformulation. Experimentally, this means standard analyses using transmission or ATR must be augmented with Thermal Gravimetric Analysis (TGA), near-IR capabilities, or high-throughput applications using automation. The need to interchange easily between techniques and applications means the spectrometer and software should offer convenient flexibility.

The Nicolet iS10 can perform a huge array of experiments in its main sample compartment. The Thermo Scientific Nicolet iZ™ 10 Auxiliary Experiment Module boosts both productivity and flexibility by providing a fully functional second sample compartment. Complete software control, including automatic recognition of the many possible configurations, permits rapid switching between the Nicolet iS10 mainframe and Nicolet iZ10 module. The powerful example shown in Figure 1 configures the Nicolet iS10 to perform diamond ATR experiments while the Nicolet iZ10 is readied for a TGA-IR analysis.

QC laboratories will have an unparalleled level of confidence in the data collected from the Nicolet iZ10, because the module passes the same ASTM-designed tests for System Performance Verification as does the Nicolet iS10. The requisite testing protocols are provided through the automatic performance verification tools. There is no need to purchase a separate verification wheel or software for the Nicolet iZ10, as the internal arrangement permits use of the same validation wheel for both the main and auxiliary sample compartments. The two compartments are separately sealed and desiccated, and the interchange is fully software controlled. Users can even enable a bar code reader to select the appropriate sample compartment, collect backgrounds and ready the instrument for sample delivery.

Thermal Gravimetric Analysis – Infrared (TGA-IR)

TGA-IR is a powerful hyphenated technique for characterizing material blends and mixtures. With great strength in analyzing polymers, rubbers and inorganics, TGA-IR provides an incisive tool for product deformulation and mixture analysis, typical concerns of analytical support laboratories. Polymer laboratories and automobile tire manufacturers commonly use TGA-IR. In the laboratory, the TGA furnace is coupled by a heated transfer line to a heated gas cell within the spectrometer. The TGA balance provides quantitative weight-loss information, while the infrared qualitatively identifies the vapors being driven off. The Nicolet iZ10 permits the heated TGA accessory to remain mounted without blocking access to the Nicolet iS10 sample compartment, as seen in Figure 1. This offers a convenient way to switch rapidly from routine measurements to TGA-IR data collection.

Figure 1: Nicolet iS10 with Smart iTR™ diamond ATR coupled with the Nicolet iZ10 and the TGA sampling accessory

Thermo SCIENTIFIC

Figure 2 shows TGA-IR data from a sample of an epoxy resin. The data imported from the TGA is seen along with the infrared spectrum from a single time point, so the gases evolved can be correlated directly to the weight loss. As this example shows, many times in TGA runs multiple gas-phase components are emerging simultaneously from the furnace, which normally complicates the analysis. However, using the OMNIC™ Specta™ software, multi-component spectra can be deconvoluted simply by any lab analyst with any level of skill. As seen in Figure 3, even with the small samples used for TGA (around 1 mg), the sensitivity and signal-to-noise of the IR spectra are very high, and OMNIC Specta's multi-component search algorithm is able to extract detailed information. The combination of tools provides a complete, powerful solution for deformulation.

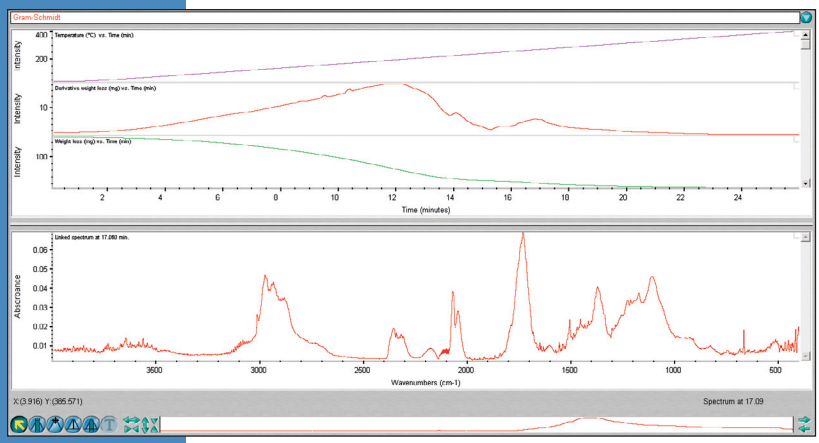

Figure 2: TGA-IR data for an epoxy resin. Top profiles show imported TGA information; lower screen shows the infrared spectrum at a particular time.

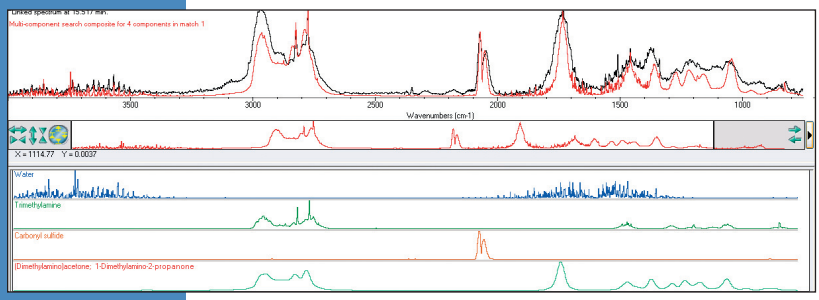

Figure 3: Multi-component search from OMNIC Specta for TGA-IR data from an epoxy. The algorithm correctly identifies four different gases being evolved.

Near-IR Integrating Sphere

A common requirement for production facilities involves incoming raw material identification. A simple way to perform this test without requiring physical contact with the sample relies on near-infrared diffuse reflectance. The Thermo Scientific Smart NIR integrating sphere is ideally suited to the needs of the QC/QA or analytical services laboratory. Shown in Figure 4, the accessory provides a flat, elevated working surface with excellent performance.

Figure 4: Nicolet iS10 with Smart iTR diamond ATR coupled with the Nicolet iZ10 containing the Smart NIR integrating sphere

A great strength of the Nicolet iS10 is the ability to configure the spectrometer for performance across the mid- and near-IR regions. Using our unique extended-range XT-KBr optics and easily swapped source, the Smart NIR integrating sphere, with its self-contained highly sensitive near-IR detector (InGaAs), provides excellent performance over the full NIR spectral range, from 4000 to 10000 cm^{-1}, while the installed DTGS continues to perform strongly across the mid-infrared and into the NIR range.

Figure 5 shows a series of spectra for polyethylene samples of varying density collected using the Smart NIR integrating sphere in the Nicolet iZ10. The samples were contained in a simple glass-bottomed cup and slowly spun over the integrating sphere window. The figure shows the calibration achieved using the TQ Analyst™ chemometrics software. This laboratory-based NIR system can provide proofs of concept for the development of calibrations useable with the Thermo Scientific Antaris™ spectrometer, a ruggedized FT-NIR designed for use in demanding environments such as loading docks or production facilities.

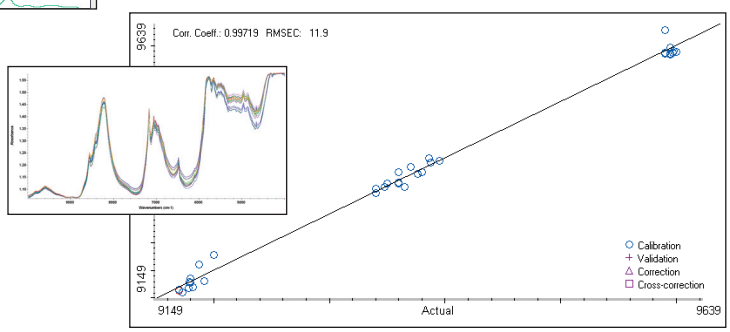

Figure 5: Spectra obtained from a series of different density polyethylene samples. The inset shows the calibration obtained using partial least squares (PLS).

High-throughput Sampling

Many modern laboratories are seeking ways to increase sample throughput without adding laboratory staff, mainly through enhanced experiment automation (an autosampler on a GC is an excellent example). The driving force may include the need for replicate measurements, or the requirement for screening multiple materials. Our Micro-well plate reader, shown in the Nicolet iS10 in Figure 6, allows the use of industry-standard or custom-designed sample plates in either transmission or diffuse reflection (DRIFTS) modes. The Array Automation™ OMNIC add-on software links data collection to the power of TQ Analyst, permitting qualitative or quantitative results to be drawn from the wells.

Figure 6: Micro-plate reader shown installed in the Nicolet iS10. Operation of the accessory is the same in either the Nicolet iS10 or Nicolet iZ10.

In the analysis shown in Figure 7, bacteria were classified in the wells via transmission.[1] The transmission configuration of the Micro plate reader carries a dedicated detector which interfaces simply to the spectrometer and OMNIC. A downward-looking CCD camera provides a visual image of the targeted sample, and the images from each well are stored in the array data file. In the bacterial analysis, each column of the plate was loaded with one class of bacteria (these were from cheese production). The colors show similarity and differences, allowing a classification analysis to be built. Use of these tools raised the daily sample throughput from less than 50 to several hundred, with automation from data collection to analysis. This is a critical productivity boost, given that screening of bacteria used in food production is coming under mounting regulatory oversight, so the sample loads are increasing rapidly. The DRIFTS form of the accessory can also be used for forensics testing of drugs or screening of powdered ore samples.

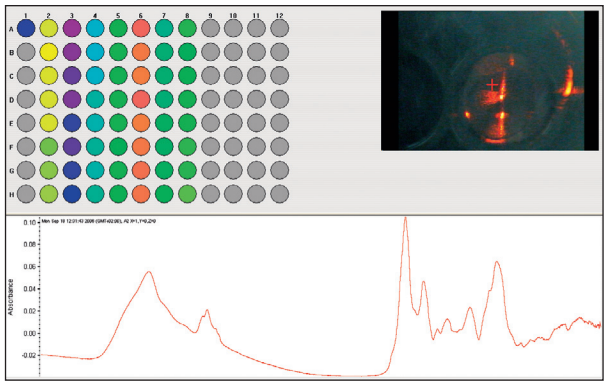

Figure 7: Array Automation software output for the classification of enzymes. See reference 1 for details.

Conclusion

The Nicolet iS10 FT-IR spectrometer paired with the Nicolet iZ10 module offers unparalleled flexibility and performance. The ability to validate the entire system automatically, using only one set of built-in standards, enhances the level of confidence in data, regardless of which sampling compartment is used. This opens tremendous possibilities in laboratories where multi-faceted approaches to problem solving are becoming the norm, without adding any complexity to the workflow or additional training. The Nicolet iZ10 essentially provides a second, economical, spectrometer to enhance productivity or provide additional analytical power to solve day to day problems in the QC, analytical or forensics laboratory.

Reference

1. Lefier, D.; Beccard, B.; Bradley, M. "Classification of Bacteria using FT-IR" Thermo Scientific Application Note 51396.

In addition to these offices, Thermo Fisher Scientific maintains a network of representative organizations throughout the world.

Africa
+43 1 333 5034 127

Australia
+61 2 8844 9500

Austria
+43 1 333 50340

Belgium
+32 2 482 30 30

Canada
+1 800 530 8447

China
+86 10 5850 3588

Denmark
+45 70 23 62 60

Europe-Other
+43 1 333 5034 127

France
+33 1 60 92 48 00

Germany
+49 6103 408 1014

India
+91 22 6742 9434

Italy
+39 02 950 591

Japan
+81 45 453 9100

Latin America
+1 608 276 5659

Middle East
+43 1 333 5034 127

Netherlands
+31 76 579 55 55

South Africa
+27 11 570 1840

Spain
+34 914 845 965

Sweden/Norway/ Finland
+46 8 556 468 00

Switzerland
+41 61 48784 00

UK
+44 1442 233555

USA
+1 800 532 4752

www.thermo.com

Thermo Electron Scientific Instruments LLC, Madison, WI USA is ISO Certified.

TN51504_E 01/08M