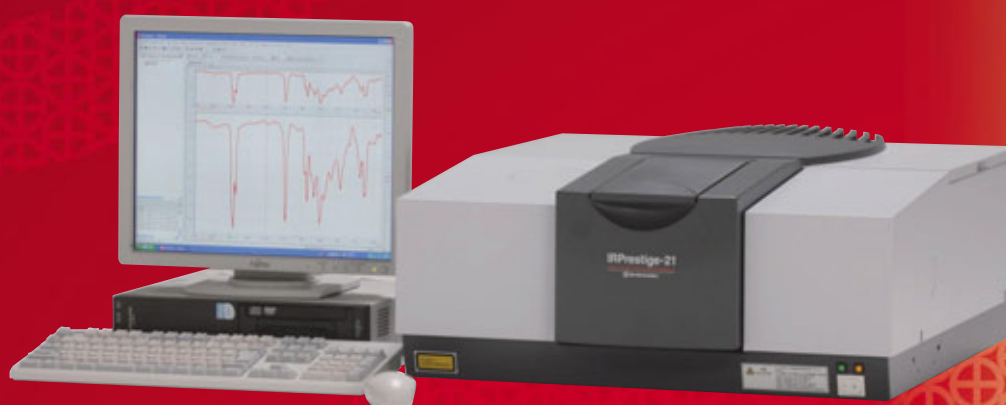


IRPrestige-21

Shimadzu
Fourier Transform
Infrared Spectrophotometer





Discover the NEW Worlds Opened
by the IRPrestige-21

IRPrestige-21

Shimadzu

Fourier Transform Infrared Spectrophotometer

IRPrestige-21 and IRsolution open up a new world for FTIR users.

High sensitivity and expanded functionality for leading-edge Research & Development

Easy software and Automatic Accessory Recognition for user-friendly operation

ADA (Advanced Dynamic Alignment) for optical system reliability

Status Monitoring and Validation Program

Near IR/Middle IR/Far IR

Wide variety of Accessories for a large range of applications

Powerful software - IRsolution - to enhance performance

Depending on the environment, the electric power consumption while measuring is reduced 25% (NOTE 1).

IRPrestige-21 and IRsolution open up a new world for FTIR users



Sensitivity

- High Signal-to-Noise Ratio; 40,000:1 or better (NOTE 2)
- High-Energy Ceramic Light Source
- High-Throughput Optics
- High-Sensitivity DLATGS Detector



Reliability

- Advanced Dynamic Alignment (Patent Pending)
- Sealed and Desiccated Interferometer
- Self Diagnostics & Status Monitoring
- JP/EP/ASTM Validation



Accessories

- NIR/MIR/FIR
- Automatic Accessory Recognition-QuickStart Accessories
- 3 Detector Selections for Various Applications
- Wide Variety of Accessories and a High-Performance IR Microscope



Software

- 32bit Windows-based IRsolution
- High Performance and Easy Operation
- Audit Trail
- FDA 21 CFR Part 11 Compliance (NOTE 3)

Contents

P 04 - Sensitivity

P 14 - NIR Accessories

P 20 - Analysis Support Programs

P 06 - Reliability

P 16 - IRsolution

P 22 - Specifications

P 08 - Expandability

(NOTE 1) Comparison with the previous Shimadzu FTIR.

(NOTE 2) 4 cm⁻¹ resolution, 1-minute accumulation, around 2,100 cm⁻¹, peak-to-peak,

(NOTE 3) IRsolution Agent software is needed to fully comply to FDA 21 CFR Part 11 regulation.

Sensitivity

Infrared spectroscopy has traditionally been used in a wide variety of applications, such as general organic chemistry, polymer science,

pharmaceuticals, and food. FTIR is now being applied in industries such as semiconductors, optical components, and electronic devices.

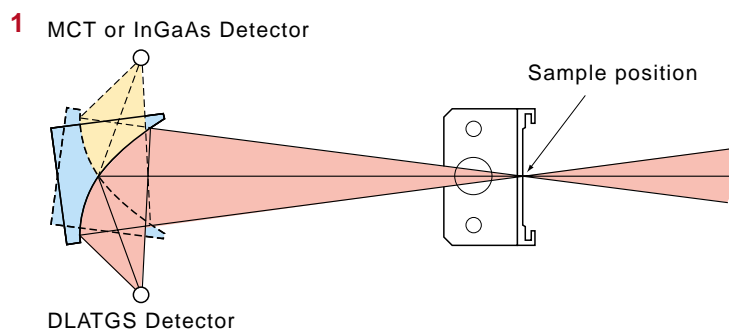
For High Sensitivity

The IRPrestige-21 uses a bright ceramic light source, high-sensitivity DLATGS detector, and high-throughput optical elements. Optimization of Optical/Electronics/Signal systems minimizes noise and maximizes the S/N ratio (40,000:1 and better)^(NOTE 1).



High-Sensitivity DLATGS Detector

IRPrestige-21 includes a high-sensitivity DLATGS (Deuterated triglycine sulfate doped with L-alanine) detector. The environment of the detection element is controlled to keep it at a specified temperature. These conditions in the IRPrestige-21 result in high sensitivity and stability^(NOTE 2).



(NOTE 1) 4 cm^{-1} resolution, 1-minute accumulation, around 2,100 cm^{-1} , peak-to-peak

(NOTE 2) Optional InGaAs detector is used for Near IR analysis. Optional MCT detector is used for small samples, dark samples, folding long path gas cell, etc. Either the InGaAs or MCT detector can be mounted on the IRPrestige with the standard DLATGS detector, but the InGaAs and MCT detectors can not be mounted on the IRPrestige at the same time.

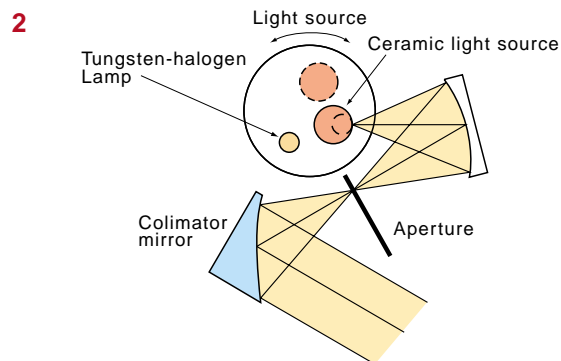
Very high sensitivity is required to analyze the thin layers or the small impurities that cause concerns in these fields. The over

40,000:1^(NOTE 1)S/N ratio of the IRPrestige-21 assists in your high-sensitivity analysis.

Bright Ceramic Light Source

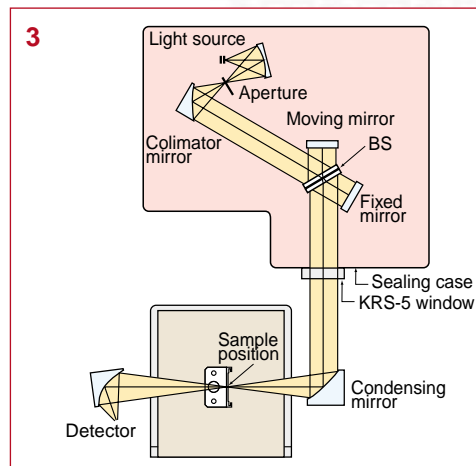
IRPrestige-21 includes a bright ceramic light source that is air cooled. This high-energy source does not require any special attachments and is extremely stable. The ceramic source is guaranteed for 3 years.

(NOTE) An optional Tungsten lamp is used for Near IR analysis.

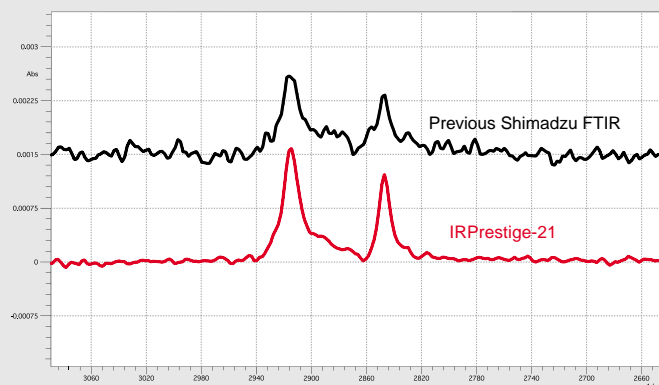


High-Energy Throughput Optical Elements

IRPrestige-21 uses high-energy throughput optical elements, such as Gold mirrors. The high-precision optics decrease energy loss in the optical path and result in increased energy at the sample. The Gold mirrors used in the IRPrestige-21 have 98% reflectance compared to the 95% reflectance of traditional Aluminum mirrors. Interferometers with Gold mirrors have greater energy throughput than those with Aluminum mirrors. The 3% reflectance difference is intensified with the number of mirrors used in the FTIR.



Application Data



Infrared Spectrum of LB Membrane on a Gold Mirror

Sample: Mono-layer of stearic acid
(around 2.5nm thickness)

Accessory: 80° Grazing angle accessory
(FT-80)

The infrared spectrum of LB membrane on the gold mirror was measured on both IRPrestige-21 and a previous Shimadzu FTIR under the same conditions. The better infrared spectrum is obtained with the high-sensitive IRPrestige-21.

Software to Support Reliability

IRPrestige-21 has many hardware and software features that improve reliability. Measurement conditions of the IRPrestige-21

are constantly monitored and reported at anytime.

Validation Program and Reporting

IRPrestige-21 comes standard with a validation program that complies with Japanese/European Pharmacopoeia and ASTM (American Society for Testing and Materials). This validation program checks the performance of the IRPrestige-21 using a polystyrene film and creates a report upon completion.

- Shape and Intensity of Power spectrum
- Measurement of Polystyrene film spectrum
 - Resolution
 - Wavenumber Accuracy
 - Wavenumber Reproducibility
 - Transmittance Reproducibility

Test Items for ASTM (ASTM1421 Level Zero)

- Energy Test by Power spectrum
- 100%T Line Test
- Polystyrene Film Test

SHIMADZU IRPrestige-21 Series Validation Report

Instrument : IRPrestige-21 Overall Judgment : PASS
 Serial No. : Temperature : 25°C
 Sample name : Polystyrene Relative Humidity : 60%
 Inspected by : Shimadzu Date/Time : 2002-09-18/14:48:47

Approved by : Date :

| 1. Power spectrum | | | | PASS |
|-------------------|----------|----------|--|------|
| Wavenumber | Measured | Standard | | |
| 4000.0 | 14.5 | 7.4 | | PASS |
| 4000.0 | 34.4 | 22.1 | | PASS |
| 3000.0 | 60.8 | 44.3 | | PASS |
| at Maximum | 73.8 | 60.0 | | PASS |
| 700.0 | 22.1 | 7.4 | | PASS |
| 500.0 | 8.3 | 1.5 | | PASS |
| 400.0 | 2.4 | 0.4 | | PASS |

| 2. Resolution | | | | PASS |
|-----------------|----------|----------|------|------|
| Wavenumber | Measured | Standard | | |
| 2570.0 | 2849.9 | 36.3 | | |
| 2551.0 | 2849.6 | 6.4 | | |
| Peak depth(1/2) | | 25.9 | 18.0 | PASS |
| 1589.0 | 1586.3 | 52.7 | | |
| 1583.0 | 1582.5 | 33.2 | | |
| Peak depth(1/2) | | 19.5 | 12.0 | PASS |

| 3. Wavenumber accuracy | | | | PASS |
|------------------------|----------|-------|-----------|------|
| Wavenumber | Measured | Error | Tolerance | |
| 3000.0 | 3000.9 | -1 | ± 1.5 | PASS |
| 2549.5 | 2549.6 | -1 | ± 1.5 | PASS |
| 1942.9 | 1943.2 | -3 | ± 1.5 | PASS |
| 1601.2 | 1600.8 | -4 | ± 1.0 | PASS |
| 1582.0 | 1582.5 | -5 | ± 1.0 | PASS |
| 1154.5 | 1154.3 | -2 | ± 1.0 | PASS |
| 1029.3 | 1029.0 | -3 | ± 1.0 | PASS |

| 4. Reproducibility of Wavenumber | | | | PASS |
|----------------------------------|--------|--------|-------|-----------|
| Wavenumber | No. 1 | No. 2 | Error | Tolerance |
| 2850.7 | 2849.6 | 2849.6 | 0.00 | ± 0.5 |
| 1601.4 | 1600.8 | 1600.8 | 0.00 | ± 1.0 |
| 1154.5 | 1154.3 | 1154.3 | 0.00 | ± 1.0 |

| 5. Reproducibility of Transmittance | | | | PASS |
|-------------------------------------|-------|-------|-------|-----------|
| Wavenumber | No. 1 | No. 2 | Error | Tolerance |
| 2850.7 | 9.4 | 9.4 | 0.0 | ± 0.5 |
| 1601.4 | 4.6 | 4.6 | 0.0 | ± 0.5 |
| 1154.5 | 42.8 | 42.8 | 0.0 | ± 0.5 |

Self Diagnostics and Status Monitoring

The self-diagnostics of the IRPrestige-21 at initialization check for optimal conditions of the Electronics, Optical, and Signal systems. If the interferometer conditions are not good, alignment is automatically performed with the ADA (Advanced Dynamic Alignment) system.

A status monitor consistently checks the condition of the light source and He-Ne laser. The system also monitors the switching of beam splitters, sets optimum scan parameters, and switches the light source and detector setting. When a QuickStart accessory is installed in the sample compartment, the status monitor recognizes it, and sets the optimum scan parameters(NOTE). The results of the self diagnostics and status monitoring are recorded onto a log file.

The light source is guaranteed for 3 years and the He-Ne laser is guaranteed for 30 months.

The light source and the beam splitter are user-replaceable parts.

(NOTE) Only when the Auto Recognized Accessories (QuickStart series) are installed.



Easy Maintenance Hardware to Enhance Reliability

The interferometer is one of the most important parts of the FTIR. For accurate data collection, the interferometer must scan with high precision. The IRPrestige-21 includes the Patented FJS system which scans the moving mirror with a smooth and stable mechanism. The optimization and stabilization of the

IRPrestige-21 interferometer by the Advanced Dynamic Alignment (ADA; Patent pending) system ensures consistent and repeatable results. Since the beam splitter within the interferometer is susceptible to moisture, the optical system of the IRPrestige-21 is sealed and desiccated.

FJS System & Advanced Dynamic Alignment

Highly precise control of the moving mirror is required to stabilize the interferogram of the FTIR instrument.

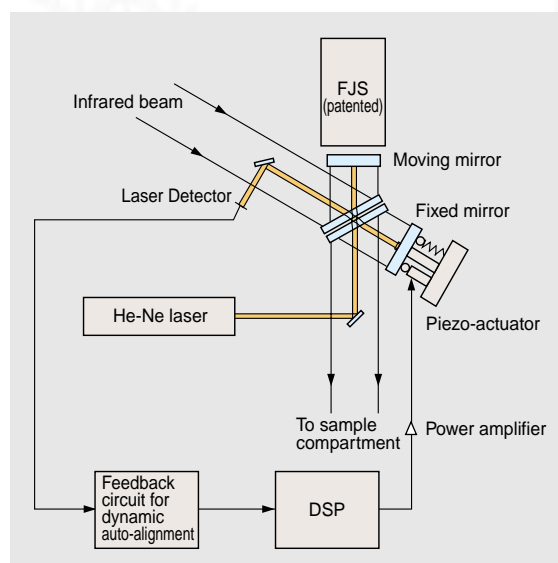
The IRPrestige-21 includes the patented FJS system - very smooth and precise moving mirror unit - and the Advanced Dynamic Alignment (ADA; Patent pending) system to optimize and stabilize the interferometer unit.

IRPrestige-21 requires only a short stabilization time and is very secure.

The ADA system automatically aligns the interferometer when the beam splitter is replaced.

Advanced Dynamic Alignment (Patent pending)

This system monitors the interferometer condition of the He-Ne laser and compares it with that of optimized conditions. Any detected discrepancies by the DSP system are corrected by automatic alignment of the piezo actuators at the fixed mirror.

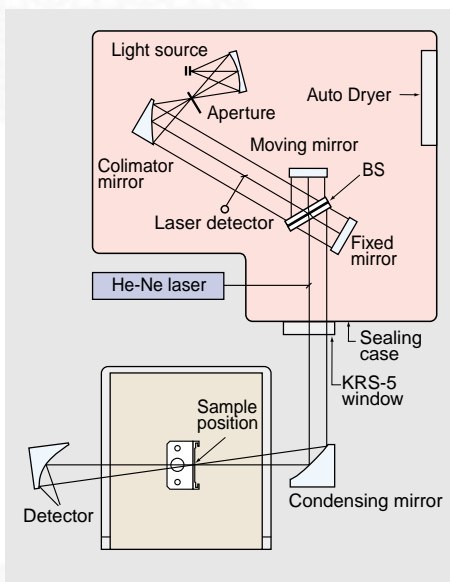


Desiccated Interferometer & Atmosphere Correction

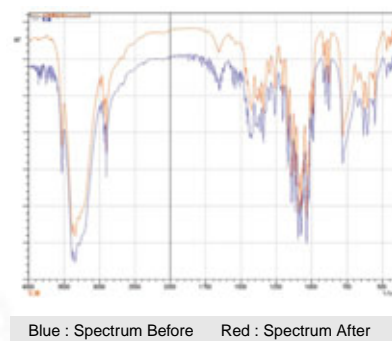
The interferometer is one of the most important parts of the FTIR. The IRPrestige-21 has 3 features to stabilize the interferometer and to protect the beam splitter.

1. Sealed optical system to create closed environment
2. Desiccated interferometer to remove moisture by the Auto Dryer (Patent pending)
3. Anti-Humidity Beam Splitter coating to provide extra protection

The Atmosphere Correction Function easily compensates for the influences of water vapor and carbon dioxide on your data. You can easily get beautiful spectra with the IRPrestige-21 even if the sample has peaks which overlap with water vapor around $2100\text{-}1300\text{ cm}^{-1}$ or $4000\text{-}3100\text{ cm}^{-1}$.



Elimination of influences of CO₂ and H₂O by Atmosphere Correction



Expandability

Near IR/Middle IR/Far IR

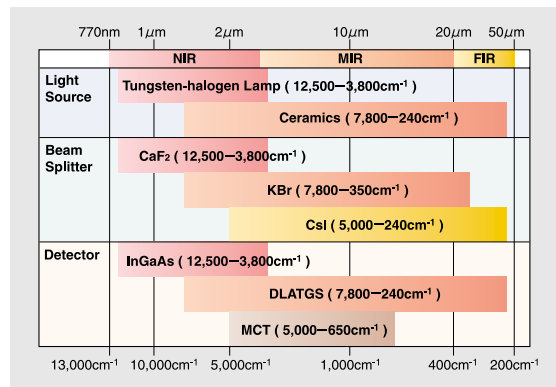
Not just a standard Middle Infrared range instrument, the IRPrestige-21 can measure Near Infrared or Far Infrared spectra with the simple exchange of an optional light source, beam splitter and detector.

In the Near IR region, harmonics of the Middle IR region peaks of organic materials exist. Glass and plastic exhibit low absorbance in the Near IR region, so samples contained in a glass or plastic container can be directly measured. Some samples can be measured directly in the Near IR region without dilution with KBr powder.

In the Far IR region, inorganic materials such as the Oxides and Halides of Metals exhibit peaks.

The changeable light source and detector can be easily selected in IRsolution software. The beam splitter can be exchanged easily by the user.

When changing the light source, beam splitter and detector, the optimum measurement parameters are automatically set. Of course, the changes are displayed in status monitor and recorded in the log file.



Scan Wavenumber with options

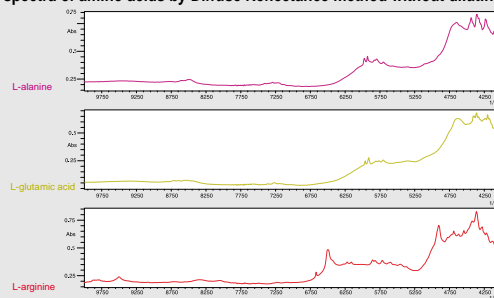


Application of Near IR

IRPrestige-21 uses an InGaAs detector (option) as a high-sensitivity Near IR detector.

Samples are analyzed without diluting by KBr.

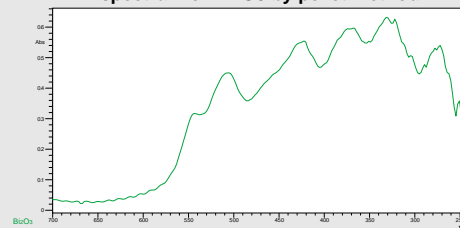
NIR spectra of amino acids by Diffuse Reflectance method without diluting by KBr



Application of Far IR

IRPrestige-21 with a CsI beam splitter can obtain high-quality spectra under 400 cm⁻¹. Inorganic materials such as Oxides and Halides of Metals have peaks in the FIR region.

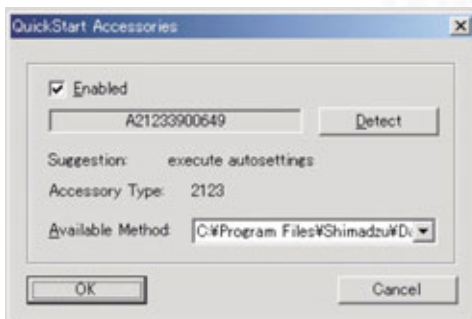
FIR spectrum of Bi₂O₃ by pellet method



Automatic Accessory Recognition

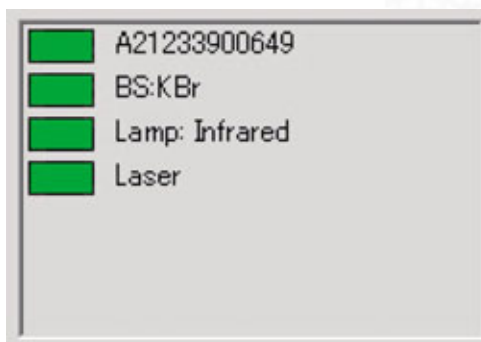
The IRPrestige-21 can recognize when QuickStart accessories are mounted in the sample compartment.

When the QuickStart accessory is installed, IRPrestige-21 automatically recognizes the accessory type and ID number. Optimum scan parameters for the accessory are automatically set.



When the QuickStart accessory is installed, IRsolution displays the type and ID number on the screen.

This information is displayed on the Status Monitor and is recorded in the log file.



The IRPrestige-21 sets the optimum scan parameters for the selected accessory.

Automatic recognition of the following accessories is available. These accessories may be used with other Shimadzu FTIR spectrometers. The IRPrestige-21 can also use other accessories without the auto-recognition feature, by manually configuring the method prior to measurement.

QuickStart Accessories

ATR Accessories

ATR-8000A
ATR-8200HA
MIRacle A
DuraSampl IR II A

Diffuse Reflectance Accessories

DRS-8000A

Reflectance Accessories

SRM-8000A
RAS-8000A

Expandability

The IRPrestige-21 may be easily customized into an application-specific measuring system using a wide variety of available accessories, such as the AIM-8800

IR microscope. These sampling accessories are available from Shimadzu Corporation and Shimadzu Partner companies, ensuring that users' needs are met.

For liquid samples

For measuring liquid samples, demountable or sealed liquid cells may be used. Additionally, the ATR (Attenuated Total Reflectance) accessories are also convenient. To measure liquids with ATR, sample preparation is as simple as dispensing the liquid onto the prism of the accessory.

The ATR correction program in the IRsolution software converts the measured ATR spectrum into a normal transmittance measurement by correcting for depth penetration differences.



ATR-8200HA (P/N 208-97240-91)

Liquid sample trough and solids flat plate prisms are available to conveniently accommodate a range of liquid, solid and film samples. The ZnSe prism is standard in most accessories. A Ge prism is available for high refractive index samples such as black rubber.

Both the ZnSe prism and the Ge prism are water resistant, so even aqueous solutions can be easily and conveniently measured.



MIRacle A (ZnSe : P/N 208-97247-95
Ge : P/N 208-97247-96)

Single-bounce ATR with a 2mm diameter prism. This accessory is suitable for liquids, solids, powders, films, and a variety of other sample types. The ZnSe prism is standard. A Ge prism is available for high refractive index samples.

For powder samples

For measuring powder samples, conventional KBr pellet methods may be used. The diffuse reflectance method is also convenient and requires less sample preparation. In the diffuse reflectance method, the sample is mixed with KBr powder and then measured; there is no need for making a pellet. Single-bounce ATR accessories may also be used for powder samples in some cases.



DRS-8000A (P/N 206-62301-91)

Sample is mixed with KBr powder, placed in a sample cup and measured.

With the Kubelka-Munk conversion in IRsolution software, the diffuse reflected spectra can be converted into transmission spectra for comparison purposes.

For gases

Various gas cells are available for gas sample measurement. The path length is selected according to the concentration of the gas. Various path length cells are available ranging from 5 cm to 20 m.

- 5 cm gas cell P/N 202-32006-30 (KRS-5 window plate)



5 cm gas cell



10 m gas cell

Automated accessories may be combined with IRsolution software to provide an automatic measuring system with high-throughput capability.

The IRPrestige-21 is a total lab solution for your FTIR measurement requirements.

For solid samples, films, cast resins

The transmission method is effective for film samples up to 100µm thick. For films thicker than 100µm, multi layer film and cast resins, ATR (Attenuated Total Reflectance) is recommended. Samples are clamped to the prism to ensure contact. With the ATR method, a spectrum is taken through a depth of a few µm within the sample. For samples with high refractive indices, the Ge prism is suitable. For hard samples, the diamond prism is preferred. With ATR correction available within IRsolution software, ATR spectra are converted into normal transmittance spectra. Another method for these sample types involves scratching the surface of the sample and measuring with a diffuse reflectance accessory.



ATR-8000A (P/N 206-62303-91)

This accessory can measure film samples clamped firmly on one or both sides of the prism. A large contact area results in good sensitivity. The KRS-5 prism is standard; a Ge prism is also available for samples with a high refractive index. The incident angle on the sample is switchable between 30/45/60°, allowing for accumulation of spectra at different depths.



ATR-8200HA (P/N 208-97240-91)

Liquid sample trough and solids flat plate prisms are available to conveniently accommodate a range of liquid, solid and film samples. The ZnSe prism is standard in most accessories. A Ge prism is available for high refractive index samples. The measuring light is reflected through the prism 10 times. The sample is clamped firmly to the prism to ensure contact with an attached clamp and easily adjust clamp pressure.

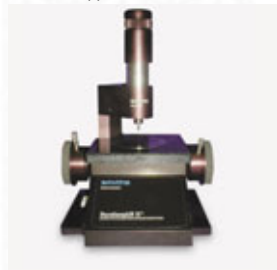


MIRacle A (ZnSe : P/N 208-97247-95) (Ge : P/N 208-97247-96)

Single-bounce ATR with a 2mm diameter prism. This accessory is suitable for liquids, solids, powders, films, and a variety of other sample types. The ZnSe prism is standard. A Ge prism is available for high refractive index samples. The sample can be easily clamped to the prism with the attached clamp, and the pressure can be adjusted. For hard samples, the Diamond MIRacle with a diamond prism is available.

DuraSamplIR II A System I DuraSamplIR II A System I DuraSamplIR II A System H (With Pressure Sensor)

(ZnSe support: P/N 208-92143-11) (ZnSe support: P/N 208-92144-11) (ZnSe support: P/N 208-92145-11)
(KRS-5 support: P/N 208-92143-12) (KRS-5 support: P/N 208-92144-12) (KRS-5 support: P/N 208-92145-12)



Single-bounce ATR with a 2mm diameter diamond prism. This accessory is good for measuring hard samples that may damage other prism types. It is also suitable for liquids, solids, powders, films, and a variety of other sample types. The System I (High Pressure Device Type) allows the sample to contact the prism easily with the attached clamp, and the pressure can be adjusted. The system with a pressure sensor is also available. The System H (ViewIR Type) allows the sample to be visually observed while clamping.



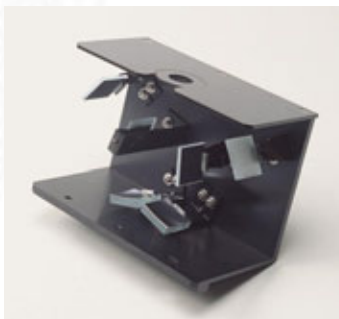
SiC Sampler (P/N 200-66750)

This sample preparation accessory has SiC emery paper that is used to scratch the sample of interest. The powder of the sample on the emery paper is directly analyzed with a Diffuse Reflectance Accessory.

Expandability

For coating films on metals or resins

For coatings, reflectance is the measurement method of choice. Selection of either the specular reflection or reflection absorption method is dependent on the thickness of the coating sample.



SRM-8000A (P/N 206-62304-91)

Specular reflectance accessory with 10° reflection. Samples are placed on the top of the accessory with the measurement side down. Analysis of μm thick thin films is possible.

The specular reflectance spectra can be converted into a transmittance spectra with Kramers-Kronig conversion in IRsolution software.



RAS-8000A (P/N 206-62302-91)

Reflection absorption spectroscopy method accessory with a 70° or 75° reflection angle. Analysis of nm thick thin films is possible. The optional GPR-8000 polarizer allows for higher sensitivity measurement.

When a polarized light beam is incident on a metal substrate, the phase of the light is changed. In vertical polarization, the vectors of the polarized light are opposite to each other, and hence no stationary waves are produced. In parallel polarization, the vectors of the polarized light meet at the point to produce stationary waves, which enhances the sensitivity of the measurement.

Accessory for automated analysis

These accessories may be combined with IRsolution for an automated analysis system.



ASC-8000T (P/N 206-63900)

ASC-8000T is an auto sample changer for performing transmission measurements on up to 18 samples. The holder is designed for 13mm diameter KBr pellets; an optional film holder or cell plates for Nujol mulls are also available.

The ASC-8000T can be easily controlled by IRsolution software.



DRS-8010ASC (P/N 206-62308)

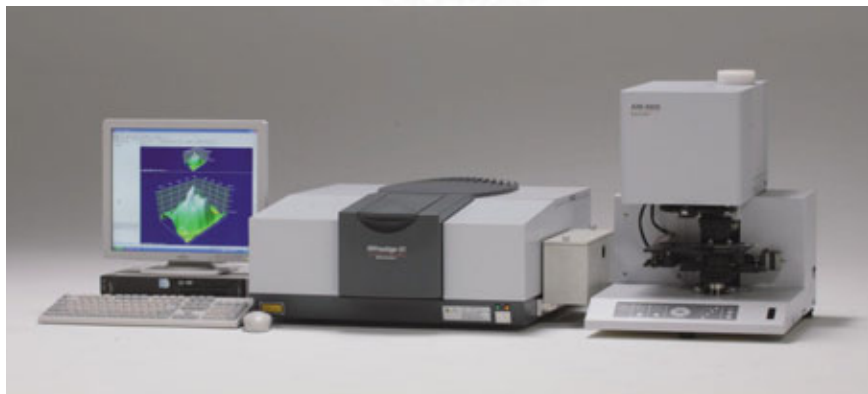
DRS-8010ASC is an automatic diffuse reflectance accessory. The DRS-8010ASC accepts up to 24 samples. The DRS-8010ASC can be easily controlled by IRsolution software.

For small samples

If the sample size is between 2 and 3 mm, a single-bounce ATR accessory such as the MIRacle or DuraSampleIR may be used for analysis. For samples between 10µm and 2mm, the FTIR microscope is the preferred method for analysis. The FTIR microscope may be operated in many measuring modes including transmission, reflectance and ATR. This versatility enables the accurate and complete analysis of small samples in various forms.



AIMView



IR Microscope AIM-8800 (P/N 206-72500-□□)

AIM-8800 is an FTIR microscope that is installed to the side of the IRPrestige-21. This infrared microscope features optimized optics and a state-of-the-art MCT detector, enabling high-sensitivity detection of micro samples. In addition, advanced functions, such as auto aperture setting and auto focusing, greatly simplify the analysis of micro samples.

Simple switching from internal measurement with the IRPrestige-21 to microscopic analysis is possible within IRsolution software.

Features

- Optimized high-throughput optical system, employing a state-of-the-art MCT detector for high-sensitivity analysis.
- Auto aperture, auto centering and auto X-Y stage functions simplify determination of the desired analysis location.
- Auto focus brings image into clear focus with a single mouse click.
- Up to 10 sample positions and 2 background measurement positions can be stored in memory with aperture settings.
- Stage movement, aperture setting and focusing, as well as switching between transmission / reflection and measurement / observation modes are all performed via the AIMView software.
- Control functions are also possible using the microscope's front panel keyboard.



ATR Objective ATR-8800M (Slide-On type) (P/N 206-70450-91)

An optional objective that may be used in the AIM-8800 for ATR measurement. The single-bounce ATR objective uses a semicircular Ge prism for analysis.

The prism is a slide type that permits easy switching between the visual observation and IR measurement modes.

Shimadzu Partners

The IRPrestige-21 enhances the flexibility of FTIR measurement via compatibility with a wide range of accessories. These include Shimadzu accessories as well as unique accessories and software from Shimadzu partners. Please refer to the Shimadzu FTIR Accessory Hand Book or contact your Shimadzu representative.

Shimadzu Partners in the World

Hardware and Accessories

- Harrick Scientific
- Infrared Analysis
- Pike Technologies
- SensIR Technologies
- Specac
- ST Japan

Software

- Bio-Rad - Sadtler

Accessories for Near Infrared Measurement

Accessories are available for easier and higher-sensitivity near IR measurement of a wide range of samples.

Each accessory is equipped with the Automatic Accessory Recognition function.

In the near IR region, absorption due to molecular vibration appears. Therefore, substances can be identified by comparing spectral patterns, and quantitatively determined from the peak intensity. Absorbance is lower in the near IR region than in the

Powder Samples



Upward-looking Diffuse Reflectance Accessory UpIR A (P/N 208-97271-91)

- Powder samples can be placed on the sample stage for measurement.
- Pretreatment such as KBr dilution is unnecessary.
- Powders can be measured directly. Alternatively, directly set the sample contained in a vinyl bag or glass bottle.
- Applications include qualitative or verification tests in acceptance inspections and quantitative analysis of powders.

Main Specifications

Measurement range : 10,000 to 3,800 cm^{-1}
Accessory Recognition function : Yes

Powders, Tablets, Paste or Pellet Samples



Near IR Integrating Sphere IntegratIR A (P/N 208-97272-91)

- Powders, tablets, liquids, paste, fibers, plastic pellets and molded samples can be placed on the sample stage for measurement (reflectance measurement).
- Pretreatment such as KBr dilution is unnecessary.
- Samples contained in a vinyl bag or glass bottle can be measured.
- Applications include qualitative or verification tests in acceptance inspections and quantitative analysis.
- A highly sensitive InGaAs detector is built-in.
- The IntegratIR installation kit (P/N 206-72715-91) must be purchased separately.

Main Specifications

Measurement range : 10,000 to 3,800 cm^{-1}
Accessory Recognition function : Yes

Differences between UpIR A and IntegratIR A

The UpIR A and IntegratIR A differ in the following aspects. Choose the accessory which suits your needs.

Advantages of the IntegratIR A

1. Peak intensities are several times higher than the UpIR A, so spectra with higher S/N ratios can be obtained.
2. High-quality data can be obtained for powder samples contained in plastic bags.
3. Pellets, paste, tablets, liquids and fabrics can be measured.

Advantages of the UpIR A

1. Lower cost
2. Specifically suited for powder samples.

mid IR region, so samples can be measured without dilution. The IRPrestige-21, which employs the Fourier transform method and offers spectra with high wavelength precision, is optimal for identifying substances by comparing spectral patterns. Samples

contained in glass or thin plastic containers can be measured directly. It is also possible to analyze a sample using a probe. Thus, sample pretreatment is easy. The near IR measurement is also suitable for measuring samples that cannot be easily unpacked.

Other



Fiber Coupler (P/N 206-72751-91)

- This is an interface for attaching a near IR optical fiber to the IRPrestige-21.
- By using a near IR optical fiber probe, samples can be measured without being placed in the sample compartment or an accessory container.
- The fiber coupler comes with two SMA connectors. Various fiber probes with SMA connectors can be connected.
- The fiber coupler and fiber probe are separate items. Please purchase both of them.
- Contact Shimadzu if using a fiber probe other than the product introduced below.

Main Specifications

Connector shape : 2 x SMA
Accessory Recognition function : Yes



Reflective Fiber Probe (P/N 206-72760-91)

- Near IR rays emitted from the probe head are directed to the sample, and the reflected light is collected for measurement.
- Pretreatment such as KBr dilution is unnecessary.
- Just insert the probe into the sample powders, or samples can be analyzed while they are contained in bags or glass bottles.

Main Specifications

Measurement range : 10,000 to 3,800 cm^{-1}
Connector shape : 2 x SMA
Probe shape : Probe head 6.4 mm dia. x 50 mm, SUS303
Handle 18 mm dia. x 100 mm, aluminum
Operating temperature : Room temperature
Permissible bending radius : 100 mm
Length : 1 m from the probe head to connector

Liquid Samples



Heating Transmission Cell Set (P/N 206-72716-91)

- Liquid samples contained in the supplied 6-mm diameter test tube can be measured while they are being heated, or maintained at a constant temperature.
- Applications include multi-component quantitative analysis of liquid samples and tracing reactions and changes in the sample under heating.
- The temperature can be set from room temperature to 120°C.
- The set comprises a transmission cell for measurement under heating and a temperature controller.

Main Specifications

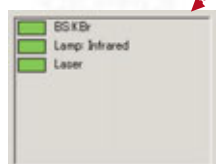
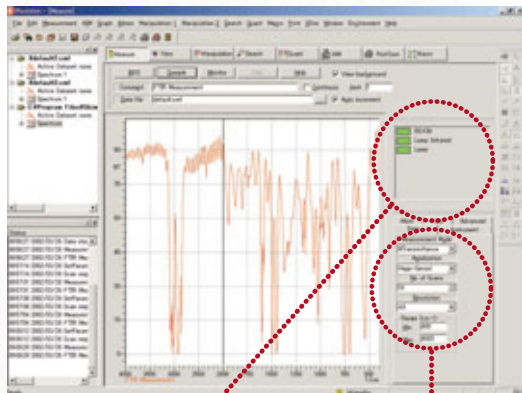
Measurement range : 12,500 to 3,800 cm^{-1}
Accessory Recognition function : Yes
Temperature range : Room temperature to 120°C (heater temperature)
Applicable test tube : 6 mm dia. x 50 mm
Output : 5A Max.
Power supply : 120/220 V selectable

IRsolution

IRsolution software provides Windows-based 32bit software control for the IRPrestige-21. With IRsolution, operations for FTIR analysis can be performed easily and quickly using dedicated analysis screens.

- Spectrum measurement
- Data display and comparison to other spectra
- Data processing, quantitation and spectral searching
- Report generation

Measurements and Status Monitor



Status Monitor



In the measurement menu of IRsolution, all measurement start buttons and dialogs to set the analysis parameters are integrated for easy operation. All measurement parameters are arranged into five dialog screens that are easily viewed.

One click will start the analysis. During measurement, a real-time spectrum is displayed on screen.

The hardware settings, including selection of light source, beam splitter, detector and accessories, are displayed on the status monitor screen.

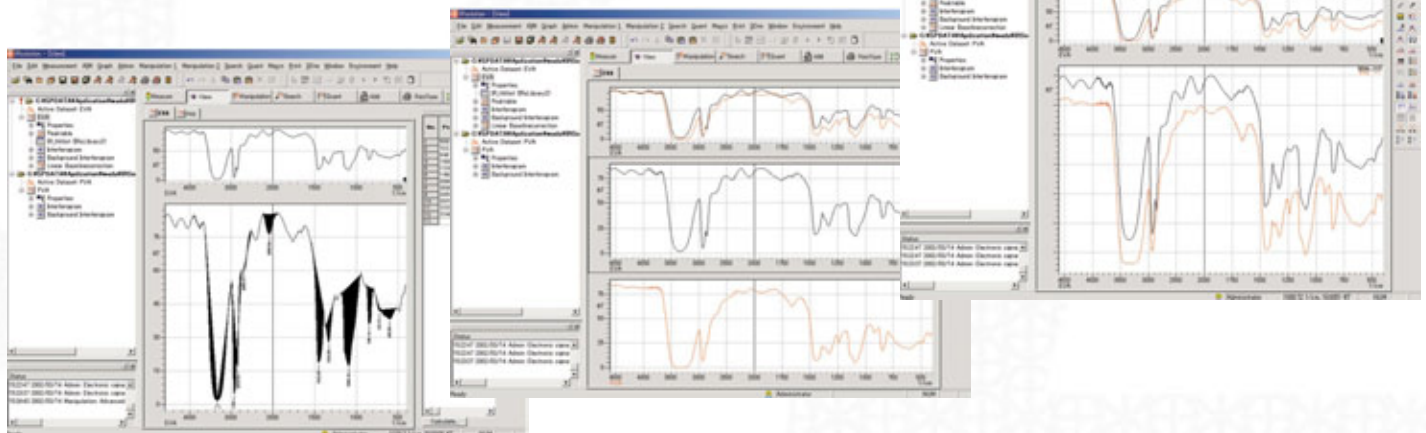
Optimum measurement parameters are automatically determined according to the hardware settings.

In addition to the normal accumulation mode, the IRPrestige-21 includes:

- Evaluation Scan which accumulates only normal data.
- Continuous Scan which continuously measures data.
- Atmosphere Correction Scan which eliminates the effects of CO₂ or H₂O on the data.

View Mode

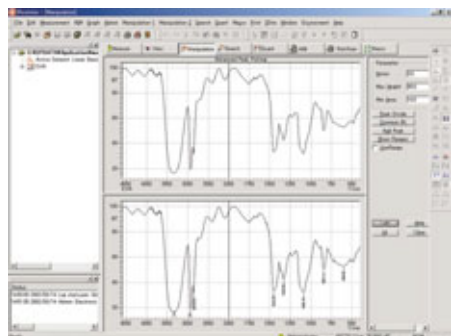
After the data is acquired, you can use the View Mode to zoom in on certain areas or compare with other spectra.



As the operation progresses, IRsolution software automatically advances into the optimum mode. Optional software modules, such as PLS quantitation and macro-programming, are available for increased versatility.

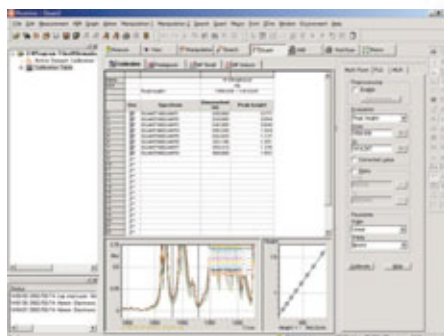
Comprehensive Help functions support the operation of the software.

Data Processing, Quantitation and Search



Peak detection

After the data acquisition has been completed, you can extract a variety of specific information from the measured spectrum. IRsolution software has many functions ranging from Peak detection, Spectral subtraction, Kubelka-Munk conversion and ATR correction to optional Spectrum searching and Quantitation. The results of data processing can be imported into Word Processing and Spreadsheet software applications.



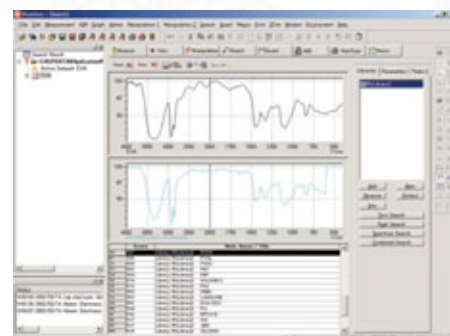
Quantitation

• Quantitation

In addition to multi-point calibration curve methods, IRsolution software offers MLR (Multi Linear Regression) and optional PLS (Partial Least Squares) analysis that is useful for Near IR measurements.

• Spectrum Search

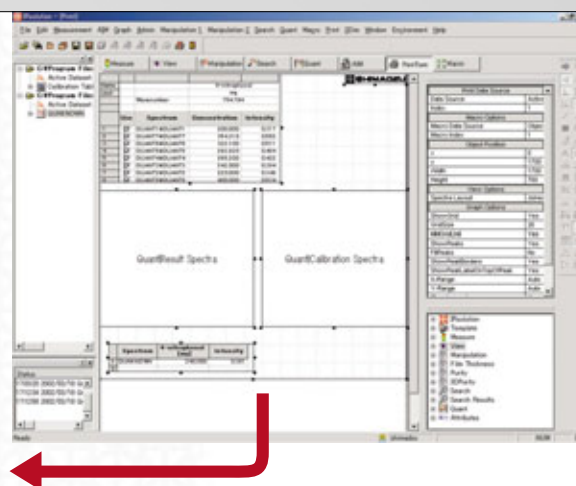
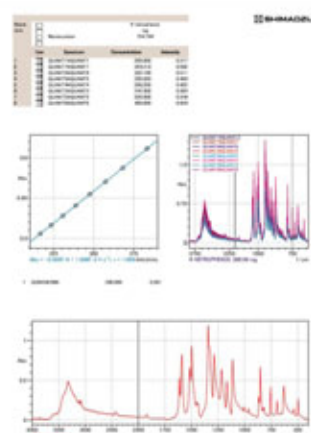
IRsolution software allows the creation of user libraries from acquired spectra, and spectral searching of user and commercial libraries.



Spectral Searching

Report Generator

Data is not useful unless you can get the results in the desired format. IRsolution software includes a powerful report generator with customized layout features. With the Report Generator, you can create reusable print templates using any data including the spectrum, calibration curve, quantitation results and peak pick tables. You can set the thickness and color of the graph lines as well as the font size. Annotations may be attached on the graph to comment on the results. The print layout can be saved as a template file for later use, ensuring accurate repeat reporting.



IRsolution

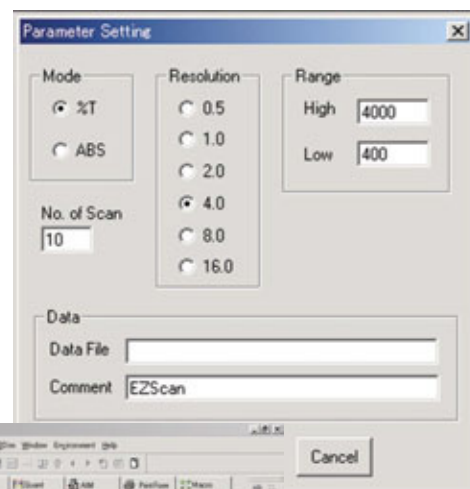
The versatility of IRsolution makes it perfect for use in high-level research and development areas. The simplicity of the software makes it perfect for

routine work within QA/QC departments or educational institutions, where operation is limited to certain functions. In either case, procedures can

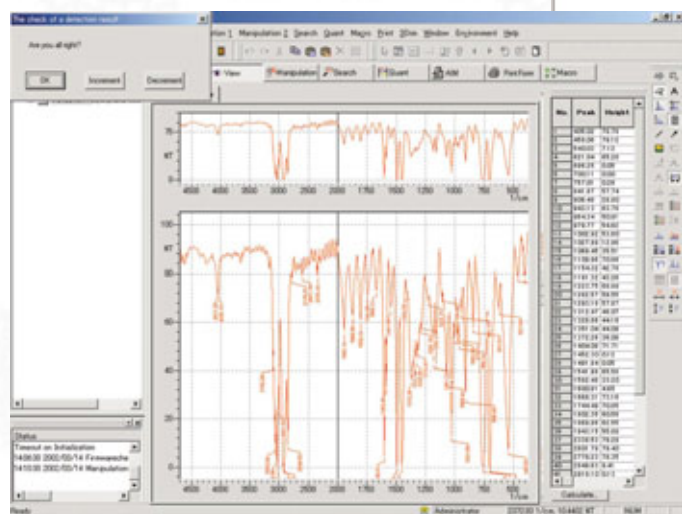
Easy Operation

IRsolution software is equipped with an Easy-Scan program. This macro program takes the user step by step through the entire analysis from spectrum measurement, peak detection, printout and saving of the result data. On-screen instructions guide the operator every step of the way. This feature decreases in the learning curve for operating IRsolution and the IRPrestige-21.

The Accessory Recognition system with the automatic scan parameters setting and the user group management system by password protection on IRsolution make the system highly secured.



Scan Parameter Setting



Peak Detection

BKG Measurement

be simplified by the standard Easy-Scan program. All procedures, including the setting of measurement parameters, analysis of the sample,

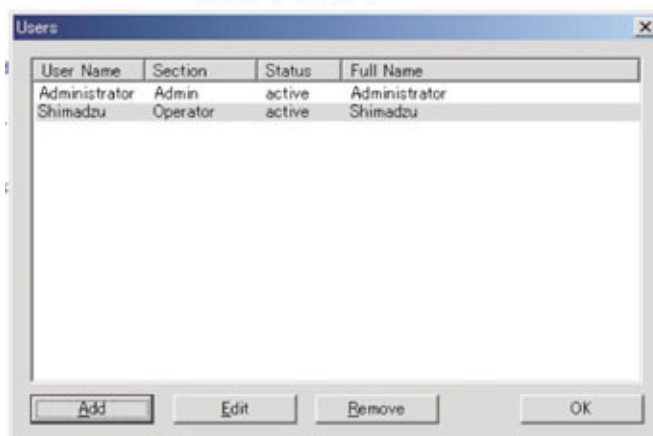
data processing, saving, and printing of the results, are performed with one-click operation.

Compliant with GLP/GMP and FDA 21 CFR Part 11

Recently, the reliability and security of the software controlling the instrument and the collected data have become more important. The FDA regulations such as 21 CFR Part 11 in the Pharmaceutical industry and GLP/GMP in the food industry are examples. The IRPrestige-21 with IRsolution and IRsolution Agent software includes the following features and supports GLP/GMP, ISO-9000 series and FDA 21 CFR Part 11.

- Security and log function with User name/Password
- Restriction of user rights by user group
- Raw data preservation including interferogram and background spectrum before FFT
- History log of data processing
- Electronic signature^(NOTE 1)

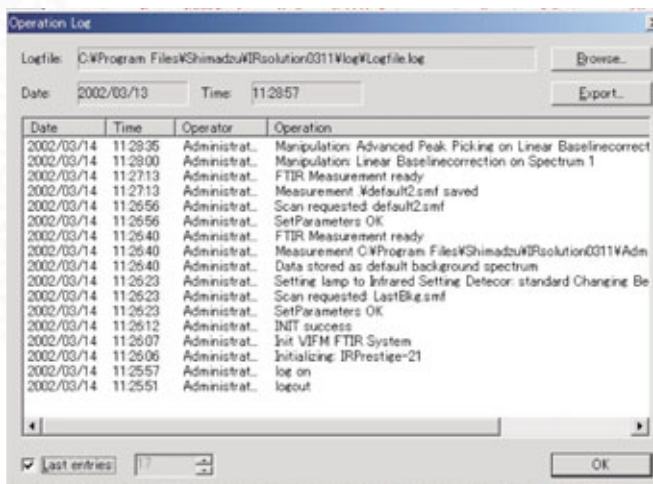
Instrument and software installation according to IQ/OQ documentation is available.



Audit Trail of the Instrument

All instrument-related information, including the power on date/time, user name, results of the instrument initialization, date/time of measurement, and attached accessories, are recorded as an audit trail.

This file can be displayed and is write-protected by IRsolution software for security.



(NOTE 1) The electronic signature should be done by IRsolution Agent software for FDA 21 CFR Part 11.

Equipped with Analysis Support Programs

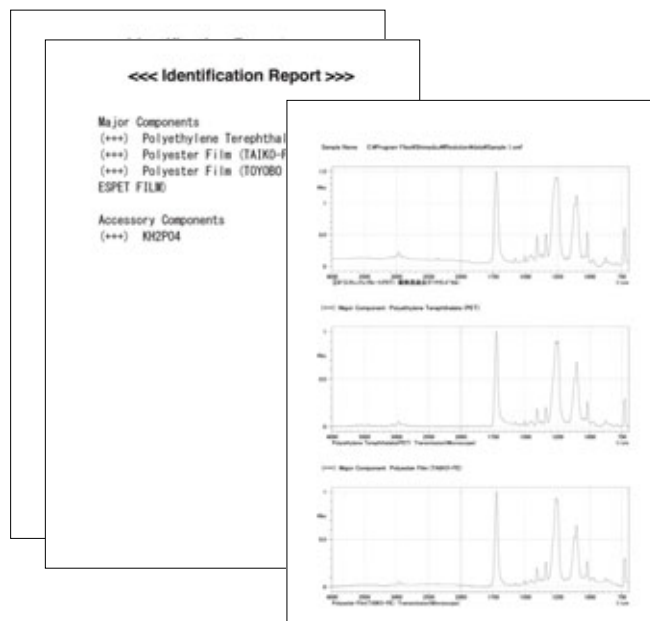
The two main applications of infrared analysis are the analysis of foreign matter and identification

tests. At Shimadzu, in order to allow operators with little experience in infrared analysis to fully

Contaminant Analysis Program (Patent pending)

By combining a library of spectra for substances that are often detected as foreign matter and Shimadzu's own algorithms, this program identifies foreign matter with a high degree of accuracy. Reports are automatically created after analysis, so operators with little knowledge of infrared analysis can perform analysis easily.

- Contains spectra for over 300 highly-selected inorganic substances, organic substances, and polymers that are often detected as foreign matter in Shimadzu's Analytical Applications Department.
- Incorporates algorithms that focus on spectral characteristics, rather than performing simple spectrum searches.
- Allows the automation of the process, including searching, judgment, and report creation.

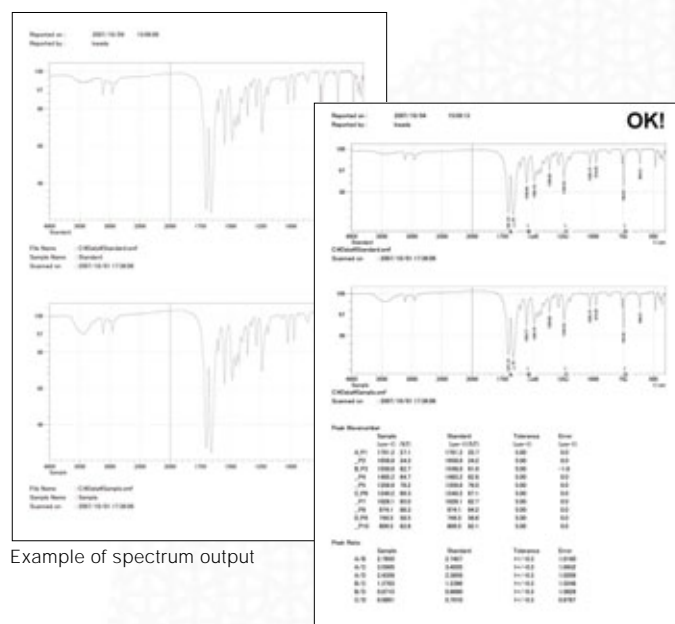


Example of report output

Pharma Report Program

This program makes pass/fail judgments about samples in accordance with the tests specified under "Infrared Spectrophotometry" in the Japanese Pharmacopoeia. In addition to identification tests for pharmaceutical products, use this program for incoming inspections and pre-shipment inspections. Its functions are described below.

- Prints out the spectra for standards and samples in order to facilitate easy comparison.
- Detection and print out of just the peaks that are specified for pass/fail judgment.
- Calculation of the differences between the peak wavenumbers for standards and samples, differences in intensity ratios between peaks, pass/fail judgments, and print out of reports.



Example of spectrum output

Example of report output

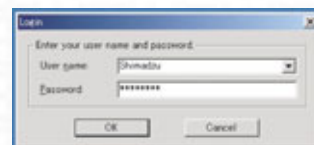
utilize the functionality of the IRPrestige-21, we have prepared analysis support programs. These

programs are useful in a variety of analysis scenarios where infrared spectra are used.

Software security by user name and password

By requiring a user name and password upon startup of IRsolution software, security can be enhanced by restricting the functions or methods for a particular user within a user group. An administrator can restrict the functionality that is available within IRsolution to each particular user and can control all the user rights.

The logon information is recorded in a log file with the date, time and user name.

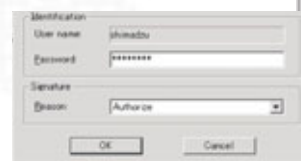


Raw data preservation and data processing history

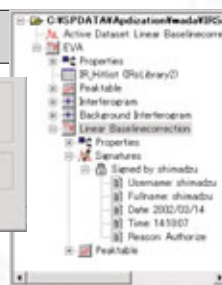
Spectra obtained by IRsolution software are stored in a container file that includes the scan parameters, background and the original interferogram.

When a data manipulation is performed, the processed data is added to the file along with the date and time of processing, user name and the manipulation method. The original data is preserved - not overwritten.

The electronic signature is also supported for FDA 21 CFR Part 11 compliance.(NOTE 1)



Electronic Signature in IRsolution

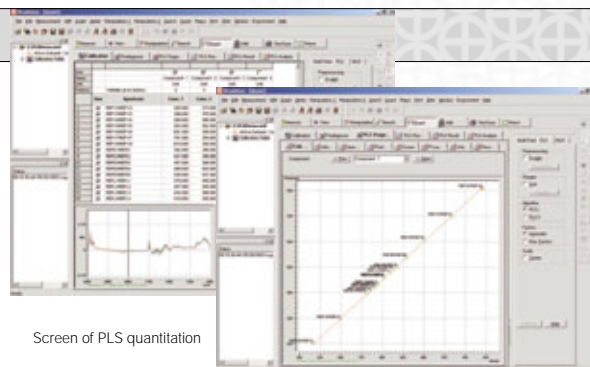


Optional programs

PLS quantitation software (P/N 206-72331-91)

PLS (Partial Least Squares) quantitation is a widely used Chemometrics method like the Multiple Linear Regression (MLR) method for quantitation of multicomponents.

IRsolution has PLS I and PLS II methods for PLS quantitation. IRsolution analyzes PLS calibration curves by calculating "Influence", "Residuals", "Scores", "Loadings", "Press Values", etc.



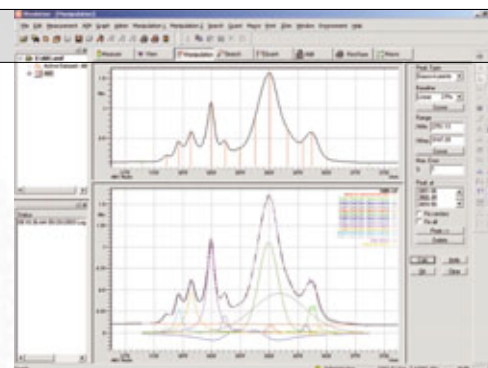
Screen of PLS quantitation

Curvefitting (Peak split) software (P/N 206-72333-91)

Usually, an IR band can consist of several overlapping peaks. Curvefitting (Peak split) software separates IR bands into individual component peaks. This software is good for many applications, such as analysis of a peak with hydrogen bond influences and analysis of hidden peaks overlapped with other peaks.

Curvefitting (Peak split) software separates the band with suitable curves from 6 types of curves such as Gaussian, Lorentian, Gaussian+Lorentian. Component peaks and a synthesized peak are displayed to evaluate the separation.

Curvefitting (Peak split) result of peak (3150-2750 cm^{-1}) of ABS resin spectrum.
Top : Target peak and specified peaks
Bottom : Component peaks and a synthesized peak



Macro Platform (P/N 206-72330-91)

Macro Platform is a module to run Macro programs provided by Shimadzu on IRsolution software. Please contact your Shimadzu representative when you need an automatic measurement system with an automatic sample changer or to perform routine operation with repeated specified operations.

(NOTE 1) The electronic signature should be done by IRsolution Agent software for FDA 21 CFR Part 11.

Specifications

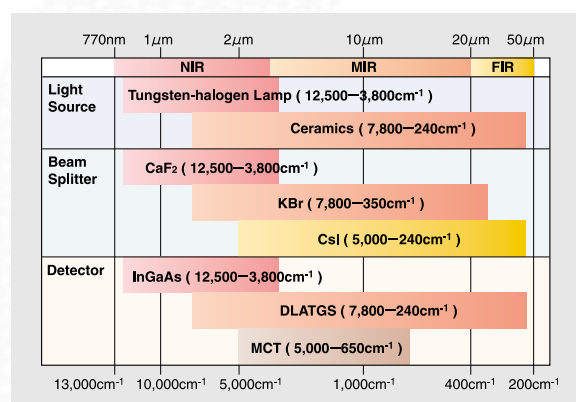
| | | |
|-----------------|--------------------|--|
| Hardware | Interferometer | Michelson interferometer (30 degree incident angle) |
| | | Advanced Dynamic Alignment system (Patent pending) |
| | | Sealed and desiccated interferometer with an automatic dryer (Patent pending) |
| | Optical system | Single beam optics |
| | Beam splitter | Germanium-coated KBr plate for Middle IR (Standard) |
| | | Germanium-coated CsI plate for Middle/Far IR (Optional) |
| | | Silicon-coated CaF ₂ plate for Near IR (Optional) |
| | Light source | Air-cooled ceramic for Middle/Far IR with 3 years guaranteed (Standard) |
| | | Tungsten lamp for Near IR (Optional) |
| | Detector | DLATGS detector with temperature control for Middle/Far IR (Standard) |
| | | MCT (Hg-Cd-Te) detector with liquid nitrogen cooling for Middle IR (Optional) |
| | | InGaAs detector for Near IR (Optional) |
| | Wavenumber range | 7,800 - 350 cm ⁻¹ |
| | | 12,500 - 240 cm ⁻¹ (Optional. See figure for detail) |
| | Resolution | 0.5 cm ⁻¹ , 1 cm ⁻¹ , 2 cm ⁻¹ , 4 cm ⁻¹ , 8 cm ⁻¹ , 16 cm ⁻¹ (Middle/Far IR) |
| | | 2 cm ⁻¹ , 4 cm ⁻¹ , 8 cm ⁻¹ , 16 cm ⁻¹ (Near IR) |
| | S/N ratio | 40,000: 1 or higher |
| | | (4 cm ⁻¹ resolution, 1-minute accumulation, around 2,100 cm ⁻¹ , peak-to-peak) |
| | Mirror speed | 3-step selection of 2.8, 5, or 9 mm/sec |
| | | Scanning at 4 cm ⁻¹ takes from 2-3 sec |
| | Data sampling | He-Ne laser with 30 months guaranteed |
| | Gain control | Automatic or manual from x1 - x128 |
| | Sample compartment | Automatic accessory recognition |
| | | 200 (W) x 230 (L) x 170 (H) mm |
| | | Center Focus |
| | Dimensions | 600 (W) x 680 (L) x 290 (H) mm |
| | Weight | 54kg |

| | | | | | |
|-------------------|---------------------|----------------------|-----------------|-------------------------------------|------------------------|
| Scan Range | Light Source | Beam Splitter | Detector | Scan Range (cm⁻¹) | Necessary Parts |
| | Tungsten | CaF ₂ | InGaAs | 12,500-3,800 | NIR Set (206-72015-91) |
| | Ceramic | KBr | DLATGS | 7,800-350 | Standard |
| | | | MCT | 5,000-720 | MCT Set (206-72017-91) |
| | | CsI | DLATGS | 5,000-240 | FIR Kit (206-72016-91) |

(Caution) The beam splitters must be kept inside the IRPrestige-21 or a desiccator.

Scan wavenumber with options

The orange bar expresses the wavenumber range which can be measured with the standard elements. The red, yellow and brown bars express the wavenumber range which can be measured with the optional elements.



| | | |
|-----------------|-----------------------------------|--|
| Software | OS | Microsoft Windows 2000 (Service Pack 2 or later), Windows XP Professional |
| | Interface | IEEE-1394 |
| | Monitor of hardware | Self-diagnosis function, Status monitor |
| | | Validation program based on Japanese Pharmacopoeia/Europe Pharmacopoeia (EP)/ASTM |
| | Data processing | Addition, Subtraction, Multiplication, Division, %T ↔ Abs conversion, Normalization, Baseline correction, Log conversion, Smoothing, Derivatives, ATR correction, Kubelka-Munk correction, Kramers-Kronig analysis, Wavenumber/wavelength conversion, Peak detection, Peak area calculation, Film thickness, Atmosphere correction, CAMP-DX conversion, ASCII conversion |
| | Quantitative processing | Peak height, Peak area, Multi-point calibration curve method using ratio, Multi-regression (MLR) method |
| | Spectrum search | Search parameter setting, Search of user library and commercial library, Creation of user library Shimadzu original library with over 800 spectra is included as standard |
| | Print | Report generator function |
| | Display | Compression of wavenumber axis, Enlargement/reduction, Auto scale, Overlap, Stack display, Shift display |
| | Edit | Copy, Cut, Paste |
| | Others | Customization of GUI |
| | Optional software | Macro programming, PLS quantification, Curve fitting, 3-D display, Mapping measurement |
| | Audit trail | Saves sample/background interferogram and saves data processing history |
| | | User administration by password and creation of user group |
| | | Log record |
| | | Function corresponds with FDA 21 CFR Part 11 ^(NOTE1) |
| | Recognition of accessories | Automatic recognition of installed accessories, Automatic setting of measurement parameters, Automatic |
| | | execution of macro program |

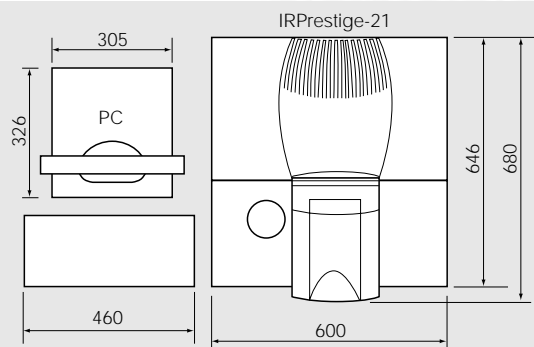
(NOTE 1) IRsolution Agent software is needed to fully comply to FDA 21 CFR Part 11.

| | | |
|--------------|---|--|
| Other | Installation site | Ambient temperature : 15-30°C |
| | | Ambient humidity : 70% or less to avoid condensation |
| | Power requirements ^(NOTE 2) | AC 100/120/220/230/240V, AC50/60Hz, 240VA, Standby power 4.5VA |

(NOTE 2) PC requires additional power.

| | | |
|------------------------------|-------------------------|---|
| Computer Requirements | Type | Desktop (IEEE 1394 interface for desktop PC is required.) Notebook (PCMCIA IEEE 1394 interface is required.) |
| | Operating system | Microsoft Windows XP Professional SP2 |
| | CPU | Celeron D processor 330 (2.66GHz) or better |
| | Video | 1024 x 768/256 color or better |
| | RAM | 512MB and more |
| | HDD | 30MB and more for free space |

Dimensions

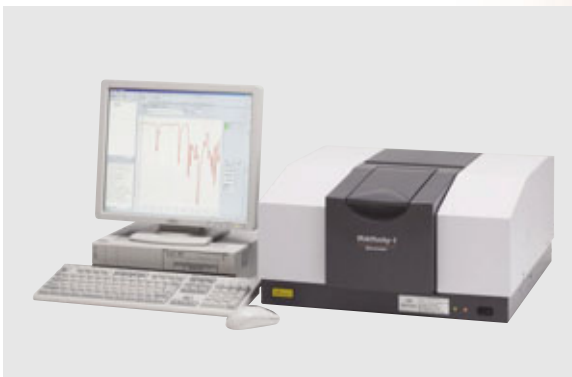


Unit : mm

High-performance entry-model FTIR

IRAffinity-1

Resolution 0.5, 1, 2, 4, 8, 16 cm^{-1}
Scan range 7800 - 350 cm^{-1}
S/N ratio 30,000 : 1 or better
Interferometer 30 degree Sealed Michelson
with Dynamic Alignment



JQA-0376

Founded in 1875, Shimadzu Corporation, a leader in the development of advanced technologies, has a distinguished history of innovation built on the foundation of contributing to society through science and technology. We maintain a global network of sales, service, technical support and applications centers on six continents, and have established long-term relationships with a host of highly trained distributors located in over 100 countries. For information about Shimadzu, and to contact your local office, please visit our Web site at www.shimadzu.com



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