

A FASTIR WAY OF GRINDING OUT SPECTRA



Figure 1. The [FastIR™](#).

INTRODUCTION

Internal reflectance spectroscopy (ATR)¹ is used widely for studying a variety of liquids, pastes, and solids. It is well suited for analyzing optically thick and opaque samples that cannot be examined via conventional transmission spectroscopy. Internal reflectance is straightforward and convenient, resulting in minimal disruption of the sample and requiring minimal sample preparation. For liquids and pastes, the sample is simply placed, as is, in contact with an internal reflectance element (IRE) and the spectrum recorded. For solids, the sample is placed on the IRE and pressure is applied to obtain good contact between the sample and the IRE.

ATR spectra are most commonly recorded using multiple reflection accessories. These accessories allow the beam to repeatedly interact with the sample to provide a greater pathlength. To direct the beam through the crystal, these accessories frequently have multiple mirrors that must be correctly positioned to optimize the performance of the accessory. Given the excellent signal-to-noise ratios of today's spectrometers, many samples do not require multiple interactions to obtain good quality spectra.

Spectra can be easily obtained using single reflection

ATR. Single reflection ATR is extremely convenient, both in terms of experimental set-up and sample analysis. The accessories are lower cost than their multiple reflection counter-parts and are very durable.

To illustrate the versatility and power of single reflection ATR, several types of samples have been examined and the results are presented herein.

PERCOLATED RESULTS AND COFFEE HOUSE DISCUSSION

The samples were analyzed using the FastIR™ (Figure 1) in a Mattson Polaris spectrometer with a DTGS detector. The FastIR™ is a horizontal sampling, single internal reflection accessory with fixed 45° incident angle.

The spectrometer collected 16 scans and 8 cm⁻¹ resolution with a 30% aperture. Background single beam spectra were recorded with the clean IRE as the reference. All the samples were examined on a flat sampling plate. The powders were compressed against the crystal using the pressure applicator and the films were cast directly onto the crystal.

Figure 2 shows the internal reflectance of two powdered hot chocolate mixes: Swiss Miss® Chocolate Sensation and Carnation® Hot Cocoa Mix. From the spectra, it is clear that the two different blends of hot

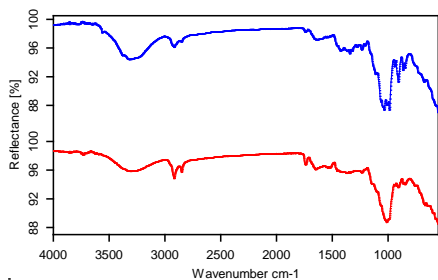


Figure 2. ATR Spectrum of Hot Chocolate Mixes: Carnation (blue) and Swiss Miss (red).

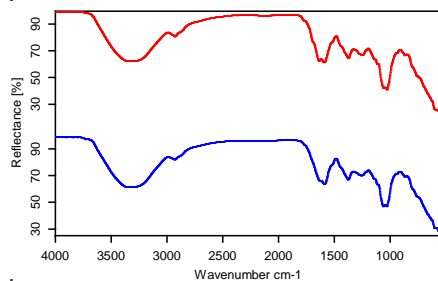


Figure 3. ATR Spectra of Instant Coffee (red) and Decaffeinated Coffee (blue).

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chocolate use similar ingredients in different proportions.

Figure 3 compares instant coffee and instant decaffeinated coffee. Both types of coffee were cast as films on the crystal. The Taster's Choice® coffees were dissolved in hot water, dripped onto the crystal of the FastIR™, and dried to form films. The coffee spectra express their differences in the 1700 cm⁻¹ region, where the decaffeinated coffee lacks some shoulder bands that are present in the non-decaffeinated coffee. These bands are probably due to caffeine or other components that are removed during the caffeine extraction.

And for those who prefer the aroma of fresh ground coffee, Figure 4 compares the spectrum of fresh coffee grounds to the Taster's Choice® instant freeze-dried powder. The instant coffee shows much weaker C-H and carbonyl bands. This is due to the lower concentration of aromatics, cellulose, and other materials that are removed during the freeze-drying process.

SUMMARY

Single, internal reflectance (ATR) measurements can be used for quantitative and/or qualitative analysis. The FastIR™ provides a convenient, quick and reliable

method of examining solids and pastes without elaborate sample handling or preparations. The FastIR™ is especially good for the last drop!

REFERENCES

¹N. J. Harrick, *Internal Reflection Spectroscopy* (Harrick Scientific Corp., Ossining, New York, 1967).

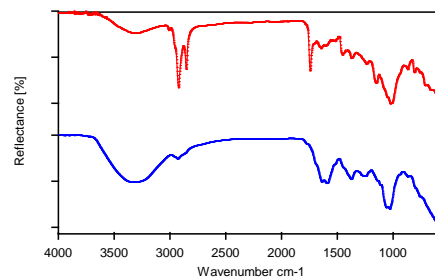


Figure 4. ATR Spectra of Fresh Grounds (red) and Instant Coffee Powder (blue).



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