C103-E148B

SHIMADZU
Excellence in Science

Fourier Transform Infrared Spectrophotometer

IRSpirit-X Series

IRSpirit™, **Ready to Run**

IRSpirit-X

FOURIER TRANSFORM INFRARED SPECTROPHOTOMETER

Space-Saving, Expandable

- Great for Small Lab Spaces
- Standard-Sized Sample Compartment in a Compact Bench

FTIR Made Easier

- IR Pilot™ Pre-built Macro Program
- Spectrum Advisor Function
- Contaminant Analysis Program
- Identification Test Program

Reliability to Deploy with Confidence

- Technology Inherited from Higher-End Models
- Reliable Parts Come with a 10-Year Warranty

  Note: This warranty does not cover consumables, accessories other than the FTIR main unit, PCs and peripherals, instruction manuals, jigs, and labor charges for the second and subsequent years.
- High Durability Due to Humidity-Resistant Design
- Internal Dehumidifier (Optional) Ensures Robustness
- Instrument Status Monitoring

Simple Operation, Confident Results

- Easy Macro – Just a Single Click Launches Routine Work
- Acquisition and Analysis of EDX and FTIR Data from a Single Computer

ANALYTICAL INTELLIGENCE

- Automated support functions utilizing digital technologies, such as M2M, IoT, and Artificial Intelligence (AI), that enable higher productivity and maximum reliability.
- Allows a system to monitor and diagnose itself, handle any issues during data acquisition without user input, and automatically behave as if it were operated by an expert.
- Supports the acquisition of high quality, reproducible data regardless of an operator's skill level for both routine and demanding applications.

Space-Saving, Expandable

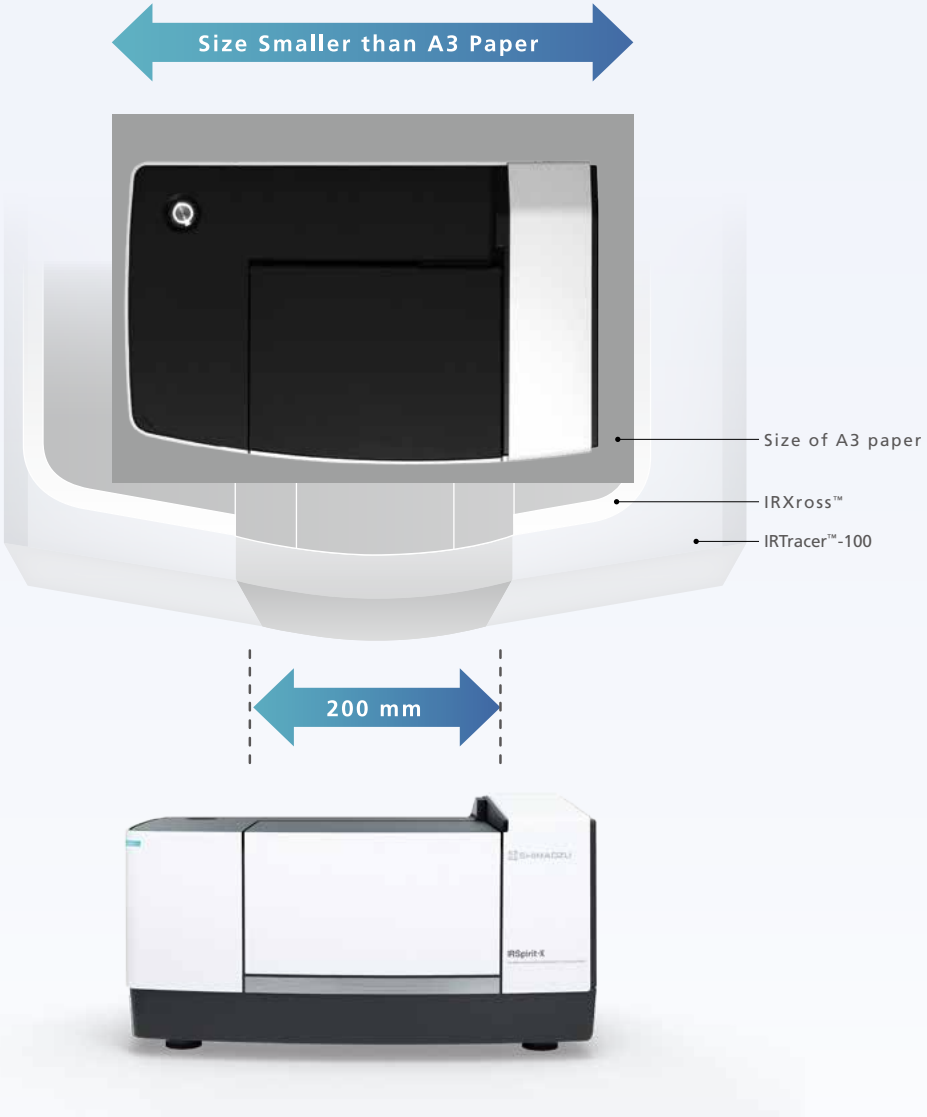
Great for Small Lab Spaces

There is a growing need for systems that can fit in tight spaces, like glove boxes and multiuse facilities, and the IRSpirit-X is perfect for those situation. Even in narrow spaces, samples can be measured with the unit positioned vertically (see images below). The start button is accessible and the humidity indicator is visible from both directions.

In addition, the ATR crystal and FTIR main unit are the same height. Therefore, samples can be placed directly on the ATR attachment, which is integrated with the sample compartment, which can eliminate the trouble of having to cut large samples.

Standard-Sized Sample Compartment in a Compact Bench

In spite of a body size smaller than a piece of A3 paper, the sample compartment width is the same as on higher-end models. This makes it compatible with many Shimadzu and 3rd party accessories, allowing it to be used for a wide variety of applications.



Fields \ Applications	Contaminant analysis	Raw materials acceptance inspection	Identification tests	Quantitative analysis	Spectral analysis
Pharmaceuticals and life sciences	●	●	●	●	●
Chemicals and petroleum	●	●	●		●
Academia			●	●	●
Environmental	●			●	●

● : Applicable

ATR

Diffuse reflectance

Specular reflectance

Gas cell

Liquid cell

FTIR Made Easier

IR Pilot™

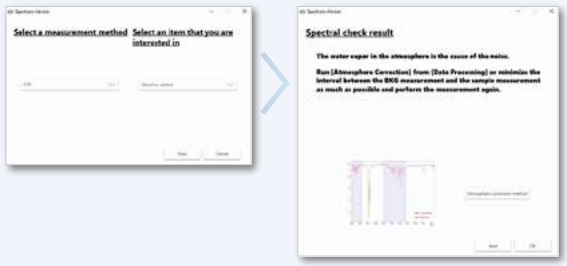
ANALYTICAL INTELLIGENCE

IR Pilot offers a total of 23 application programs as standard, making it easy for operators with minimal FTIR experience to analyze samples by simply selecting the analysis purpose and accessory. There is no need to set parameters. Once a workflow has been determined, it can be recorded, which means that for analyses with the same procedures, the sequence from measurement to data analysis and printing can be performed with a few clicks.

* Quantitative analysis function cannot be used when using IR Pilot with LabSolutions DB/CS.

Spectrum Advisor Function
(patent pending)

Corrective measures are proposed by comparing the measured spectrum to optimal spectrum examples. Troubleshooting advice is provided on scan parameters, accessories, and post-processing data. As a result, better quality data can be acquired.



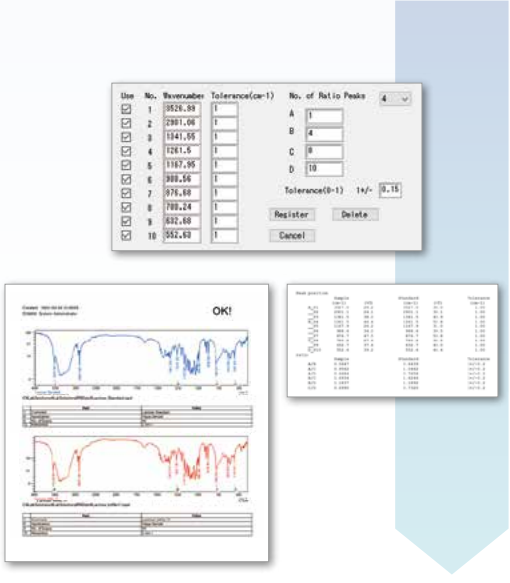
Contaminant Analysis Program

ANALYTICAL INTELLIGENCE

The contaminant analysis program identifies measured contaminants using Shimadzu's proprietary identification algorithm (Japanese Patent No. 5205918) in combination with a spectral library containing more than 550 spectra for substances commonly detected as contaminants. After data analysis, it automatically makes a pass/fail judgment and creates a report. Even if the contaminant is a mixture, it searches for major and minor components and displays their ranks. Since the number of components in the mixture does not need to be specified, even operators with minimal infrared analysis experience can easily analyze samples. It takes just seconds between selecting the spectrum and displaying the analysis results.

Identification Test Program

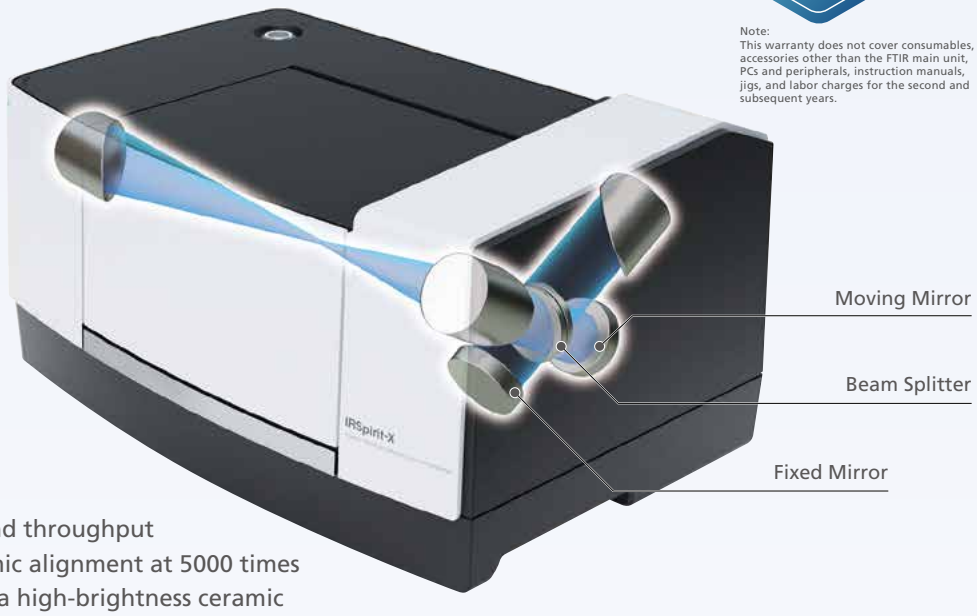
The identification test program calculates the difference in peak wavenumbers and peak ratio intensities between standard and test sample data, and then summarizes the pass/fail judgment results in a printed report. This program can be used if the standard is described in the national pharmacopoeia or official law. Spectra of 57 substances included in Japan's Specifications and Standards for Food Additives are also included in this program.



Reliability to Deploy with Confidence

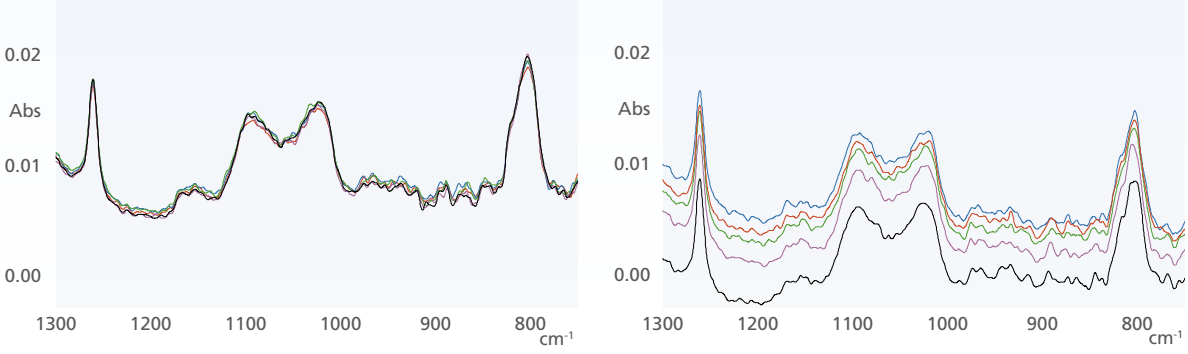
Technology Inherited from Higher-End Models

Note:
This warranty does not cover consumables, accessories other than the FTIR main unit, PCs and peripherals, instruction manuals, jigs, and labor charges for the second and subsequent years.



- High stability and throughput
  (Features dynamic alignment at 5000 times per second and a high-brightness ceramic light source)
- High sensitivity comparable to standard models (IRSpirit-TX)
  (DLATGS detector with temperature control function)

The silicone oil content in paraffin oil (1.0%) was obtained by repeating a single-reflection ATR method five times. Data obtained using the DLATGS detector with temperature control is shown on the left and data obtained using the DLATGS detector without temperature control is shown on the right. The internal heat in the instrument and the environmental temperature caused large baseline data fluctuations without temperature control. In contrast, using the detector with temperature control resulted in highly repeatable data.



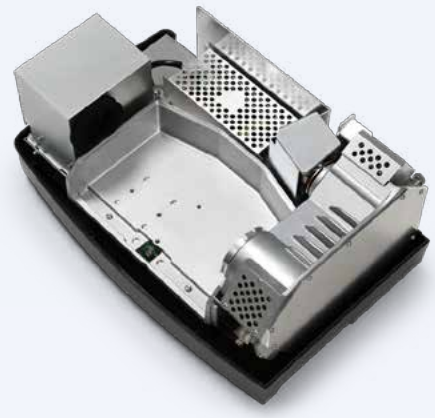
ATR Spectra of Silicone Oil Content in Paraffin Oil (measurement repeated five times)

High Durability Due to Humidity-Resistant Design

The robust optics are designed to ensure the system can be used reliably even under harsh temperature and humidity conditions.

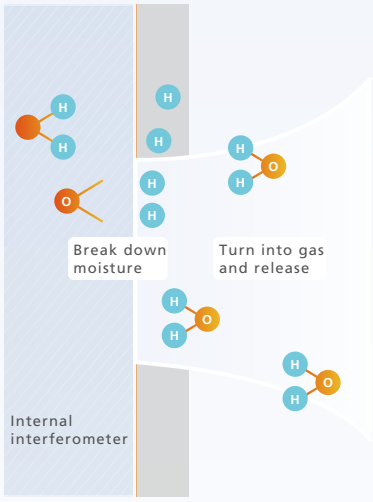
- KBr beam splitter includes a humidity-resistant coating (IRSpirit-TX/LX), or ZnSe beam splitter (IRSpirit-ZX)*1
- Optics sealed in an aluminum die cast housing
- Status monitor function features electrical and paper-based indicators.
- Select from a KBr window (to 70% RH) or a KRS-5 window (to 90% RH); both include a humidity-resistant coating.*2, *3
- Optional electric dehumidifier can be installed.*4

*1 The measurement wavenumber range will be 6,000 to 550 cm^{-1} with the IRSpirit-ZX, which is equipped with a ZnSe beam splitter.
*2 No condensation
*3 The KRS-5 window plate is used with the IRSpirit-ZX.
*4 Not required with the IRSpirit-ZX.



Aluminum Die Cast
Interferometer Housing

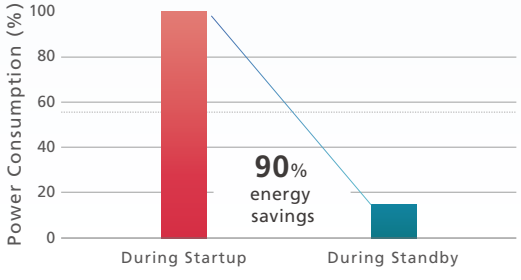
Window	KBr 	KRS-5 
Humidity Resistance	With humidity-resistant coating Max. humidity at installation site: 70 %RH (with no condensation)	Max. humidity at installation site: 90 %RH (provided no condensation at temperatures up to 30 °C)
Wavenumber Range	350 to 7,800 cm^{-1}	
Transmittance	About 90 %T	About 70 %T
Characteristics	• High transmittance and high sensitivity • Could deliquesce in humid environments	Compared to KBr window: • Higher humidity-resistance • Lower S/N due to lower transmittance



The Principle of a Dehumidifier

Internal Dehumidifier (Optional) Ensures Robustness

This dehumidifier removes moisture from inside the interferometer electrolytically using a solid polymer electrolytic membrane. It maintains low humidity levels inside the interferometer without leaving the light source ON. Using the dehumidifier alone can reduce power consumption by about 90 % compared to leaving the light source illuminated. Note that a dehumidifier is not required as the ZnSe beam splitter adopted for the IRSpirit-ZX features high resistance to humidity.



IRSpirit-X series power consumption during Startup (with Start Switch ON) and during Standby (with Start Switch OFF and Dehumidifier ON)

Instrument Status Monitoring

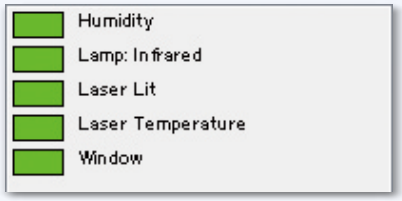
Instrument status is automatically verified during start-up and results are saved in a report. This feature is especially convenient for instrument management. Pharmacopoeia-compliant validation programs convenient for routine inspections are also included.

Self-diagnostic function

A self-diagnostic function inspects the signal system and optics during instrument initialization. It obtains a variety of information and automatically outputs the results in one file, making instrument management easy. The instrument status history can also be confirmed.

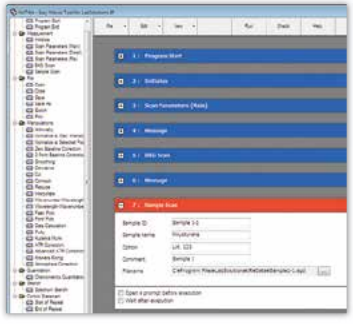
Status monitor function

This function continuously monitors and manages information about the light source, semiconductor laser, humidity inside the instrument, the window plate connection (interlock), and accessories.



Simple Operation, Confident Results

LabSolutions™ IR automates routine work, such as scanning, data manipulation, reporting, identification tests, and contaminants analysis. Launch programs from the Launcher or your PC.



Easy Macro – Just a Single Click Launches Routine Work

- ✓ Initialization of FTIR, configuration of scan parameters, spectrum measurement
- ✓ Data manipulations, search, quantitation, printing
- ✓ Repeat measurements, displaying messages, alarm sounds, external program execution

The “Easy Macro” function will create macros that are suitable for routine work, particularly when repetitive operations are used. The macro builder allows macros to be constructed by simply selecting and aligning operations from a list. Once constructed, the macros can be registered with the Launcher and Desktop for quick execution. Operators who are not familiar with FTIR can easily operate the instrument.

Acquisition and Analysis of EDX and FTIR Data from a Single Computer

Both EDX and FTIR models can be controlled with a single computer. The efficiency of time-consuming contaminant analysis can be improved by installing EDXIR-Analysis™, an integrated EDX/FTIR analysis program, on the computer.

Integrated Data Analysis for Contaminants

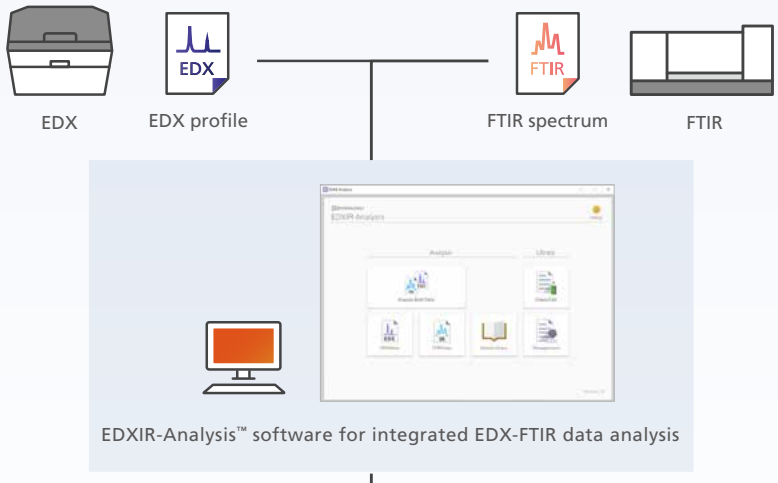
- ✓ To perform qualitative analysis automatically, simply click “Analyze Both Data” and select the EDX/FTIR data.*1
- ✓ This enhances the efficiency of time-consuming analyses that were traditionally left to the analyst, and provides strong support for contaminant analysis.
- ✓ In addition to a list of hits, the integrated data analysis results show EDX profiles and FTIR spectra found as hits from the library.

Data Comparisons for Identification Tests

- ✓ A Data Comparison function calculates the degree of matching between the actual measured data and the data registered in the library.
- ✓ The software can be used for countermeasures against "silent change" and for other confirmation tests.
- ✓ Clicking the "Print" button prints the results in a fixed format and also saves them in Word format.*2

*1 Using the EDX profile, data are classified as organic, inorganic, and mixture. Integrated data analysis is performed by applying priority levels to each classification (Patent No. 06638537).

*2 Microsoft® Word must be installed.



Integrated Data Analysis Results for a Black Rubber Contaminant

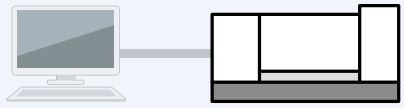
Data Comparison Results for a PVC Examination Object and the Standard Product

Reliable LabSolutions™ Software

In addition to LabSolutions IR, which provides basic functionality, Shimadzu also offers LabSolutions DB IR and LabSolutions CS IR to meet the requirements of ER/ES regulations.

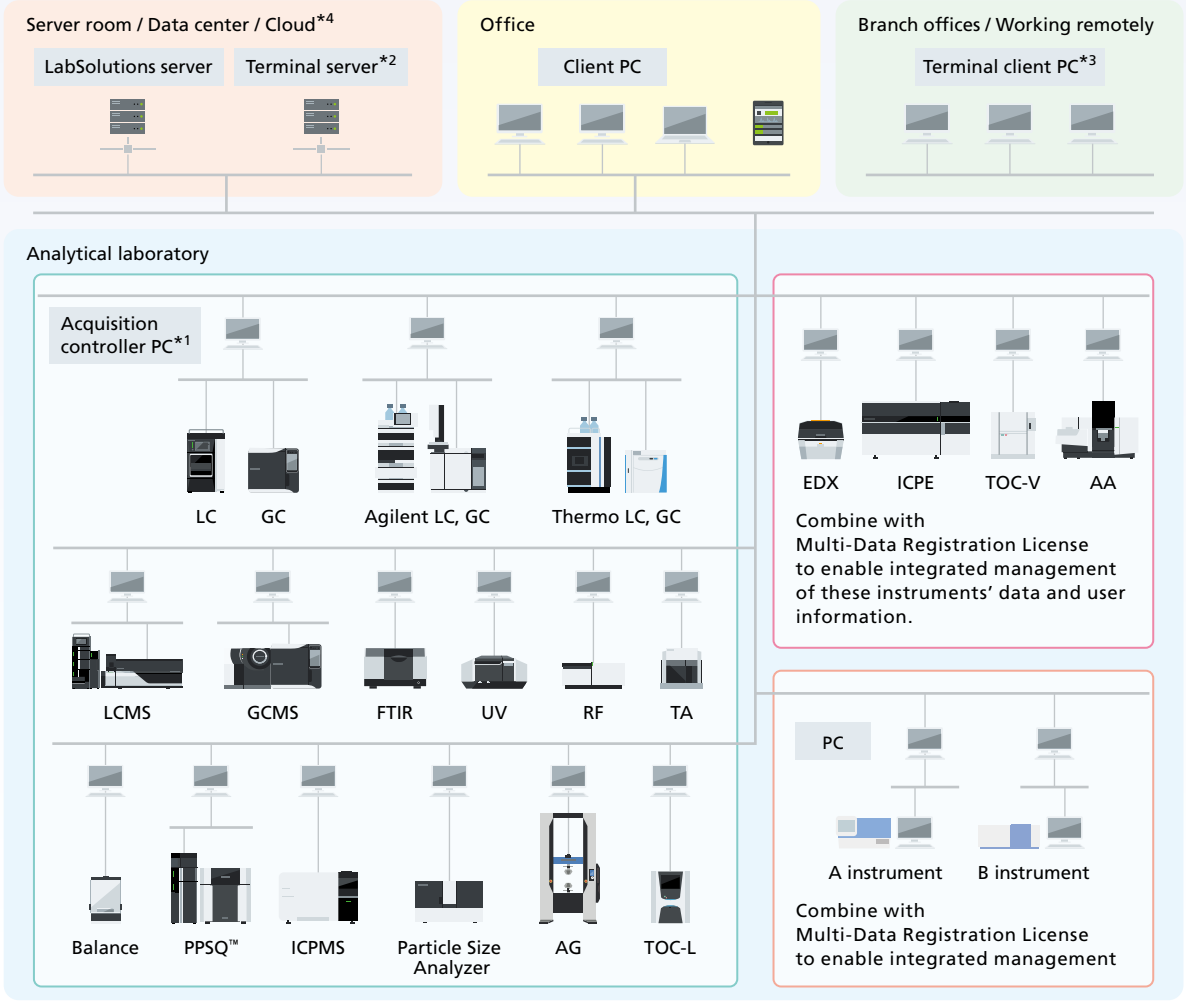
LabSolutions DB IR

LabSolutions DB IR allows for secure data management by integrating a data management function with LabSolutions IR. Compliant with ER/ES regulations, the software is optimally configured for customers using a PC. It is recommended for facilities that do not require network connections and want to be ER/ES compliant.



LabSolutions CS IR

LabSolutions CS, which is freely accessible to the analysis network, can be connected to LabSolutions IR, eliminating the need for connecting a PC to the instrument. Since all the data are managed on a server, LabSolutions CS IR can be read from any personal computer on a network. With terminal service, LabSolutions IR can be controlled from a client PC without installing LabSolutions IR on it. It is recommended for facilities that have a large number of users, manage data in a database, and want to be ER/ES compliant.



*1 The acquisition controller PC controls analytical instruments.
*2 A terminal server is a server for using terminal services. Users can view data reports and perform electronic signature operations through terminal services. It is ideal for remote connections because of the low network load. Only LC, GC, LCMS, and GCMS support analysis and postrun operations through terminal services.
*3 If a terminal service is used, LabSolutions software does not need to be installed on client PCs or tablets.
*4 Servers can be built on various clouds (IaaS). AWS (Amazon Web Services), Microsoft® Azure®, GCP™ (Google Cloud Platform™)

Data Integrity Compliance

High Security

An audit trail to ensure the reliability of data and document e-mail transmission functions when any event occurs in the system can be set up. User accounts are managed using passwords, where password length, complexity and term of validity must satisfy specified requirements. It is also possible to set lockout functions to prevent illegal access, and set a registered user's deletion and change in status. In addition, a box can be selected to prevent overwriting a data file and outputting an item to a report.

Essential Information Is Managed for Every Project

LabSolutions DB IR and CS IR provide a project management function enabling control suited to tasks and system operations. This function enables equipment and user management, security policy, and data processing to be set on a project by project basis, thereby improving the efficiency of data searches and management tasks.

Visualization of the Sequence of Analysis Operations

Report set includes test methods and test results for a series of samples analyzed as well as a corresponding operation log (a record of all operating events from login to logout), which is automatically extracted from the data and summarized in a single report. It provides visibility of the individual analytical operations, and helps to check for operating errors and improve the efficiency and reliability of checking processes.

Applications and Options

Pharmaceutical

MHP-1

This is a compact, inexpensive hand-driven press used to produce 4 mm dia KBr pellets. A pellet produced in the frame is directly measured using the dedicated holder, which ensures exceptional simplicity of operation. No dies or a vacuum pump are required. (Samples That Can Be Measured: Powders)

DRS-8000A

Although powder samples are mixed with KBr, as with the KBr pellet method, the DRS-8000A analyzes the samples in their original state; creating pellets is not necessary. For plastic moldings, emery paper attached to the SiC sampler (P/N 200-66750-01) scrapes off part of the surface, forming a powdered sample that can be analyzed. Easily obtain diffuse reflectance spectra similar to transmittance spectra using the built-in Kubelka-Munk conversion function in LabSolutions IR software. Functionality is included for automatically recognizing attached accessories. (Samples That Can Be Measured: Powders, Moldings)

SiC sampler

Chemicals and Polymer

QATR™-S

This is a single reflection ATR measurement attachment. The prism is made entirely of diamond, so the measurement wavenumber range is up to 400 cm^{-1} (wide-band). With a liquid sample, simply place a drop on the prism to measure spectra. For other samples, clamp the sample closely against the prism surface before measurement on the sample surface The incident angle is 45 degrees. Four prism materials are available: diamond, (wide-band, high-throughput), germanium (Ge) or zinc selenide (ZnSe). The Ge prism is best suited for samples with a high refractive index.

Dehumidifier Unit

This is the same electric dehumidifier unit used in our higher-end models (IRXross™ and IRTracer™-100). The dehumidifier is driven by a stand-by power, so it is possible to maintain a low level of humidity inside the interferometer even when the FTIR is not used (AC power supply). It can reduce the labor and maintenance costs associated with replacing the silica gel.

Image of Dehumidifier

Back side of IRSpirit-X series

Contaminant Library for LabSolutions IR

This is Shimadzu's latest original library. It is an effective tool for analyzing contaminants in tap water and food. In addition to containing information on actual sample contaminants and information about water supply maintenance parts commercially available in Japan, the library also includes X-ray fluorescence profiles (PDF files) to significantly improve the accuracy of contaminant searches. Unlike existing libraries, this library contains data on mixed compounds and incorporates the depth of knowledge and experience needed to make qualitative assessments.

KnowItAll® Bundle

Activate John Wiley & Sons, Inc. KnowItAll from a button in the LabSolutions IR software to automatically transfer the active spectrum. With KnowItAll, you can perform searches using a rich library, analysis of constituent components and constituent ratios by mixture analysis, and functional group analysis by searching for functional groups of specified peaks.

* LabSolutions IR does not work with KnowItAll Version 2018 and earlier.

EDXIR-Analysis™ Software

EDXIR-Analysis software is specially designed to perform
qualitative analysis using data acquired by an energy dispersive X-ray (EDX) fluorescence spectrometer and a Fourier transform infrared (FTIR) spectrophotometer. This software is used to perform an integrated analysis of data from FTIR, which is excellent at the identification and qualification of organic compounds, and from EDX, which is excellent at the elementary analysis of metals, inorganic compounds and other content. It then pursues identification results and the degree of matching. It can also be used to perform EDX or FTIR data analysis individually. The library used for data analysis (containing 485 data files) is original to Shimadzu, and was created through cooperation with water supply agencies and food manufacturers. Additional data can be registered to the library, as can image files and document files in PDF format. It is also effective for the linked storage of various types of data as electronic files.

EDXIR-Holder™

This foldable holder consists of an adhesive layer with samples attached and polypropylene film designed for X-ray fluorescence analysis. It provides measurement by keeping the samples in the holder with EDX and FTIR. When using EDX for measurement, close the holder and place the polypropylene film directly to the irradiation side (downside). When using FTIR for measurement, open the holder and press the samples attached to the adhesive layer against the ATR prism. Close the holder after the measurement and it can be used as sample storage.

Image of measurement with EDX

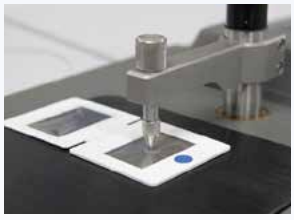
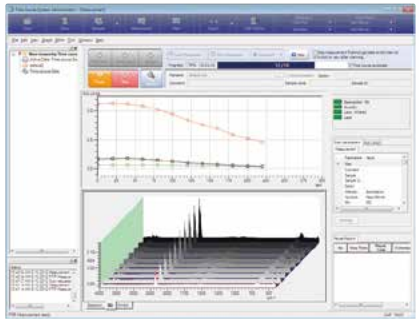


Image of measurement with FTIR

Semiconductor

Time Course Software

The time course program is used to collect spectra in regular intervals and creates a time course dataset used to follow reactions as a function of time. Changes in peak height and peak area can be used to calculate values related to reaction kinetics. Time course information is saved and displayed in 3D or in a contour plot.



Fourier Transform Infrared Spectrophotometer Plastic Analysis System

Plastic Analyzer

When analyzing plastics, libraries are used to qualify their material properties. However, infrared spectra of plastics that have been denatured (have deteriorated) due to heat or UV rays differ in shape from standard spectra, and qualifying them can sometimes be difficult. To address this, the Plastic Analyzer includes a deterioration library, so highly accurate qualification can be performed reflecting the state of deterioration.

Plastic Analyzer consists of the following.

- Fourier transform infrared spectrophotometer
- Single-re ection ATR attachment
- Plastic Analyzer method package
  1. UV-Damaged Plastics Library
  2. Thermal-Damaged Plastics Library
  3. Macro Program for IR Pilot/Parameter File

IRSpirit-X+QATR-S System

1. UV-Damaged Plastics Library*1

Unlike previous libraries, this library includes information about plastics degraded by ultraviolet rays. Because many contaminants are degraded, this library is especially useful for such cases. It is also useful for analyzing microplas-tics.

*1 Plastics degraded using an Iwasaki Electric super accelerated weathering tester were measured and compiled as a library by Shimadzu Corporation.

2. Thermal-Damaged Plastics Library*2

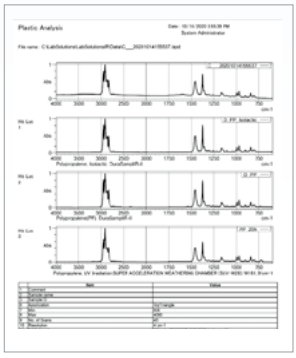
Unlike previous libraries, this library includes information about plastics that have degraded due to oxidation associated with heat. The library is especially useful for analyzing contaminants, which are commonly degraded.

*2 Spectra were measured and acquired at the Hamamatsu Industrial Research Institute of Shizuoka Prefecture and compiled as a library by Shimadzu Corporation.

3. Macro Program and Parameters

The system includes plastic measurement parameters and IR Pilot, a special program for IRSpirit-X that simplifies spectral measurementsand the creation of reports, enabling analysts to perform everything from the measurement of target samples to data analysis easily. Even users unfamiliar with FTIR analysis can start work immediately.

IR Pilot, a Special Program for IRSpirit-X

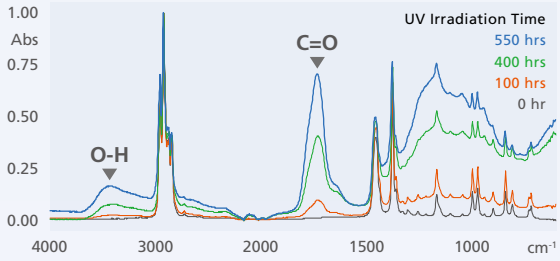


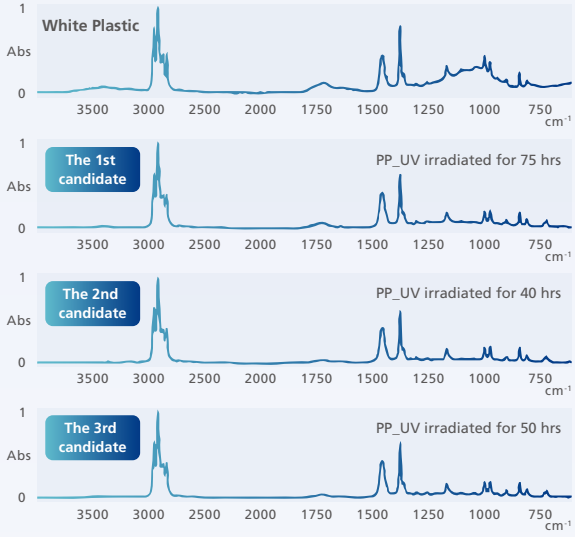
Report Output

Sample Positioning

Analysis Example with Plastic Analyzer

Evaluation of Deteriorated Samples





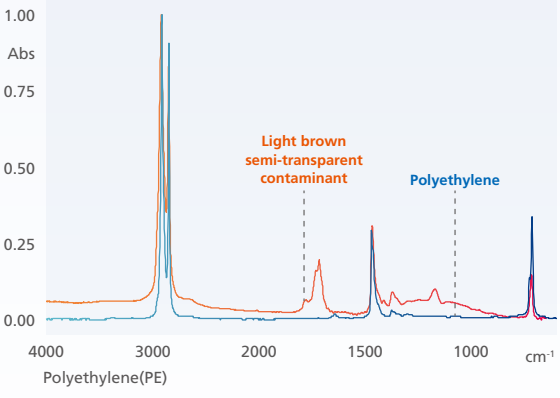
Plastics degrade as they experience molecular cleavage and cross-linking due to heat and light. As a result, in fault analysis and failure analysis, the qualities of deteriorated samples must be analyzed.

The above left figure shows the infrared spectrum of a polypropylene (PP) sample that has been irradiated with UV rays. The UV irradiation has caused the plastic to deteriorate, and it is evident that the shape of the infrared spectrum has changed.

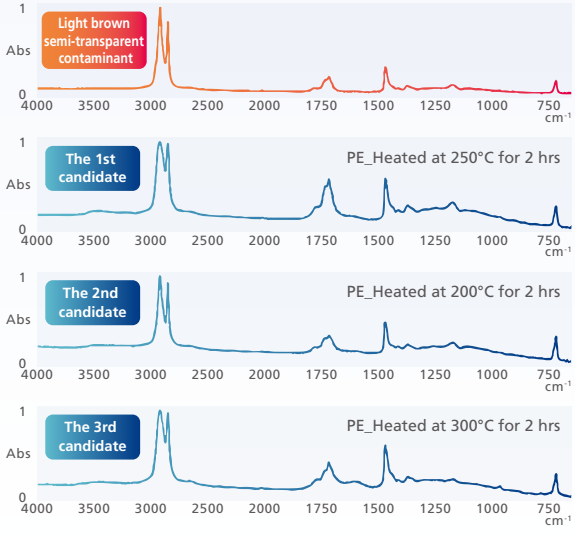
The top right figure shows the search results from measurements by Plastic Analyzer of a white plastic (PP material) that was left outdoors for an extended period and exposed to UV rays.

The infrared spectrum of the sample exposed to UV rays differs from the standard spectrum. Accordingly, in general library searches, different plastics such as polybutene are at the top of the results. In contrast, with Plastic Analyzer, PP denatured by UV rays is the top result.

Contaminant Analysis (Contaminants in Processed Items)



A light brown semi-transparent contaminant on a plated item



The measurement of a light brown semi-transparent contaminant on a plated item was performed. The figure above shows that the spectral pattern of the acquired infrared spectrum differs from the standard polyethylene (PE).

Plastic Analyzer shows the best match is heated PE. The Thermal-Damaged Library makes it useful for surmising the thermal history of the plastic.


HOMEDY

Transporting and Moving the Instrument

When transporting and moving the instrument, avoid vibrations, falls, or other strong impacts. When transporting it over long distances, such as to another building, use the original packaging. Note that Shimadzu is not responsible for performance deterioration resulting from transportation or movement of the instrument.

This product is certified as Shimadzu's Eco-products Plus.
Energy savings: 62% reduction as compared to the conventional model*
Space savings: 76% reduction of weight as compared to the conventional model*
70% reduction of installation area as compared to the conventional model*
*: The comparison with our conventional model.

Shimadzu Corporation
www.shimadzu.com/an/