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ATR Accessory

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The ATR, a journey into performance and value:

The ATR Accessory is a performance single-reflection ATR accessory from ATL designed for laboratory spectroscopic sample analysis in the mid- and far-infrared. With an innovative optical design and durable monolithic diamond ATR crystal option, this product sets the benchmark in performance and value for ATR spectroscopy.

In its standard configuration, the ATR Accessory has a strong and durable monolithic diamond ATR crystal which is ideal for analysing hard inflexible solid materials without risk of being scratched or damaged even for extreme point loads. Coupled with diamond's inherent chemical resilience, this allows the ATR Accessory to be used with the broadest range of sample types. A 1.8mm diameter diamond sample area means that good contact can be achieved even with the smallest amount of material available for analysis.

The ATR Accessory features an all-reflective optical design, based around ATL's proprietary Synopti-Focal Array technology. This comprises precision-molded aspheric mirrors and gold-coated optics as standard, and provides the ATR Accessory with high transmission throughput and an extended wavelength range capability to match that of your mid- and far-infrared FTIR instrument. Together with an optimised angle of incidence on the ATR crystal, these features ensure outstanding quality of spectra.

Four easily-interchangeable crystal pucks are available for use with the ATR Accessory: a high-throughput diamond puck for mid-infrared analysis (7800 to 400 cm^{-1}), an extended wavelength range diamond puck for the mid- and far-infrared (10000 to 40 cm^{-1}), a ZnSe crystal puck for softer materials, and a Ge crystal puck for strongly absorbing samples. These ATR crystals are mounted in a durable stainless steel puck and held in place against a robust metal seal to ensure compatibility with a broad range of sample types.

Repeatable and reproducible sample loads are enabled by a full-function pressure tower. This has an audible click' to indicate at the preset pressure limit, and features a swing anvil arm to allow easy access to the ATR crystal puck. Both plane and pellet anvils are provided with the accessory to allow analysis of samples of various shapes. These anvils are easily interchangeable and stored on the top plate when not in use.

Note that the ATR Accessory is Benchmark Baseplate compatible.

Features:

- Strong and durable monolithic diamond
- Extended wavelength capability from 10,000 to 40 wavenumbers
- High spectral quality and high throughput capability
- Interchangeable Diamond, ZnSe and Ge ATR crystal puck options

The Benchmark Baseplate System:

ATL believe that your accessory should be able to be quickly and easily switched from instrument to instrument in your laboratory. To facilitate this, we have developed the "Benchmark Baseplate" system as an interface between the accessory and instrument, and to which the accessory can be fitted with a single thumbscrew fixing. The Benchmark Baseplate is unique to the instrument model being used (a baseplate is supplied with the ATR Accessory), and can be left in the sample compartment, if required, for use with other ATL Benchmark compatible accessories. You should specify your spectrometer when ordering your Quest.

Why is a monolithic diamond important?:

'Diamond' ATR Accessories on the market are generally available in two forms: those that feature a solid monolithic diamond and those with a thin diamond wafer supported by an optical element (typically ZnSe). Monolithic diamond ATR accessories are seen to benefit from the inherent robustness and durability of a solid diamond element, and are particularly resilient to high point loads typically encountered when analysing hard irregularly-formed samples. They can also take advantage of the broad transmission window of diamond (10,000 to 40 cm^{-1}).

Conversely, diamond wafer ATR accessories are seen to be more fragile under point loads, can suffer de-lamination from the supporting element, and have a useable transmission range that is often limited by the support material. However, featuring a thinner diamond, they also have weaker diamond absorption features at 2000 to 2500 cm^{-1}.

Ordering Information:

- Complete ATR Accessory

20-10800-X : ATR Diamond Accessory
20-10801-X : ATR Diamond Extended RangeAccessory
20-10802-X : ATR ZnSe Accessory
20-10803-X : ATR Ge Accessory

- Please specify spectrometer make & model

X represents Top Plate colour, the colours available are: Black colour, Orange colour, Red colour, Green colour, Yellow colour, Aqua colour & Purple colour.

- ATR Puck Only

20-10810 : ATR Diamond Crystal Puck
20-10811 : ATR Diamond Extended Range Crystal Puck
20-10812 : ATR ZnSe Crystal Puck
20-10813 : ATR Germanium Crystal Puck

- Spares and Accessories

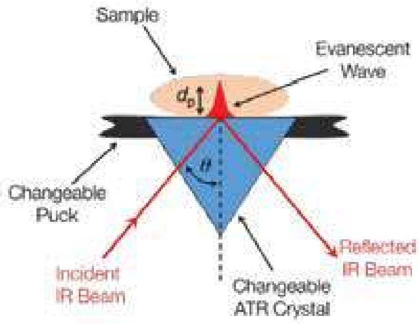
20-10820 : ATR Stainless Steel FlatAnvil
20-10821 : ATR Stainless Steel Pellet Anvil
20-10825 : ATR Volatiles Cover
20-10707 : Purge Bellows (Pair)

How the ATR accessory works:

TRADITIONALLY, recording IR spectra of samples involved making KBr discs or dissolving the sample in solvents.
However, this is an inefficient and time consuming practice, especially for multiple recordings.
Furthermore, solvents present hazards and can be expensive, while making KBr discs requires user training.
Diluting samples in this way helps to prevent the intense absorption bands saturating the detector.
Attenuated Total Reflectance (ATR) eliminates these issues because little or no sample preparation is needed.
ATR is an effective FTIR sampling technique to produce qualitative or quantitative spectra of a broad range of samples.
Therefore, using the Specac ATR can save time and money for researchers and industry professionals.
In this document, we will show you how ATR is a very efficient spectral analysis technique.

So how does it work?

Figure 1 demonstrates the principle behind the single bounce ATR, where IR light from a spectrometer is internally reflected in the ATR crystal and interacts with the sample at the crystal interface.
Partial penetration of the IR light by an evanescent wave allows an absorption spectrum to be recorded.



Graphical representation of a single bounce ATR.

The absorbance and depth of penetration (dp) of the evanescent wave depend on the following factors:
- the refractive index of the crystal, n_1
- the refractive index of the sample, n_2
- the angle of incidence, θ
- the wavelength of the light, λ

$$d_p = \frac{\lambda}{2\pi\sqrt{(n_1^2\, sin^2\theta - n_2^2)}}$$

Table 1 shows the physical properties of different ATR crystals and the value of dp when n2 = 1.5, 0 - 45° and λ = 10 μm. The typical value of dp ranges from 2-4 μm depending on the crystal.

Crystal	n_1	d_p/μm	IR range/cm-1	Uses	Part no.
ZnSe	2.4	2.01	7800-500	General	20-10812
Diamond	2.4	2.01	7800-400	Harder & chemically resistant	20-10810
Extended Diamond	2.4	2.01	10000-400	Shorter freq.	20-10811
Ge	4.0	0.66	5500-480	Highly conc.samples	20-10813

Table 1: Physical properties of the ATR crystals.

For example, a Ge crystal provides a shorter sample penetration depth than a ZnSe crystal, which is ideal for strongly absorbing samples.
However, its effective IR absorption range is limited,whereas a range of 4000-400cm^{-1} can be achieved by using the extended mono-crystalline type IIIa diamond crystal.
The Specac ATR allows the user to change the crystal to suit the experimental requirements by swapping the top-plate puck.

Figure 2 shows that ZnSe and Diamond have similar refractive indices and hence have similar penetration depths, while Ge is significantly different, so provides a lower penetration depth.

Intensity Corrections

At higher frequencies, the relative absorbance of a sample is lower in the spectrum recorded using the ATR.

This is because the penetration depth of IR light into the sample depends on the refractive index of the crystal, which changes as a function of frequency.

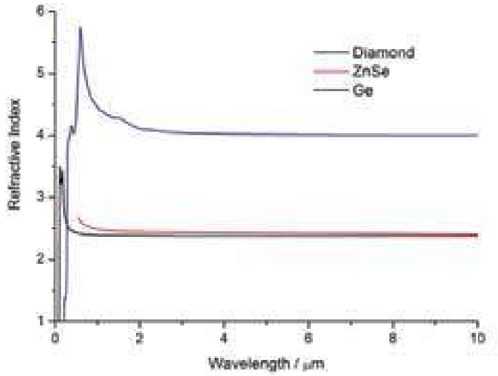


Figure 2: The refractive index of Ge, ZnSe and Diamond.

Figure 3 shows in more detail how the refractive index of ZnSe changes with wavelength at standard room temperature and pressure.

Consequently, the depth of penetration changes with the refractive index and hence the amount of light absorbed by the sample. Most FTIR spectrometers come with a correction package.

Figure 4 shows the transmission spectra of DuPont Krytox Gpl205 lubricant recorded using a traditional transmission method and the ATR.

Using a transmission measurement technique, there is a strong absorption by the bands around the fingerprint region (1500-500 cm^{-1}) as well as some saturation at 1250 cm^{-1} But the peaks are more resolved using the ATR because of its short effective pathlength.

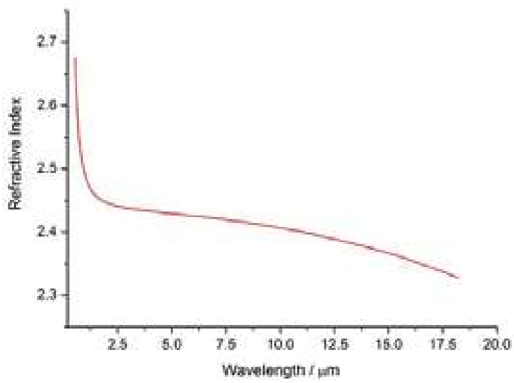


Figure 3: The refractive index of ZnSe

Conclusions

The ATR is a single bounce ATR that provides a quicker alternative for acquiring IR spectra for a range of sample types, such as gels, pastes, liquids and powders.

As the IR light frequency decreases, so does the crystal's refractive index, which results in an increase in sample absorbance. Interchangeable pucks with 4 different crystals allow the user to control the IR light penetration depth and effective pathlength, as well as the spectral range.

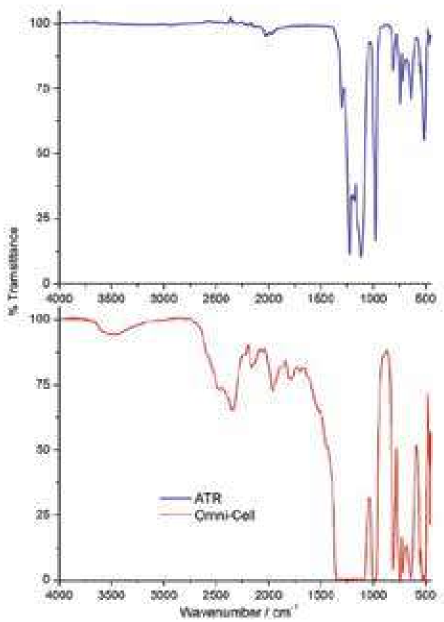


Figure 4: Transmission spectra of Gpl205 lubricant.

References

Berge Tatian, "Fitting refractive-index data with the Sellmeier dispersion formula," Appl. Opt. 23, 4477-4485 (1984)

Norman P. Barnes and Martin S. Piltch, "Temperature-dependent Sellmeier coefficients and nonlinear optics average power limit for germanium," J. Opt. Soc. Am. 69, 178-180 (1979)

H. R. Phillip and E. A. Taft, "Kramers-Kronig Analysis of Reflectance Data for Diamond," Phys. Rev. 136, A1445 (1964)

Narcotic analysis using the ATR accessory

NARCOTICS HAVE BEEN CONSUMED for cultural and personal reasons throughout the ages. Security agencies are continually looking to enhance their methods of substance detection and testing, in an endless arms race of drug smuggling and dealing.

Any controlled narcotic or illegal 'street' drug needs to be routinely submitted for chemical analysis that has a fast turnaround time with minimal user error. Security services require non-destructive techniques so that samples can be presented as evidence after testing.

Attenuated Total Reflectance (ATR) spectroscopy is a fast method of analyzing liquid and solid drug samples non-destructively. The ATR accessory allows users to quickly record qualitative and quantitative spectra, in order to test which drugs are present in the sample and in what proportions.

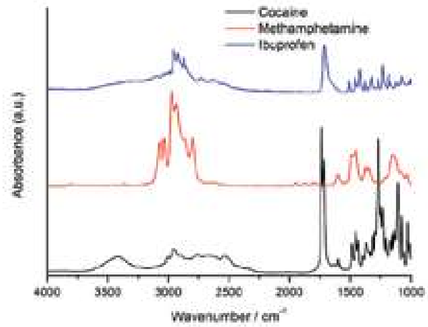


Figure 1: ATR spectra of cocaine, methamphetamine & ibuprofen

This note demonstrates how you can distinguish several common different narcotics easily and quickly.

Powdered samples

Figure 1 shows the ATR spectra of cocaine, methamphetamine and ibuprofen. All three can be seen as fine white powders, but they each absorb different quantities of infrared light. The sharp peak at ~1750 $cm^{-1}$is only present in cocaine and ibuprofen. Even more differences can be seen at the lower wavenumber region, often called the fingerprint region.

Cocaine

There are several stages in the chemical process followed to make cocaine.

For instance, the coca leaves first need to be harvested before cocaine paste is extracted, which is then converted to the cocaine base. Finally this is turned into Cocaine HCl.

ATR spectroscopy can tell these two different forms apart, as shown in Figure 2. Such a capability is useful for forensics agents to immediately tell what stage of the process criminals have reached and the street value of their drugs.

Contaminants and cutting agents are sometimes found in narcotics (rat poison, baking soda, caffeine, etc). ATR spectroscopy can detect them all.

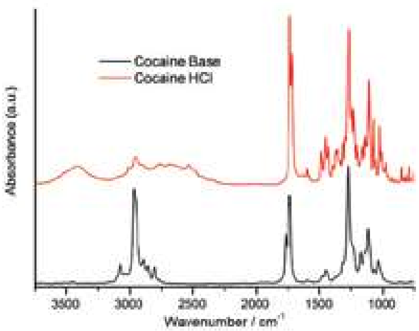


Figure 2: ATR spectra of cocaine base vs cocaine HCl

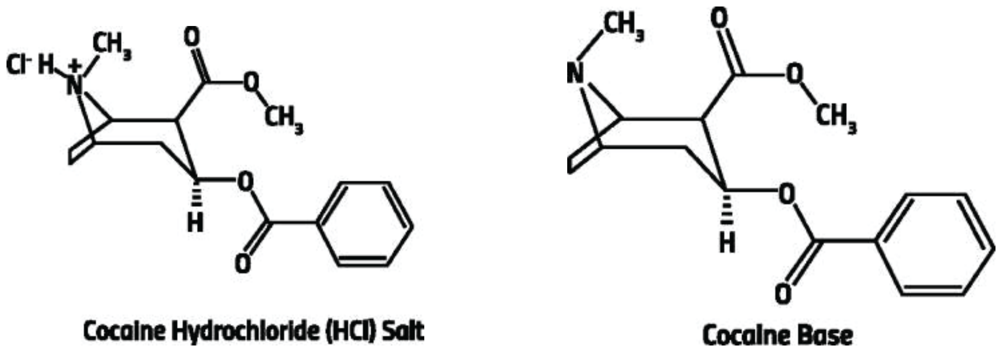


Figure 3: Cocaine HCl & Cocaine Base molecules

Awkward narcotic sample-types

Some narcotics, like cannabis, are not powders but resins, sticky solids or oils. The ATR can still distinguish non-powdered substances than may be found on a crime scene.

Figure 4 shows the spectra of cannabis leaf, some hemp rope and an ordinary garden flower. Although each sample shares a noticeable water absorption band at 330 cm^{-1}, there are clear differences around the lower wavenumber region.

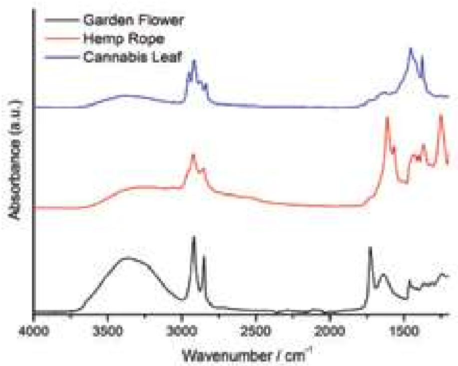


Figure 4: ATR spectra of Cannabis Leaf, Hemp Rope & Garden Flower

In conclusion…

Modern forensic scientists and government security agencies need fast, reliable analysis techniques that allow them to determine what a substance is, in a nondestructive way.

The ATL ATR is the perfect tool for analyzing many samples quickly, without sample preparation. It is also very user friendly and gives reproducible results.

This note shows different legal and illegal drug samples analyzed using the ATR accessory. Each chemical absorbs different quantities of IR light, and spectroscopy is a key way to rapidly confirm what the sample contains.

Acknowledgements

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Richard A. Larson, Spectral Consulting

Acknowledgements

1. Koulis, C. V., Hymes, K. J., Rawlins, J. L. Journal of Forensic Sciences, 2000, 45, 876.
2. An ATR library of 455 compounds was provided by the Illinois State Police Department.

ATL ATR: Analysing Pharma Theophylline

ATL ATR accessory lets the user test various samples without the need for any sample preparation.

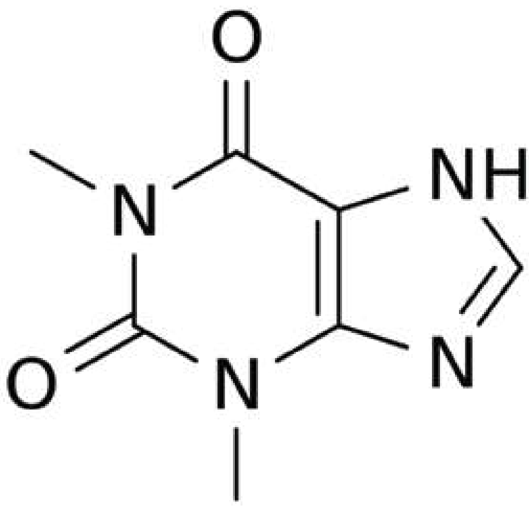
IN COMPLIANCE WITH Japanese Pharmacopoeia regulations, pharmaceutical samples are required to have IR spectral data spanning 4000-400 cm^{-1} (2.5 µm to 25 µm).

Traditionally, KBr windows have been used as part of liquid cells for this range. However, their structural integrity can be compromised if the sample contains any aqueous component.

Dry solid samples can be analysed within a KBr matrix too. But this is a time consuming method and the quality of the spectra produced depends on the sample, the structural integrity of the KBr pellets and the user.

An alternative method available for the recording of IR spectra is Attenuated Total Reflectance (ATR). Here samples are brought into direct contact with an ATR crystal.

An important pharmaceutical, Theophylline.



The IR light from the spectrometer is internally reflected in the crystal and interacts with the samples at the crystal interface.

The spectral range accessible by the ATR technique depends on the ATR crystal used. A range of 4000-400 cm^{-1} can be achieved with a mono crystalline type IIIa diamond crystal.

This application note compares both methods of spectroscopy by examining the white crystalline powder Theophylline ($C_7H_8N_4O_2$).

Experimental

The Specac Basic Solid Pack contains all the necessary equipment to make a KBr pellet of the sample, as shown in Table 1.

A small amount of Theophylline was added to a 99% excess of spectroscopic grade KBr Powder and ground together with a mortar and pestle.

A small amount of Theophylline was added to a 99% excess of spectroscopic grade KBr Powder and ground together with a mortar and pestle.

Equipment	Part Number
Mini-Pellet Press (2T)	GS03940
7 mm Pellet Die + Ring Holder	GS03950
Spare Ring Holder	GS03951
Pestle and Mortar	GS03600
50 g KBr Powder	GS03610
7 mm Disc Holder Mount	GS03960

Table 1: Part numbers of the Basic Solid Pack.

For the ATR measurements, the solid samples were placed onto the extended range diamond crystal in the ATL ATR without any preparation, demonstrating its suitability for FTIR spectral acquisition in a quick and reliable fashion.

A set load from the anvil arm on the ATL was used to ensure contact between the samples with the ATR crystal. The Spectra were collected using an FTIR spectrometer with a resolution of 1 cm^{-1} and an average of 16 scans.

The Specac ATL ATR accessory.

Discussion

The IR spectra for Theophylline recorded using a KBr pellet and the ATL are shown in Figures 1 and 2 respectively.

There is a stronger absorbance for the KBr pellet, but this is a consequence of the longer pathlength in the pellet (~1 mm) compared to the ATR (~2 µm).

The signature peaks and their positions in the spectrum collected using the ATR are identical to those collected wth KBr pellets.

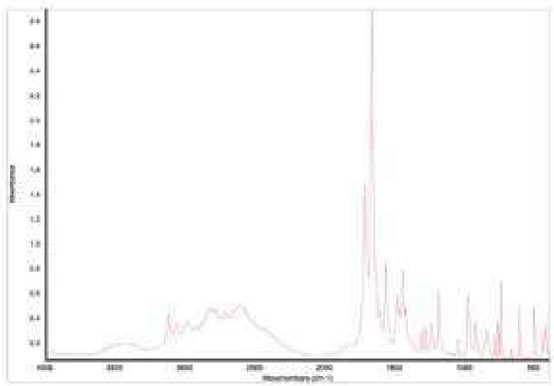


Figure 1: IR spectrum of a 7 mm KBr Pellet of Theophylline.

However, the peak intensities are different for the two different techniques. Specifically, at a higher frequency, the relative absorbance is lower in the spectrum recorded using the ATR.

This is a well-known consequence of the ATR technique and corrections are commonly applied.

Some weak spectral features in the higher frequency region of an IR spectrum may not be easily observed if analysing the sample via the ATR technique. An important comparison to make is the ease of sample handling.

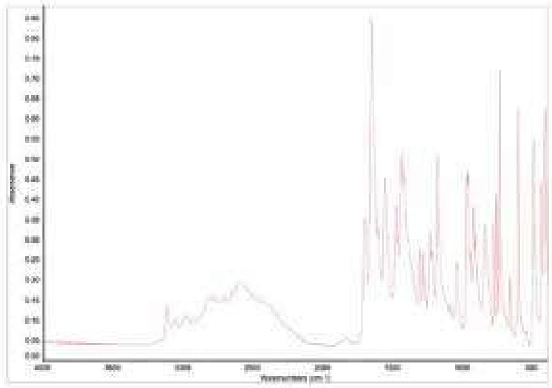


Figure 2: IR spectrum of Theophylline using the ATL ATR

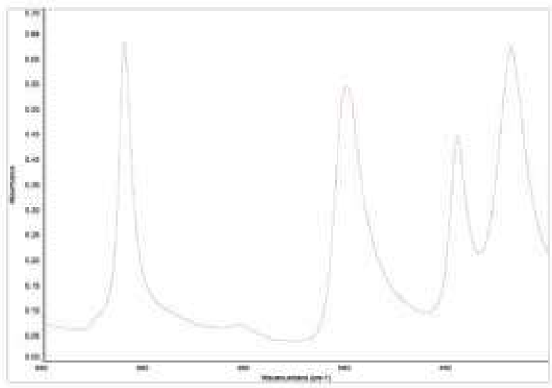


Figure 3: IR spectrum of Theophylline using the ATL ATR

Conclusion

Transmission spectroscopy using KBr pellets tends to produce more accurate qualitative IR spectra, but the quality varies with the pellet's integrity, sample preparation and the user.

Conversely, the ATR technique is ideal for performing quick and reproducible qualitative and quantitative measurements. Spectral acquisition is faster with the ATL because samples can be analysed 'as is', i.e. without prior preparation. This requires less user training.

Furthermore, the ATR can more easily handle a wide range of sample types, including gels, solids, oils and aqueous liquids.

Analyse leather with the ATL ATR

ATR-FTIR is ideal for fast & accurate leather analysis.

ANIMAL SKINS HAVE BEEN USED to make leather since ancient times and their texture and properties depend on which animal they come from. Chemical treatment with vegetable tannins modifies the skins to produce strong and flexible materials that resist decay.

Commercially, IR spectroscopy is used to test for consistency in batches of leather and to uncover fraud.Attenuated Total Reflectance (ATR) accessories like the ATL allow users to test a variety of leathers quickly and efficiently.

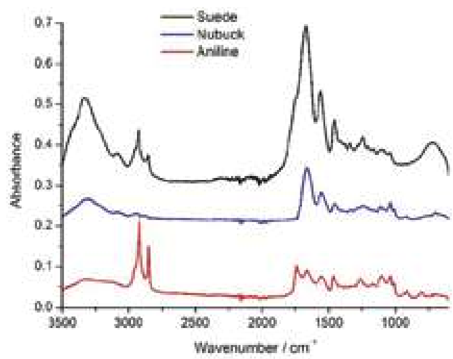


Figure 1: IR spectra of three leather samples

This note shows how ATR spectroscopy can be a fast and reliable technique to distinguish different leathers.

Results

Figure 1 shows the IR spectra of three material samples of nubuck, suede and aniline-dyed leather recorded using the ATL ATR accessory in a commercially available spectrometer.

The spectra were recorded by simply placing the leathers onto the ATR device for 20 seconds. Therefore, the turnover for sample analysis is significantly faster than traditional solid analysis methods.

Suede is primarily made from the lambskin, while nubuck is a cowhide leather that has been made to feel like suede.

Aniline leather is a leather made with soluble dyes that cover the material surface. The chemical makeup of all three samples is different and as such, their IR spectra are different.

If we focus on the lower wavenumber region of 1800-600 cm^{-1}, we can see the amide I and II band intensities differ for each material.

Therefore, the ATR technique allows for a fast and effective distinction of a large number of different samples.

Conclusions

IR spectroscopy allows users to assess the quality of fabrics in a reliable, consistent and fast way, without contaminating or damaging the material.

No sample preparation or solvents are needed for sample analysis, unlike alternative analytical techniques.

ATR-FTIR is the best spectroscopic method for reliable at-line analysis, providing manufacturing control and supply-chain checks. Complementary methods of analysis for more in depth studies on material adulteration and for the detection of fraud include SEM, as well as microscope surface mapping for quality control purposes.

Acknowledgements & references

Institute for Creative Leather Technologies, University of Northampton.

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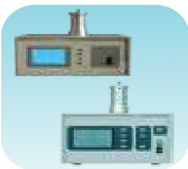
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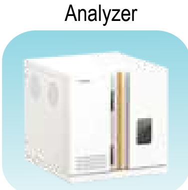
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