Thermo Scientific
Smart Accessories

sampling tools

for Thermo Scientific Nicolet FT-IR Systems

Thermo
SCIENTIFIC

Smart Accessories

Speed Sample Preparation and Improve the Results in your Laboratory

An Accessory For Every Need

Thermo Scientific Smart Accessories offer an extensive line of sampling choices for Thermo Scientific products including the Thermo Scientific Nicolet iS10 and Thermo Scientific Nicolet iS50 FT-IR spectrometers to address a variety of sample types and laboratory needs, from routine to advanced.

- The basic Smart Accessories™, such as the Thermo Scientific Smart Multi-bounce HATR and the Thermo Scientific Smart Diffuse Reflectance, are ideal for the routine measurements done in quality control or teaching laboratories. These accessories provide affordable tools that offer sampling speed and ease of use.
- The research Smart Accessories, such as the Thermo Scientific Smart ARK, Thermo Scientific Smart iTR and Thermo Scientific Smart SAGA, are geared toward the research environment to provide the highest quality data and the greatest degree of flexibility.

- Smart Accessories are optimized for ease of use and universal sample compatibility.

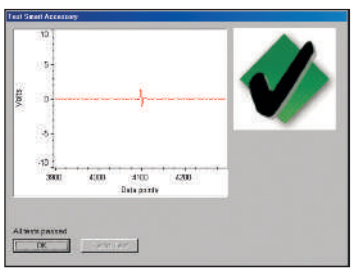
All Smart Accessories are compatible with Thermo Scientific Nicolet iS10, Nicolet iZ10, Nicolet iS50, Nicolet 380 and Nicolet x700 series spectrometers.

Designed For Ease

The most dramatic feature of a Smart Accessory is its integration with the software and the spectrometer, bringing an unprecedented level of convenience and speed. When you place a Smart Accessory in the instrument, you are instantly ready to collect spectra. There is no need for manual or mechanical alignment of accessories and no need to constantly adjust data collection parameter files.

Automated Experiment Set-up

Like every smart component on a Nicolet FT-IR spectrometer, Smart Accessories are recognized by the system as soon as they are installed. When a Smart Accessory is placed in the spectrometer, an Experiment file containing the software and hardware parameters for that measurement is automatically loaded. The FT-IR system will set everything for you, so you are free to concentrate on your work.



Optimal, Reliable Performance

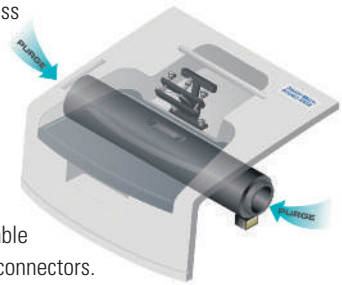
We pioneered Smart Accessories, the only FT-IR accessories that use permanently aligned optical systems. Permanent alignment means there are no time consuming adjustments necessary before you can collect spectra. With a Smart Accessory you can be confident that everything is positioned properly, making your results more reproducible and reliable.

Confidence Through Diagnostics

Once the experiment parameters are set, the system will run diagnostic tests to validate the performance of your spectrometer, giving you maximum confidence in your results. These tests save time and improve results by identifying common user errors such as improperly cleaning a previous sample from a transmission cell. They also proactively help in addressing problems to maximize productivity.

Automatic Purge

Smart Accessories are constructed around a central-sealed optics tube. If your bench is purged, the accessory will automatically be purged when it is inserted. Because the purged volume of a Smart Accessory is small, purge is achieved quickly. Over time, the small purge volume will also show less fluctuation than the relatively large volumes of a full-sized sample compartment – your results are much more reproducible.



In addition, the design eliminates the need for adjustable purge seals or separate purge connectors. Traditional accessories either do not have purge seals or require adjustments to seal the accessory.

Expertise When You Need It

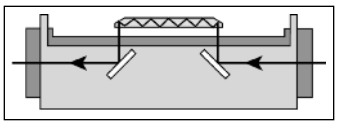
Multimedia on-line tutorials for our Thermo Scientific OMNIC software help you choose the right accessory for your application, show you how to use and care for your accessory, and demonstrate how to prepare a sample. OMNIC™ software can monitor your spectra as you collect them using spectral quality checks to look for common sampling mistakes, then prompt you with situation specific tips and tutorials that can sharpen your skills and improve your results.

How does it work?

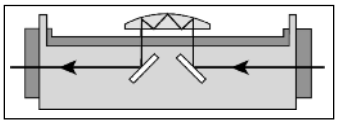
An Overview of Basic FT-IR Sampling Techniques

Attenuated Total Refection (ATR)

An attenuated total reflection accessory operates by measuring the changes that occur in a totally internally reflected infrared beam when the beam comes into contact with a sample. An infrared beam is directed onto an optically dense crystal with a high refractive index at a certain angle greater than the critical incident angle. The resulting internal reflectance creates an evanescent wave that extends beyond the surface of the crystal into the sample held in contact with the crystal. In regions of the infrared spectrum where the sample absorbs energy, the evanescent wave will be attenuated. The altered (attenuated) energy from each evanescent wave is passed back to the IR beam, which then exits the opposite end of the crystal and is directed at the detector in the IR spectrometer. The detector records the attenuated IR beam as an interferogram signal, which can then be used to generate an infrared spectrum.



Beam path for a multi-bounce ATR

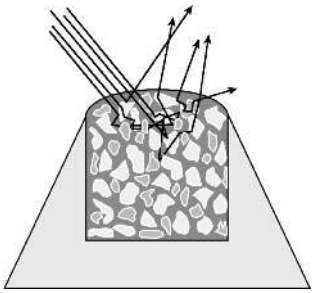


Beam path for a single-bounce ATR

Diffuse Reflectance (DR)

When an infrared beam is focused onto a particulate material, the incident beam can react with the particle in one of several ways. The radiation can be reflected off the top surface of a single particle or multiple particles without penetrating the particle, a process called specular reflectance. Diffuse reflectance results from the penetration of the incident radiation into one or more sample particles and subsequent scatter from the sample matrix.

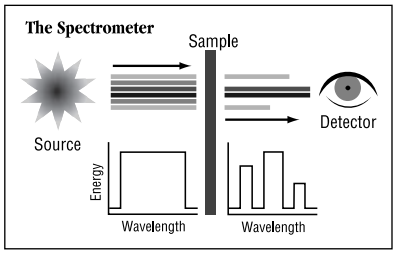
A diffuse reflectance accessory operates by directing the infrared energy into a sample cup filled with the neat solid powder or a mixture of the sample and an infrared transparent matrix (such as KBr). The infrared radiation then interacts with the particles causing the light to "diffuse" or scatter as it moves throughout the sample. The output mirror collects the diffusely scattered energy, which is directed to the detector in the spectrometer. The detector records the altered IR beam as an interferogram signal, which can then be used to generate a spectrum. Typically, a background is collected with the diffuse reflectance accessory in place and the cup filled with just the IR transparent matrix. Excellent quantitative data can be collected with proper sample preparation.



The IR beam interacting with a sample in a diffuse reflectance experiment

Transmission

The transmission technique does not require a separate accessory. The user simply places a sample within the sample compartment of an infrared spectrometer. The infrared beam passes through the sample and the energy that comes through the sample is measured to generate a spectrum. However, sample preparation is often necessary to ensure a thin uniform sample.



Conceptual diagram of a beam path

Specular Reflectance/Reflection-Absorption

Specular reflectance is a surface measurement technique that works on the principle of reflective efficiencies. This principle states that every sample has a refractive index that varies with the frequency of light to which it is exposed. Instead of examining the energy that passes through the sample, specular reflectance measures the energy that is reflected off the surface of a sample. By examining the frequency bands in which the rate of change in the refractive index is high, users can make assumptions regarding the absorbency of the sample. The specular reflectance technique provides excellent quantitative and qualitative data. Reflection-Absorption works on the same principle, but due to sample properties, some of the energy that passes through the surface layer is absorbed into the bulk of the sample and then reflects off of a substrate below the surface layer. A combination of specular reflectance and reflection-absorption can occur when criteria for both techniques are met. If a qualitative comparison of specular reflectance to transmission spectra is desired, users can apply the Kramers-Kronig correction to the data to remove the effects of dispersion.

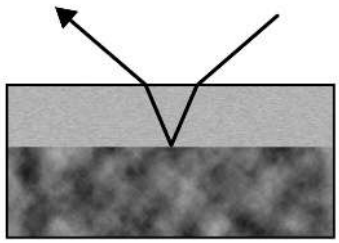


Diagram of Reflection-Absorption

Smart iTR

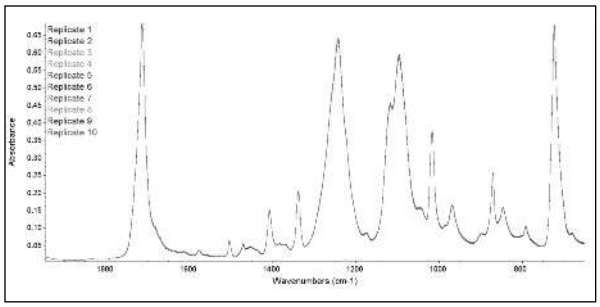
For Multi-purpose ATR Sampling

The Thermo Scientific Smart iTR is an ultra-high-performance, versatile Attenuated Total Reflectance (ATR) sampling accessory. Primarily designed for use with a single bounce diamond crystal, the Smart iTR™ also offers other options for full configurability. Each of the ATR crystals is designed for maximum infrared throughput and spectroscopic performance.

ATR is the technique of choice for infrared and the Smart iTR is the accessory of choice for Thermo Scientific spectrometers. It provides exceptional sensitivity and IR throughput. ATR crystals come in a variety of configurations suitable for every need. Solid materials can be pressed onto the ATR crystal using a high pressure tower to provide consistent results. Single bounce ATR works for many strongly absorbing materials like polymers, chemicals, etc.

Example Applications

- Most solids
- Liquids ranging from pH 1 to 14
- Acidic or alkaline materials
- Fibers
- Hard or oddly shaped samples
- Abrasive, caustic or corrosive materials
- Large or small samples
- Paint chips



Ten replicated PET spectra collected from different locations on the same sample using a Nicolet iS10 spectrometer with the Smart iTR

Unique Features

The Smart iTR is a versatile ATR for analysis of solids, liquids, pastes and gels. It is available with different crystal materials for different sampling needs. Single reflection ATR provides general purpose use, while an optional three reflection ATR can be used to optimize analysis of minor components. Crystal plates are pinned in place and easily switched with no alignment required. ATR crystal plates are backed with a ZnSe focusing optic for optimal performance. An optional specular plate gives extra flexibility when analyzing coatings on reflective materials.

The black top plate is over seven inches wide at the front, and more than five inches from front to back, providing excellent space for most samples. The plate is Teflon™ coated and lifts clear easily, making clean-up very simple. Precision machining and an unreactive-gasket provide a tight interface between the top plate and the crystal housing, so spills are not a problem. A quick-release mounting of the crystals provides rapid and reproducible crystal insertion and removal for cleaning or swapping.

The Smart iTR's high pressure clamp comes with interchangeable tips for hard, soft and pellet shaped samples. The clamp is calibrated to deliver over 10,000 psi of pressure when applied to the single reflection crystal plates.

The Smart iTR accessory is compatible with the Thermo Scientific Nicolet iS10, Nicolet iS50, Nicolet 6700, Nicolet 8700 FT-IR spectrometers and the Nicolet iZ™10 auxiliary module.

Choice of ATR Crystal Materials

The Smart iTR accessory can be ordered with three common ATR crystals fixed in stainless steel as standard: diamond, ZnSe and germanium. Each crystal performs strongly under specific circumstances.

The diamond crystal is excellent for the analysis of hard, abrasive, reactive, caustic or corrosive materials, since it is inert and robust. It is also a multi-purpose ATR with a depth of penetration of over 2 microns at 1000 cm^{-1} and is used with a wide variety of samples. Its disadvantage is the intrinsic absorbtion from approximately 2300 to 1800 cm^{-1}.

The ZnSe crystal offers similarly outstanding throughput and a depth of penetration similar to diamond. It can be used for a wide variety of samples, but over time it can be etched by acids and scratched by hard samples. ZnSe is soft and not as chemically inert as the other crystals, but provides an excellent performing, lower cost option for general analyses.

A five-year warranty is provided with the diamond ATR crystal. Both the diamond and ZnSe configurations can be validated.

Germanium is also hard and inert (although not as robust as diamond). Germanium provides a much shallower depth of penetration, making it ideal for highly absorbing or scattering samples such as carbon-black containing rubbers. The exclusive germanium crystal used in the Smart iTR provides huge performance through the mid-IR range, with upwards of 50% transmittance. Germanium has a limited range, but offers good chemical resistivity to both acids and bases.

An additional ATR crystal that can be added to any of the accessories is silicon. Silicon is a very hard ATR crystal with a high refractive index. This makes it useful for strong absorbers or abrasive samples. Silicon withstands thermal shock, so it is suitable for temperature studies. Silicon is typically absorbing below 1500 cm^{-1}, but the composite design results in a much broader range.

Specifications

Diamond ATR Crystal: Diamond is one of the most rugged optical materials available.

- Low wavenumber cutoff 650 cm^{-1} (due to ZnSe lens)
- Depth of penetration 2.03 micrometers at 1000 cm^{-1}
- Refractive index 2.4
- Useful pH range 1–14
- Incident angle 42

ZnSe ATR Crystal: ZnSe is the most common ATR crystal. It has limited uses with strong acids, alkalis. The surface can be scratched by hard materials, which will eventually reduce sensitivity. Complexing agents (EDTA and ammonium) will also attack the crystal surface.

- Low wavenumber cutoff 650 cm^{-1}
- Depth of penetration 2.03 micrometers at 1000 cm^{-1}
- Refractive index 2.4
- Useful pH range 5–9
- Incident angle 42

Germanium ATR Crystal: Ge is a hard ATR crystal with a high refractive index. This makes it useful for strong absorbers or samples with a high refractive index. The novel germanium design provides enormous through-put over an extended range.

- Low wavenumber cutoff 700 cm^{-1}
- Depth of penetration 0.67 micrometers at 1000 cm^{-1}
- Refractive index 4.0
- Useful pH range 1–14
- Incident angle 42

Silicon ATR Crystal: Si is a very hard ATR crystal with a high refractive index.

- Low wavenumber cutoff 700 cm^{-1}
- Depth of penetration 0.84 micrometers at 1000 cm^{-1}
- Refractive index 3.4
- Useful pH range 1–12
- Incident angle 42

Active Sample Area: The ATR active sample area is 1.5 mm for the single bounce ATR and 6 mm for the 3 bounce ATR.

Specular Plate: Spectral range dependent on spectrometer. Incident angle is 45 degrees.

Ordering Information

Accessory	Part Number
Smart iTR with Diamond Plate	222-247000
Smart iTR with ZnSe Plate	222-247100
Smart iTR with Diamond and Ge Plate	222-247200
Smart iTR with ZnSe and Ge Plate	222-247300

Check configuration guide or contact Thermo Fisher Scientific representative for additional options.