206-94965E

INSTRUCTION MANUAL
USER SYSTEM GUIDE
IRPrestige-21 (P/N 206-72010)

SHIMADZU FOURIER TRANSFORM INFRARED SPECTROPHOTOMETER

Read this instruction manual thoroughly before operation. Store the manual in a convenient location for future reference.

SHIMADZU CORPORATION
ANALYTICAL & MEASURING INSTRUMENTS DIVISION
KYOTO, JAPAN

Safety Precautions

The IRPrestige-21, a Fourier transform infrared spectrophotometer, is used for qualitative and quantitative analysis.

Strictly observe the following precautions for safe operation. Failure to comply may lead to a dangerous situation.

1. Use only for the specified types of analyses.
2. Follow Instruction Manual procedures. If not, hazardous situation may occur.
3. Observe all warnings and precautions.
4. Do not disassemble or modify the unit without the express approval of an authorized Shimadzu representative.
5. For service or repair, contact your Shimadzu representative.
6. The pages colored pink shows installation procedure for a service personel. Do not instal this instrament by customers by themselves.

CAUTION SYMBOLS

WARNING **Indicates a potentially hazardous situation which may result in moderate to serious injury, or death.**

CAUTION **Indicates a potentially hazardous situation which may result in instrument damage or minor injury.**

NOTE **Emphasizes essential information**

SAFETY SYMBOLS

 **High voltage**

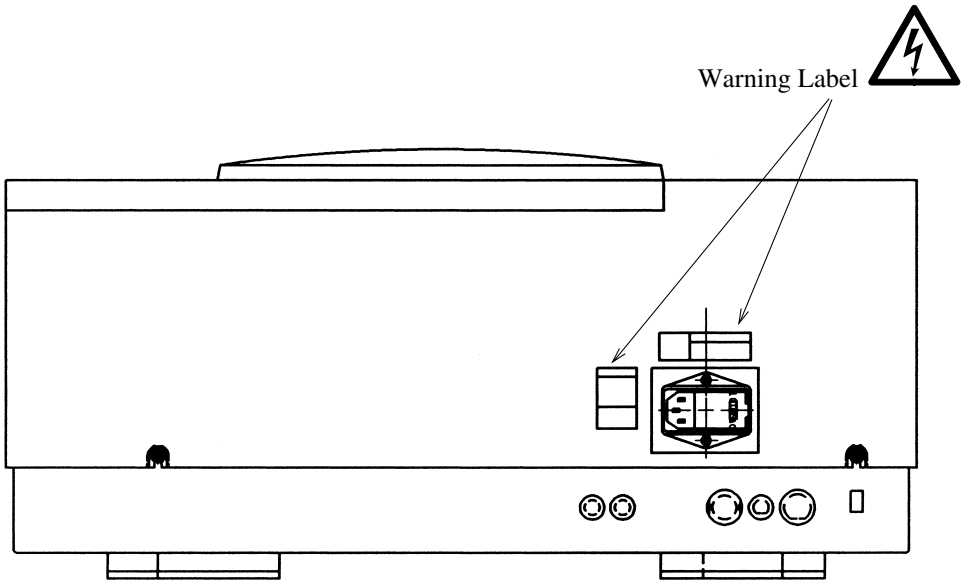
 **For operation and handling, refer to the instruction manual.**

Unit Warning Labels

WARNING

RISK OF ELECTRIC SHOCK

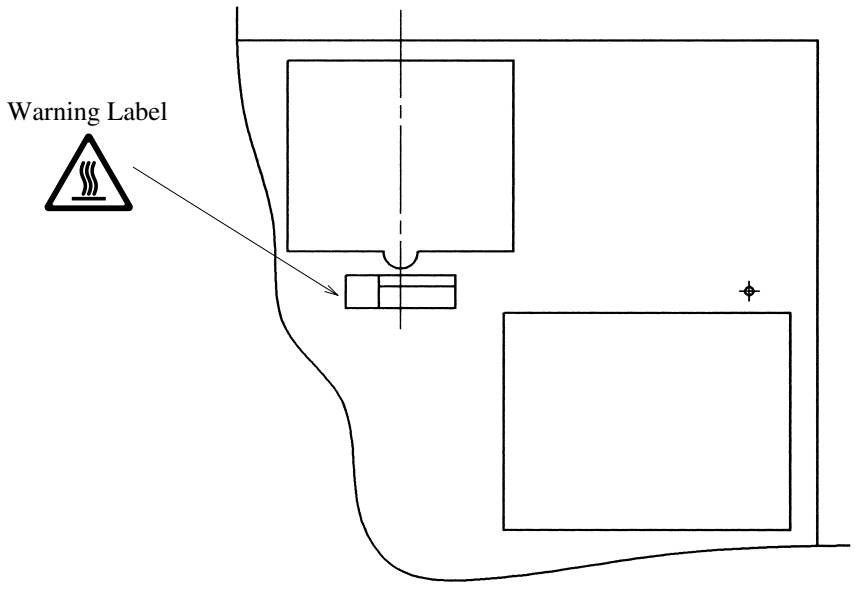
Do NOT remove cover. Contact your Shimadzu representative for service.



WARNING

RISK OF ELECTRIC SHOCK

Read instructions before changing a fuse or the inlet voltage.

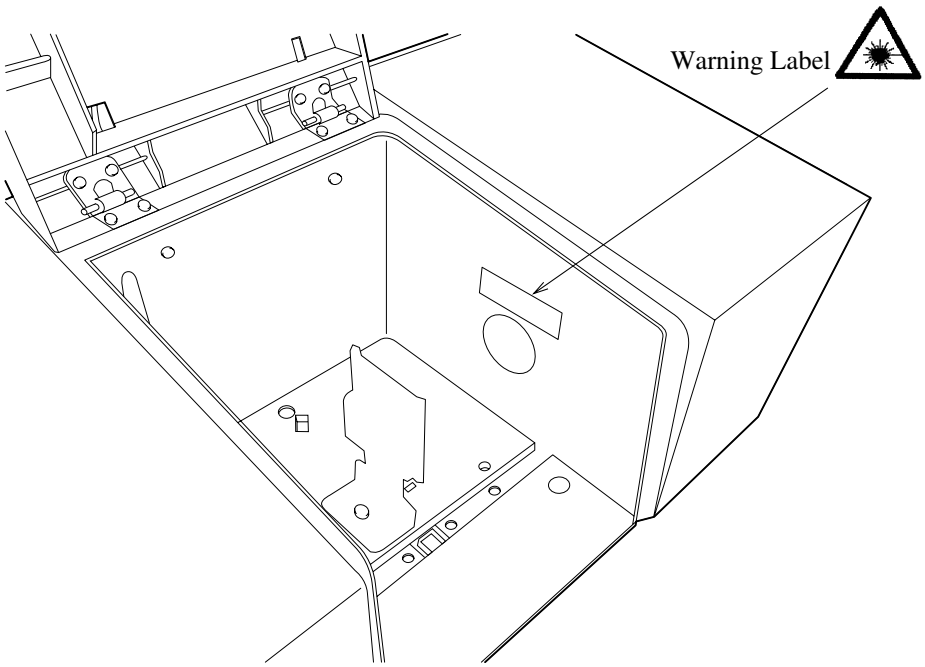


WARNING

LASER RADIATION

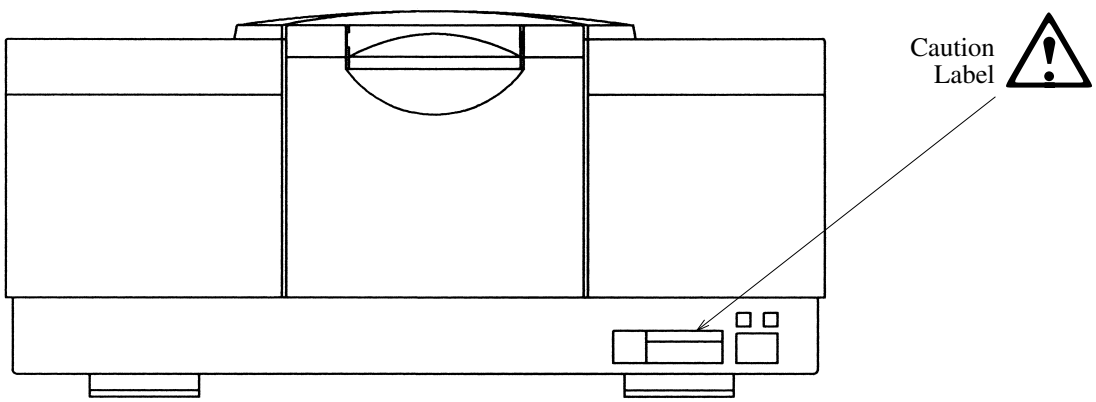
Do not stare into beam.

0.5mW max	Cw 632.8nm
CIASS2 Laser product	IEC 825-1 (1993)



CAUTION

When orange lamp is lighting, inside desicator is working.
If this orange lamp is not lighting, refer to instruction manual: user's system guide-troubleshooting immediately.



CAUTION Safety Precautions for Laser Users

The IRPrestige-21 uses a helium neon laser with an output of 0.5 mW, the strongest made by JDS Unipnase. When the IRPrestige-21 is on, the laser, Class II in the HEW classification (The Center for Devices and Rodiological Health, the U.S. Department of Health, Education and Welfare), is emitted continuously. It has two purposes in the system: sampling signal generation and optical axis adjustment. When the FTIR cover is on, the sampling signal laser is not visible. However, the optical alignment laser, a weak beam with 1/5 of the laser output (0.1 mW, maximum), is continuously emitted into the work area. Do not look directly at the laser beam.

Laser CAUTION label

Symbols found on the IRPrestige-21

Symbol	Definition
~	Current (AC)
|	Power ON.
○	Power OFF.

Regulatory Information

For Europe:

This product complies with the requirements of EMC Directive 89/336/EEC, Directive 93/68/EEC amending Directive 89/336/EEC, and Low Voltage Directive 73/23/EEC.

Product name	Fourier Transform Infrared Spectrophotometer
Model name	IRPrestige-21
Manufacturer	SHIMADZU CORPORATION ANALYTICAL INSTRUMENTS DIVISION
Address	1, Nishinokyo-Kuwabara-cho, Nakagyo-ku, Kyoto, 604-8511, Japan
Authorized Representative in EU	SHIMADZU EUROPA GmbH Albert-Hahn-Strasse 6-10, D-47269 Duisuburg, F.R.Germany
Authorized Representative in US	SHIMADZU SCIENTIFIC INSTRUMENTS, INC. 7102 Riverwood Drive Columbia, MD 21046 USA

Use of This Instruction Manual

The IRPrestige-21 Instruction Manual: User System Guide primarily describes the IRPrestige-21 hardware, including its unit description, installation and maintenance. Refer to the Instruction Manual: Operation Guide for operation procedures such as data acquisition and processing, and to the “Help” document which is included in IRsolution software itself for a detailed description of each command. For information about your PC and printer, refer to their individual product manuals.

This instruction manual consists of

Safety Precautions

1. Principles, Description and Function of IRPrestige-21
2. Specifications
3. Installation
4. Maintenance and Inspection
5. Troubleshooting
6. Index

When you want to know FTIR principles, Description or Functions, refer to Chapter 1 and 2.
When you want to know FTIR Installation or move to another room, refer to chopter 3.
When you want to know FTIR maintenance or trouble, refer to Chapter 4 and 5.

CONTENTS

Chapter 1 Principles, Description, and Functions of the IRPrestige-21

CONTENTS

1.1 Principle and Construction

The Fourier Transform InfraRed spectrophotometer measures an infrared spectrum by Fourier-transform of an interferogram.

The Physics of Fourier Transform Spectrophotometry

An FTIR uses one of several optical systems; the IRPrestige-21 relies on a Michelson interferometer (Fig. 1.1). After passing through the aperture, light is turned into a parallel beam by the collimator mirror and enters the beam splitter. A germanium film, deposited on a potassium bromide substrate via evaporation, comprises the beam splitter; it splits the single beam into two, reflecting one to the fixed mirror and transmitting the other to the moving mirror. Both mirrors reflect their beams back to the beam splitter; part of each returning beam is reflected and transmitted. The transmitted light from the fixed mirror and the reflected light from the moving mirror recombine and interfere with each other as they travel towards the collecting mirror. The interference is either constructive or destructive.

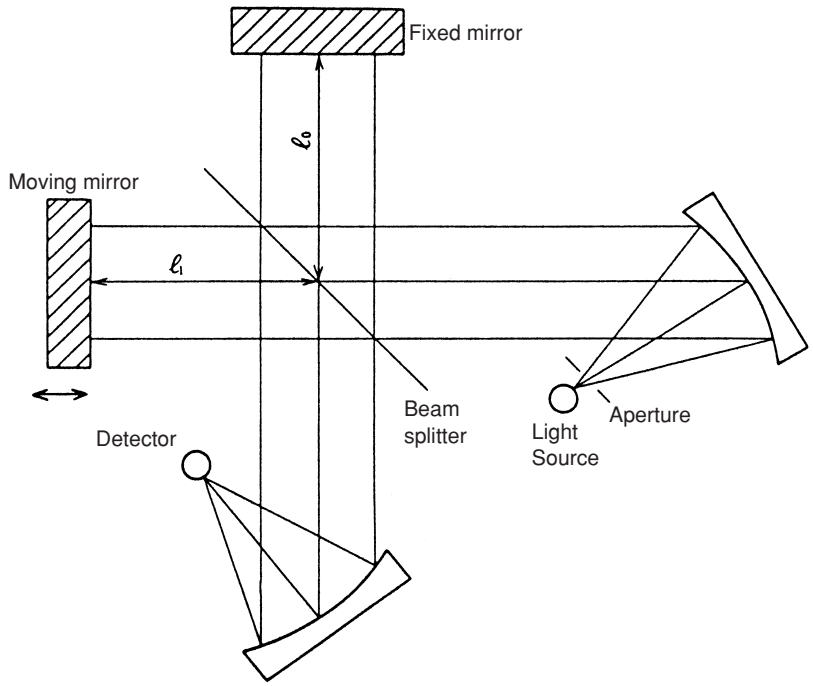


Fig. 1.1 Michelson Interferometer

Assume that the light source emits monochromatic light of wavelength λ (cm). When the distance l_0 between the fixed mirror and the beam splitter is equal to the distance l_1 between the moving mirror and the beam splitter, the optical path difference between the two beams, $\chi = 2 (l_1 - l_0)$, is equal to zero, and the beams are in phase. While in phase, the beams interfere constructively with each other (Fig. 1.2 A, B). As the moving mirror is displaced λ/4 cm, the optical path

difference becomes λ/2 cm, and the two beams are out of phase, interfering destructively (Fig. 1.2 A, C). Thus, the two beams interfere constructively with each other when $\chi = n\lambda$ and destructively when $\chi = (n + 1/2)\lambda$ where n is an integer.

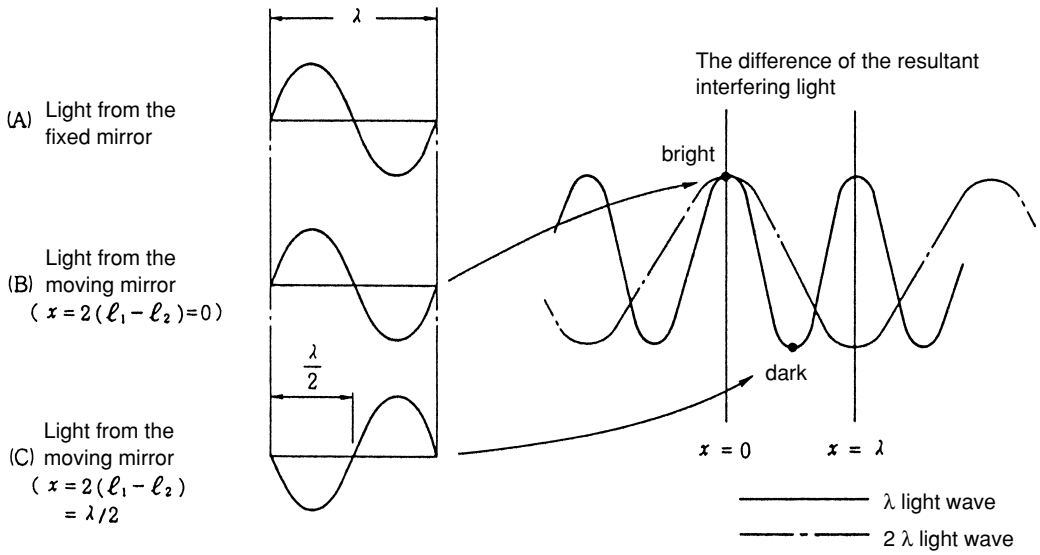


Fig. 1.2 Interference

Equation 1.1, extrapolated from the above principles, calculates the intensity I*(χ) of light (wavelength λ) incident to the detector.

$$I^*(\chi) = 4RTS(\lambda)\left[\frac{1}{2} + \frac{1}{2}\cos 2\pi\frac{\chi}{1}\right] \quad \text{..... (1.1)}$$

where R: energy reflected by the beam splitter
T: energy transmitted by the beam splitter
S (λ): radiation energy from the light source

The intensity of the light observed by the detector is a function of Equation 1.1. I(χ) denotes the light intensity, and the wave number σ (cm^{-1}) replaces the wavelength λ.

$$I(x) = 4RTS(\lambda) \bullet \frac{1}{2}\cos 2\pi\sigma\chi$$

$$= B(\sigma)\cos 2\pi\sigma\chi \quad \text{..... (1.2)}$$

where $B(\sigma) = 4RTS(\lambda) \bullet 1/2$

The signal I(χ) observed by the detector is called an interferogram, and 4RT is labeled beam splitter efficiency.

If polychromatic light is emitted instead of monochromatic light, I(χ) is given by the integration of 1.2 with respect to wave number.

$$I(\chi) = \int_0^{\infty} B(\sigma) \cos 2\pi\sigma\chi \, \delta\sigma \quad \text{.....} \quad (1.3)$$

Equation 1.3 demonstrates that I(χ) is a Fourier cosine transform of spectrum B(σ). Thus, an inverse Fourier cosine transform of I(χ) recovers the original spectrum B(σ).

$$B(\sigma) = \int_{-\infty}^{+\infty} I(\chi) \cos 2\pi\sigma\chi d\chi \quad \text{.....} \quad (1.4)$$

While the conventional dispersive spectrometer directly determines the intensity of B(σ) at certain wave numbers, the FTIR detector observes the interferogram I(χ) which must be Fourier transformed to obtain the spectrum.

1.2 Resolution and Apodization

Although Equation 1.4 maintains that the interferogram should be recorded from $-\infty$ to $+\infty$, such limits are impractical. In reality, the integration is limited to an optical path difference L, determined by the range of the moving mirror. The experimental spectrum B'(σ) differs from the theoretical spectrum B(σ) accordingly.

$$B'(\sigma) = \int_{-L}^{L} I(\chi)\cos 2\pi\sigma\chi d\chi$$

$$= \int_{-\infty}^{+\infty} A(\chi) I(\chi)\cos 2\pi\sigma\chi d\chi \quad \text{..... (1.5)}$$

$$\text{where} \quad A(\chi) = \begin{cases} 1 & \text{if } (\chi) \le L \\ 0 & \text{if } (\chi) > L \end{cases} \quad \text{..... (1.6)}$$

According to Convolution Theory,

$$B'(\sigma) = B(\sigma) * F(\sigma) \quad \text{..... (1.7)}$$

Where F(σ) is a Fourier transform of the function A(χ) in Equation 1.6.

$$F(\sigma) = 2L \sin(2\pi\sigma L)/(2\pi\sigma L)$$

$$= 2L \sin\chi(2\sigma L) \quad \text{..... (1.8)}$$

The measured spectrum B'(σ) is a convolution of theoretical spectrum B(σ) with F(σ). F(σ), a Fourier transform of A(χ), is called instrument function or instrumental line shape ILS.

Functions A(χ) and F(σ), represented by Equations 1.6 and 1.8 respectively, are given in Figure 1.3 (a). The function F(σ), as defined by Equation 1.8, first becomes zero at (= ± (1/2L), where the half-width value is 0.605/L. The greater the optical path difference L, the smaller the half-value width; when the moving mirror is driven further, the resolution improves.

The instrument function F(σ) involves marked submaxima, called side-lobes [Fig. 1.3 (a)]. If A(χ), as defined by 1.6, is replaced by the triangular function defined by 1.9, Equation 1.10 gives its Fourier transform.

$$A(\chi) = \begin{cases} 1 - |\chi/L| & \text{for } |\chi| \le L \\ 0 & \text{for } |\chi| > L \end{cases} \quad \text{..... (1.9)}$$

$$F(s) = L\sin^2(\pi\sigma L)/(\pi\sigma L)^2 = L\sin\chi^2(\sigma L) \quad \text{..... (1.10)}$$

Figure 1.3 (b) illustrates that the instrument function defined by 1.10 has worse separation, but smaller submaxima, than that defined by 1.8. Using A(χ) to reduce the instrument function submaxima called apodization; A(χ) is called the apodization function.

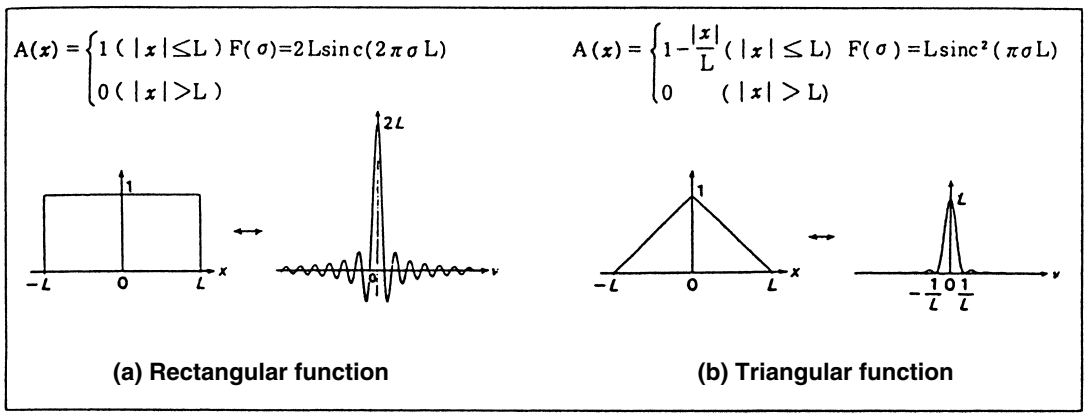


Fig. 1.3 Apodization with Rectangular and Triangular Functions

Table 1.1 lists the IRPrestige-21 apodization parameters and their characteristics.

Table 1.1 Apodization Function

Parameter	Apodization Function	Instrument Function	Half-width value	Submaxima residue
None, Box Car	$A(\chi) = 1$	$2L\,\mathrm{sinc}(2\pi\sigma L)$	0.605/L	− 21%
Triang	$A(\chi) = 1 - \frac{\lvert\chi\rvert}{L}$	$L\,\mathrm{sinc}^2(\pi\sigma L)$	0.88/L	+ 4.5%
Sqr. Triang	$A(\chi) = (1 - \frac{\lvert\chi\rvert}{L})^2$	$\{\frac{4L}{(2\pi\sigma L)^2}\}\,1 - \mathrm{sinc}(2\pi\sigma L)$	1.18/L	0.7%
Bessel	$A(\chi) = \{1 - (\frac{\chi}{L})^2\}^2$	$L\,(2\pi\times\sigma)^{5/2}\,J_{5/2}(2\pi\times\sigma)$	0.952/L	− 4.1%
Cos	$A(\chi) = \frac{1}{2}\{1 + \cos(\frac{\pi\bullet\chi}{L})\}$	$\frac{\mathrm{sinc}(2\pi\sigma L)}{2\pi\sigma(1 - 4L^2\sigma^2)}$	1.00/L	− 2.7%
Happ	$A(\chi) = 0.54 + 0.46\cos(\frac{\pi\chi}{L})$	$\{\frac{0.54}{\pi\sigma} + \frac{(0.46)\bullet 4\pi\sigma L^2}{\pi^2 - (2\pi\sigma L)^2}\}\sin(2\pi\sigma L)$	0.91/L	− 0.6%

Notes: (a) $A(\chi) = 0\ (|\chi| > L)$

(b) Ratio of the maximum submaxima peak size to the center peak size (shown in %).

The information in Table 1.1 supports using the None or Box Car (Rectangular Function) parameter for samples requiring high resolution, such as gas, and the Happ (Happ-Genzel Function) parameter, which has fewer submaxima peaks, when high resolution is unnecessary.

1.3 The FTIR Advantage

FTIR spectrophotometry offers at least three advantages: multiplex advantage (Fellgett advantage), aperture advantage (Throughput (Jacquinot) advantage), and wave number accuracy (Connes) advantage.

The multiplex advantage results from the accumulation and sorting of data. In one second with one scan, the FTIR measures a spectrum of all wave numbers. By continuing to scan for a specified period, one minute for example, and accumulating the results, a spectrum with a high S/N ratio is obtained.

The aperture advantage is created by the large FTIR aperture. FTIR results depend on the aperture area and the incident angle of light. When a large aperture is used, more of the light source is available to maintain a high-throughput optical system, giving the spectrum a high S/N ratio.

The wave number precision, or Cones, advantage is the result of the IRPrestige-21 He-Ne laser. The laser emits extremely stable monochromatic light, creating a spectrum with high wave number accuracy.

The three FTIR advantages extend many benefits:

1. Higher sensitivity measurement
2. Measures samples with low transmittance, a small sample size, or a thin layer of film on its surface.
3. Higher speed measurement
4. Higher wave number accuracy
5. Highly accurate spectrum subtraction

1.4 System Configuration of IRPrestige-21

This section briefly describes the system configuration of the IRPrestige-21.

The IRPrestige-21 consists of the interferometer and a personal computer.

The IEEE-1394 interface is used for communication between the interferometer and the personal computer.

Install the software "IRsolution" for controlling the FTIR to the personal computer, then operate the interferometer and execute data processing.

Two types of personal computers, the desktop type and the notebook type, are available. However, when using the infrared microscope which handles image data, the notebook type is not available.

Caution The software "IRsolution" for controlling the FTIR operates normally only in the Windows2000 (Service Pack 2 or later). In some personal computers, the IRsolution may not operate normally due to the effect of another software. While using the personal computer for operating the FTIR, do not start up any other software as much as possible.

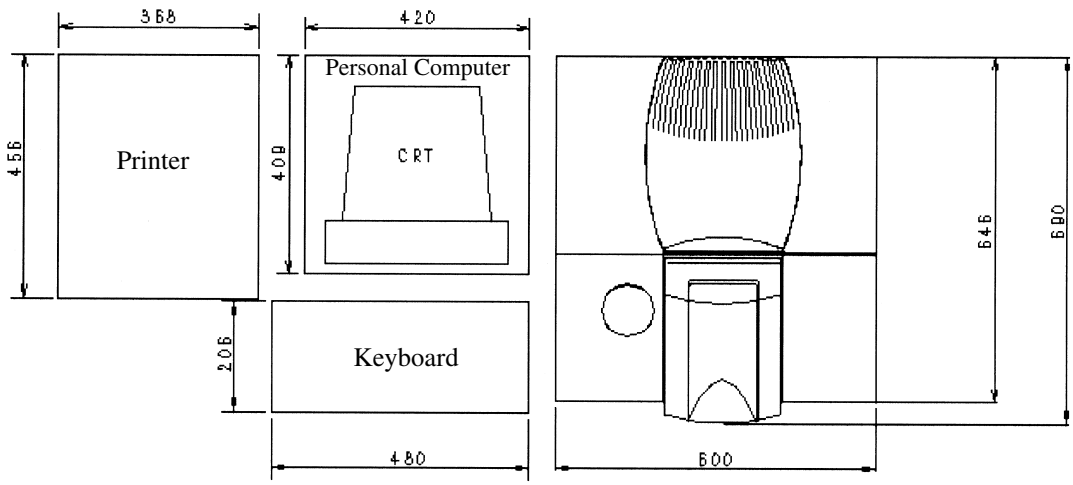


Fig. 1.4 Standard layout example of IRPrestige-21 system

1.5 Interferometer

1.5.1 Appearance

This section briefly describes the appearance and the functions of the interferometer.

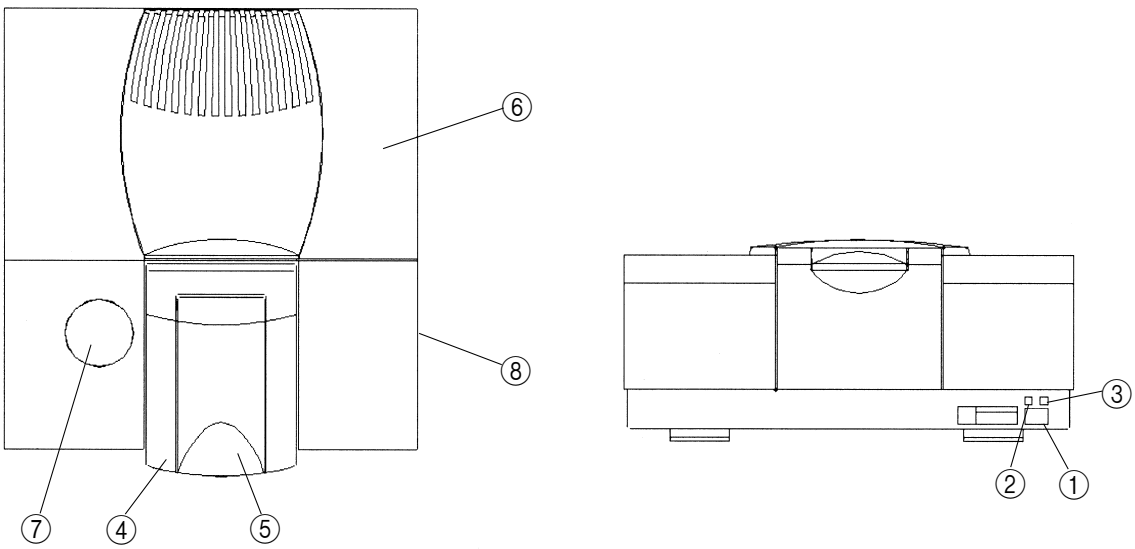


Fig. 1.5 Appearance (front view and top view) of interferometer

① Main power switch : Press the " | " side to turn on the main power of the interferometer. Press the " ○ " side to turn off the main power of the interferometer.

② Power indicator lamp (green) : Lights up when the main power of the interferometer is turned on.

③ Standby power indicator lamp (orange) : Lights up while the standby power of the interferometer is ON. means AC Cable is connected to power source While the standby power is ON, the dry unit inside the interferometer is operating.

④ Sample compartment cover : Open this cover to set an optional accessory to the sample compartment or measuring a large sample, then set the accessory or the sample.

⑤ Sample compartment lid : Open this lid to measure a small sample such as liquid cell or tablet, then set the sample to the sample compartment.

⑥ Top cover : Open this cover to replace the beam splitter with one of another type offered as an option or replace the light source, and open the cover inside the interferometer, then replace the beam splitter or the light source.

⑦ Cover for MCT : Remove this cover to install the MCT detector offered as an option,.

⑧ External beam outlet cover : To install the option such as infrared microscope, remove this cover and connect it.

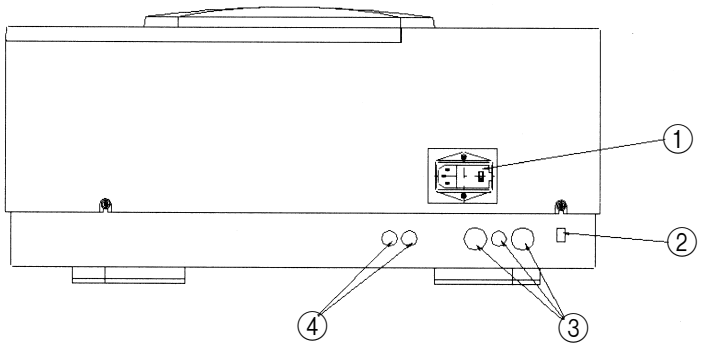


Fig. 1.6 Appearance of interferometer (rear view)

① AC inlet (with fuse holder) : Connect the power cable here. Two fuses are accommodated here.

② IEEE-1394 connector : Connect IEEE-1394 cable here to the personal computer.

③ Optional connector mounting holes : Connect the connector here to use an optional MCT detector such as infrared microscope. Caps are attached here. Not remove them unless using options.

④ Purge tube inlets : Insert tubes here and connect the tubes to the piping inside the interferometer to purge the interferometer or the sample compartment with dry air, etc.

1.5.2 Inside of sample compartment

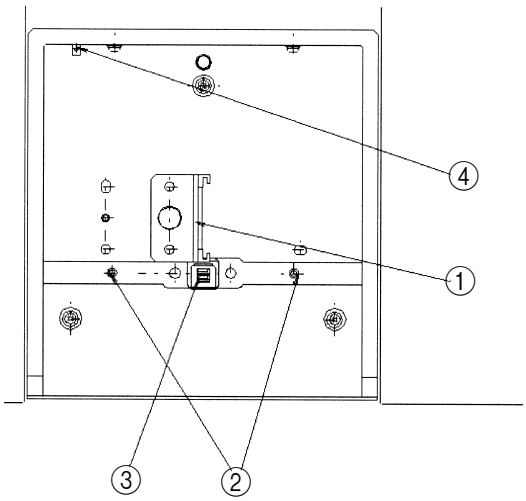


Fig. 1.7 Inside view of sample compartment

① Cassette : When using a liquid cell or 5 cm gas cell slide it into the groove here from the top. When using a KBr tablet, insert it into the cassette hole from the right side. Remove the M5 mounting screws to remove the cassette. When using a 10 cm gas cell, install the cassette to the mounting holes on the left side of the usual installation position.

② Accessory mounting guide pins : When installing an option such as diffuse reflectance attachment or ATR attachment, install it so that these guide pins are aligned with the guide holes on the rear of the attachment.

③ Accessory recognition terminal : When installing an option with the accessory recognition function to the sample compartment, connect it to the sample compartment through this terminal so that the option type can be recognized. Take care not to touch this terminal or spill liquid on it.

④ Auto sample changer connector : To use an option with the auto sample changer, connect it here.

1.5.3 Optical system

The figure below shows the optical system of the IRPrestige-21.

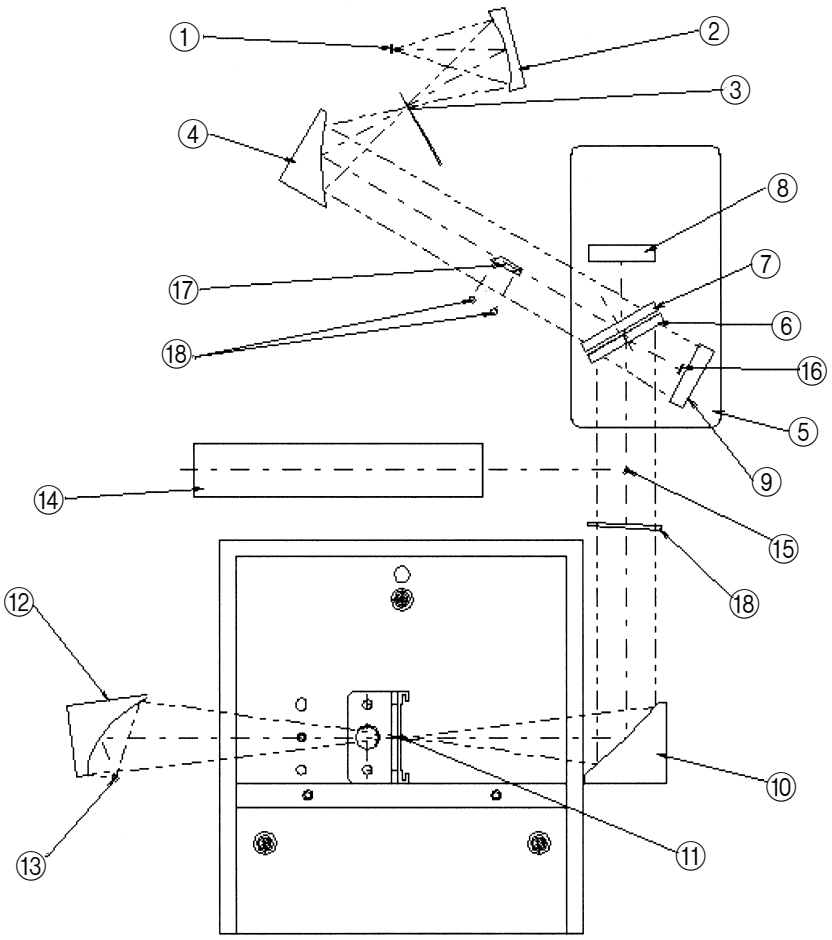


Fig. 1.8 Optical system of IRPrestige-21

The beam from the light source ① is reflected once by the spherical mirror ②, then converged in the aperture ③ position. The beam which has passed through the aperture is reflected by the collimator ④, made into parallel beam, then introduced into the interfer-

ometer ⑤. The IRPrestige-21 has the Michelson interferometer whose incident angle is 30°.

The infrared beam introduced into the interferometer is divided by the beam splitter into the moving mirror ⑧ and the fixed mirror ⑨. Each reflected beam becomes the interfered beam on the beam splitter, and goes to the converging mirror ⑩. This fixed converging mirror is equipped with the auto alignment function which always realizes the maximum interference efficiency.

By the converging mirror ⑩, the parallel infrared interfered beam makes a light source image ⑪ in the center of the sample compartment. Usually, set a sample in this center of the sample compartment, then measure it. The beam which has passed through a sample is reflected by the converging mirror ⑫, converged in the detector ⑬, then detected as the interferogram.

The aperture size is automatically selected in accordance with measurement and resolution. And the aperture can be set manually without regard to measurement and resolution. For the details, refer to the "Help" document included in the software.

The image size in the sample compartment in each resolution is as follows (when the standard light source is used).

4 cm^{-1} or more	: Approx. □10 mm
2 cm^{-1}	: Approx. ϕ6.8 mm
1 cm^{-1}	: Approx. ϕ4.7 mm
0.5 cm^{-1}	: Approx. ϕ3.4 mm

When using an accessory such as KBr tablet which limits the image size in the center of the sample compartment, the optical aperture effect is obtained. As a result, peak wavenumber deviation way occurs depending on existence of an option. To cope with this, execute background measurement by using a same option (without sample) used in sample measurement.

1.5.4 Light source

For the IRPrestige-21, the ceramic light source of high luminance and long life is used as standard. This light source can be used together with the optional, low wavenumber type beam splitter (cesium iodide = CsI).

When the near infrared type beam splitter (fluorine calcium = CaF_2) is used, use the WI (tungsten halogen) lamp as the light source. In this case, install the optional light source selector unit so that the light source to be used can be changed over.

1.5.5 Beam splitter

For the IRPrestige-21, the beam splitter which Ge (germanium) is evaporated on the KBr (potassium bromide) substrate is used as standard.

The measurement wavenumber range is from 7,800 to 350 cm^{-1}.

When measuring up to low wavenumber (5,000 to 240 cm^{-1}), replace the standard beam splitter with the optional beam splitter with the CsI (cesium iodide) substrate.

Caution Because these beam splitters have deliquescence and are very weak to humidity, take care to handle them. If their element surface is damaged by dew condensation, etc. once, they cannot be used any more. To cope with this, moisture resistant coating is applied on these beam splitters used in the IRPrestige-21, and the auto dry unit is built in the main unit. Usually, no problem is expected while the IRPrestige-21 is operating. However, when replacing the beam splitter or removing it from the main unit and storing it individually, pay rigid attention to the temperature and the humidity of the room and the storage area. And never touch the surface of the beam splitter. (Even if it becomes stained, cleaning is impossible.)

The storage humidify of the beam splitter is 40%RH or less. When removing it from the main unit and storing it individually, use a commercial desiccator, etc.

1.5.6 Detector

For the IRPrestige-21, the DLATGS detector of high sensitivity equipped with the temperature controller is used as standard. This detector can be used together with the low wavenumber type option (CsI beam splitter) or the near infrared type option (WI lamp and CaF_2 beam splitter). However, it is not recommended to use this detector for near infrared measurement because the sensitivity is not enough for such measurement. Accordingly, when using the near infrared type option, use the InGaAs (indium/gallium/arsenic) detector with higher sensitivity. In this case, separately install the detector selector unit so that the detector to be used can be changed over.

The table below shows the relationship among each measurement wavenumber range, light source, beam splitter and detector.

	Measurement wavenumber range	Light source	Beam splitter	Detector
Standard	7800 to 350 cm^{-1}	Ceramic	KBr	DLATGS
Low wavenumber	5000 to 240 cm^{-1}	Ceramic	CsI	DLATGS
Near infrared	12500 to 3800 cm^{-1}	WI	CaF_2	InGaAs

1.5.7 Dry unit

The IRPrestige-21 keeps the inside of the interferometer at low humidity by driving the dry unit even while the IRPrestige-21 is not used. Accordingly, always let the power plug of the IRPrestige-21 be connected to the AC power supply to keep power supply. Confirm that the orange LED (standby power indicator lamp) in the lower right portion of the front face is lit. If it is expected that the main power supply will be OFF for a long time, remove the beam splitter and individually store it in the desiccator, or put new silica gel into the silica gel case of the interferometer main unit. While the main power supply is OFF, silica gel should be replaced once in approximately two weeks.

Note When samples with reflectivity such as optical filters or films are scanned in the Middle IR mode, pseudo peaks may be obtained at the doubled frequency (Near IR region) of the original absorption because IR beam is returned to the interferometer. Please use the NIR kit to avoid this phenomenon.

1.6 Electrical System

After reaching the detector, the interferogram undergoes several treatments before being sent to the computer. It is amplified by the preamplifier and the automatic gain amplifier, passes through high-pass and low-pass filters, and is digitized by the 20-bit A/D converter. After the signal is digitized into the interferometer memory, it travels through the SCSI interface to the PC where IRsolution transforms the interferogram into a spectrum.

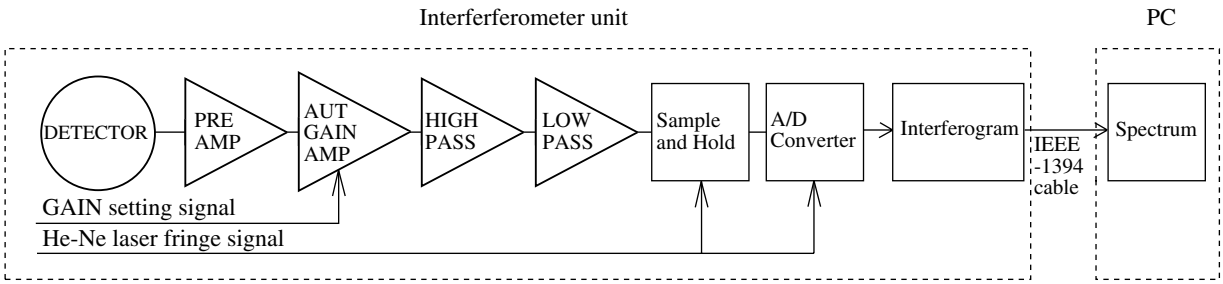


Fig. 1.9 Signal Processing System in the IRPrestige-21

Chapter 2 Specifications

CONTENTS

2. 1 IRPrestige-21 Specifications

The specifications of IRPrestige-21 is as follows.

The IRPrestige is not conformance with IEC60601.

2.1.1 Hardware (except PC)

Interferometer	Michelson interferometer (incident angle is 30˚C)
	Advanced Dynamic alignment system
	With auto drier, sealed interferometer
Optical system	Single beam
Beam splitter	Ge coated on KBr (for mid infrared, standard)
	Ge coated on CsI (for mid/far infrared, option)
	Si coated on CaF_2 (for near infrared, option)
Light source	Cooling type ceramic (for mid/far infrared, standard) (guaranteed for 3 years)
	Tungsten lamp (for near infrared, option)
Detector	DLATGS detector with temperature control system (for mid/far infrared, standard)
	MCT (Hg-Cd-Te) detector, liquid nitrogen cooling type (for mid infrared, option)
	InGaAs detector (for near infrared, option) (Note 1)
Wavenumber range	7800 to 350cm^{-1} (standard)
	5000 to 240cm^{-1} (FIR option)
	12500 to 3800cm^{-1} (NIR option)
Resolution	0.5cm^{-1}, 1cm^{-1}, 2cm^{-1}, 4cm^{-1}, 8cm^{-1}, 16cm^{-1} (mid/far infrared)
	2cm^{-1}, 4cm^{-1} , 8cm^{-1}, 16cm^{-1} (near infrared)
Wavenumber accuracy	± 0.125cm^{-1} (Note 2 and 3 below)
S/N ratio	40,000 : 1 (mid infrared)
	(Peak-Peak, Resolution 4cm^{-1}, around 2100cm^{-1}, integrated for 1 minute)
Mirror speed	3 step (2.8, 5, 9mm/sec.) (mid/far infrared) In the case of NIR, only 28mm/sec
	One times integration at 4cm-1 takes about 2.0 to 3.0 sec. (mid/far infrared)
Data sampling	He-Ne laser used (guaranteed for 30 months)
Gain	Automatic or manual (× 1 to × 128)
Sample compartment	Automatic recognition system of accessories
	200 (W) × 230 (D) × 170 (H) mm
	Center focus
Dimensions	620 (W) × 680 (D) × 290 (H) mm
Weight	54kg

(Note 1) MCT detector and InGaAs detector can not be used at the same time.

(Note 2) Resolution and wavenumber accuracy of the FTIR are determined by the wavenumber interval of spectral data. Since the maximum data interval of IRPrestige-21 is 0.25cm^{-1}, the peak position can be read at an accuracy of ± 0.125cm^{-1}. In case of the asymmetric peak, however, the accuracy for reading the peak position should be ± 0.25cm^{-1}.

(Note 3) The calculation wavenumber accuracy based on the wavelength of the He-Ne laser is ± 0.0lcm^{-1}.

2.1.2 Software

OS	Microsoft Windows 2000 (Service Pack 2 or later)
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
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
Print	Report generator function
Display	Compression of wavenumber axis, Enlargement/reduction, Auto scale, Overlap, Stack display, Shift display
Edit	Copy, Cut, Paste
Others	Customize 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 to FDA 21CFR Part11
Recognition of accessories	Automatic recognition of installed accessories, Automatic setting of measurement parameters, Automatic execution of macro program

2.1.3 Others

Installation site	Temperature : 15 to 30˚C
	Humidity : 70% or less, No dewing condensation
Utility (Note 1)	100/120/220/230 VAC, 50/60 Hz, 240 VA (at used), 4.5 VA (at standby)

(Note 1) The power for a computer is required separately.

Chapter 3 Installation

CONTENTS

3. 1 Inspecting Standard Accessories

Warning The Shimadzu service engineer shall install the IRPrestige-21 to assure safety. The customer shall not install it.

Note If the cold IRPrestige-21 is brought into a warm room, leave the IRPrestige-21 for approximately 2 hours to prevent dew condensation in the interferometer, then unpack the interferometer (especially in winter).

After unpacking, confirm that all parts are included in accordance with the standard accessory list shown below.

Table 3.1 Standard Accessories

	Part name	Quantity	Part No.
1	IRPrestige-21 Interferometer ASSY	1	206-72010-91 (100V) -92 (120V) -38 (220V/230V/240V)
2	Beam splitter ASSY	1	206-71721-91
3	IRsolution	1	206-72328-91
4	Polystyrene film	1	202-30689-01
5	AC cable (110V/120V)	1	206-13774
	or (220V/230V/240V)	1	071-60814-06
6	Fuse 6.3A (110V/120V)	1	072-02004-24
	or 4.0A (220V/230V/240V)	1	072-02004-22
7	Silica gel	1	200-53655
8	Instruction manual (User's System Guide)	1	206-94965
9	Instruction manual (Operation Guide)	1	206-94967
10	Instruction manual (Validation)	1	206-94978
11	Supplemental Disk	1	206-72407-91

Note

1. The personal computer, the IEEE-1394 interface and the printer are not included in standard accessories. Separately prepare them. We can offer the preinstall package in which the interface and the software are already installed. Omit “3.7 Introduction of Software” to use the preinstall package,.
2. The IRPrestige-21 is equipped with the minimum required instruction manual in the printed form under consideration of the global environment. The detailed description of commands required to operate the IRPrestige-21 is given in the electronic document (Help) attached to the software. Refer to it.

3. 2 Installation Environment for Equipment

Note Install the IRPrestige-21 at the following site.

1) Free from the location of strong vibration.
2) Free from the location of much dust and corrosive gas.
3) Free from the location where is exposed to direct sunlight.
4) Free from the location of high temperature and high humidity.
   Temperature and humidity range for assuring performance ; 5 to 30°C, RH 70% or less
   Temperature and humidity range for installation environment; 5 to 35°C, RH 70% or less (60% or less if 30°C or more)
   If the installation environment exceeds the above range, we recommend that you shall use an air conditioner. In addition, avoid the location where easily generates the dew condensation (near the heater).
5) Install the equipment far from the device which generates strong magnetic field and high frequency.
6) Total weight of the interferometer and the personal computer is about 100kg. Install the equipment on the flat table that withstands this weight.
7) The slit for ventilation is provided in the rear portion on the top of the IRPrestige-21. Avoid any layout in which this slit is covered.
8) For the IRPrestige-21, the internal dry unit is operating even while the power switch on the front is OFF. Accordingly, when the power should be completely turned off due to an abnormal occasion, the power plug should be disconnected. Adopt a layout in which the power plug can be easily disconnected.
9) Make sure to install it in a room equipped with a ventilation device to use the IRPrestige-21 after purge with N_2 gas. Usually, use N_2 gas for industrial use (whose purity is 99.99%) though the requirement of the purity may vary depending on the purpose of analysis.

The figure below shows the standard installation layout of the IRPrestige-21.

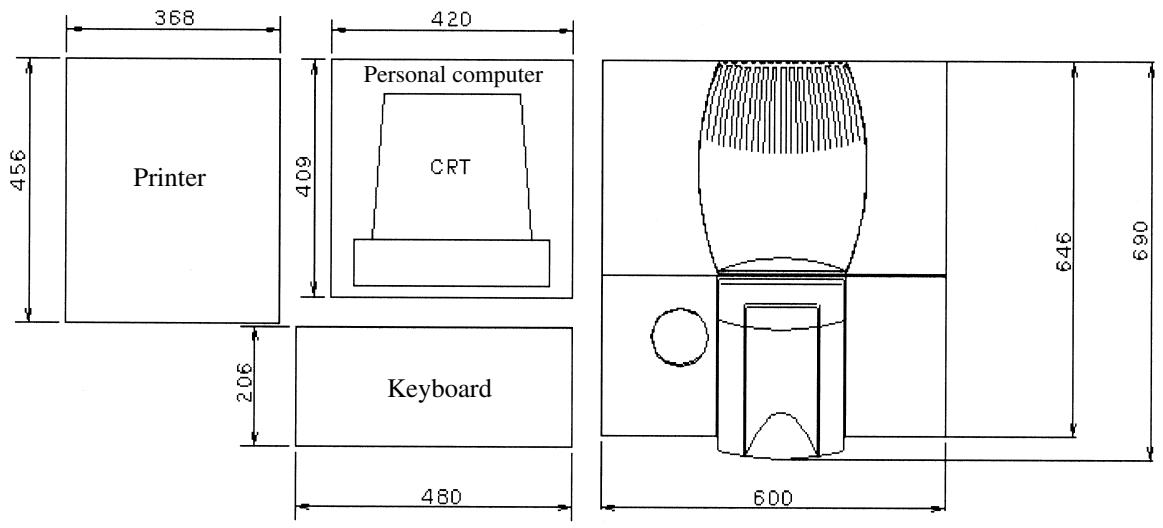


Fig. 3.1 Standard layout example of IRPrestige-21 System

3. 3 Installing the Interferometer and Removing the Clamp

Warning Installation of this equipment is to be performed by our service engineer. Do not install by the users by themselves.

Caution When the equipment is carried in the warm room, wait approximately two hours before opening the package of the interferometer in order to prevent dew condensation on it. (Especially cold term)

1) Unpack the interferometer ASSY and place it on the table to bring the back of the unit forward. When carrying the interferometer, hold the bottom of the chassis. Since the interferometer ASSY weighs about 55kg, carry it with two or more persons.
2) Loosen six screws fixing the external cover of the interferometer and remove the cover.
3) Loosen two screws (① in the figure 3.2) that clamp the optical bench of the interferometer. Completely remove front one of them.
4) Next, remove the clamp rod of the moving mirror of the interferometer. First, loosen and open the lid (② in the figure 3.2) to see the top of the moving mirror clamp rod (③ in the figure 3.2).
5) Insert the removed M5 screw into this screw hole of the clamp rod and pull it out to remove it. Attach this removed clamp rod into the optical bench hole (④ in the figure 3.2) for storage. Also, attach the M5 screw on the previous position. (Do not tighten)
6) Close the lid of internal cover removed in 4) again.
7) Attach the external cover removed in step 2).

Note Before transporting the equipment, be sure to clamp the moving mirror and the optical bench in the reversed step of above procedure. If the system is transported without being clamped, it may be damaged. In the case, for example when moving the system from one table to another table in the room, clamping is not necessary, but be careful not to drop or give strong impact.

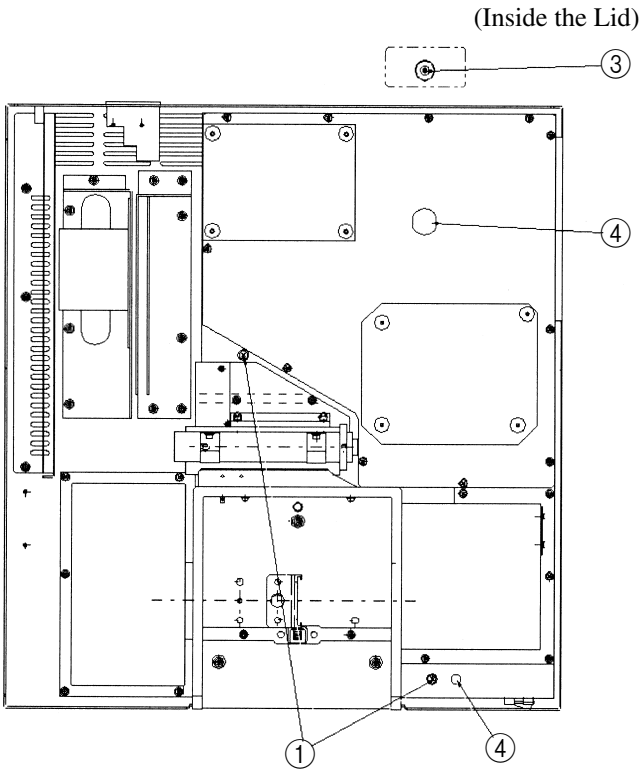


Fig. 3.2 Removing the clamp

3. 4 Confirming the Power Selector Switch and Fuse

1) The setting of input power for the interferometer unit of IRPrestige-21 is normally adjust to the supply voltage in the area where the equipment is used. By using the voltage selector switch and by changing the fuse and AC cable of AC inlet (① in the figure 1.6), voltage of 100V, 120V, 220V, or 230V AC can be used. Before use, check that the power supply switch indicates the supply voltage used. For input of 220 VAC, use the inlet voltage at 230 VAC.

2) Follow the procedure shown below for changing the voltage or replacing the fuse.

Caution Rating and type of fuse
Be sure to replace the fuse specified as below.
Supply voltages ; 100V, 120V : Part No. 072-02004-24, 125V, 6.3AT
Supply voltages ; 220V, 230V : Part No. 072-02004-22, 250V, 4.0AT

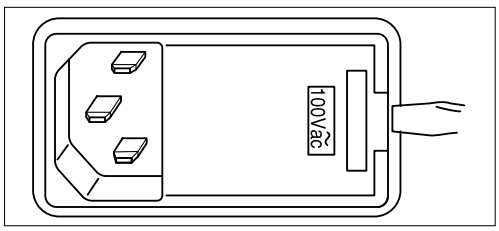


Fig. 3.3 (a)

1) Be sure to disconnect AC cable. Insert the Fillister head screwdriver, softly twist it to open the lid of AC inlet.

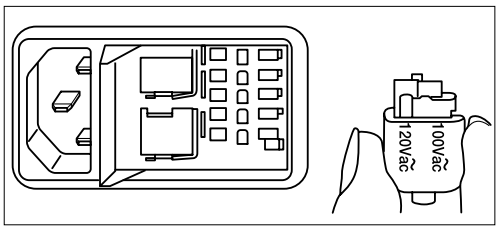


Fig. 3.3 (b)

2) To change the setting of voltage setting drum, once remove the drum.

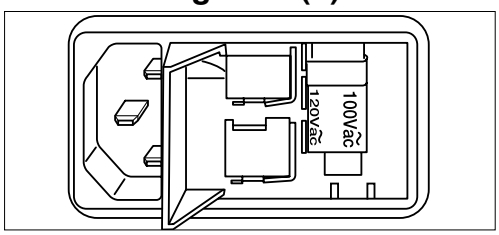


Fig. 3.3 (c)

3) Mount the drum so that the display of the set voltage is arranged to the upper portion.

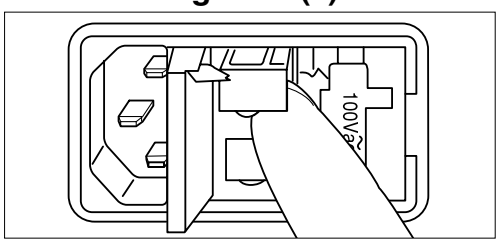


Fig. 3.3 (d)

4) Place your finger to the ↓ lever to pull out the fuse box. If the fuse differs from the given power capacity and type, put the new fuse in the fuse box and return it to the previous status. Put it so that the arrow of the fuse box is set at ↓ direction.

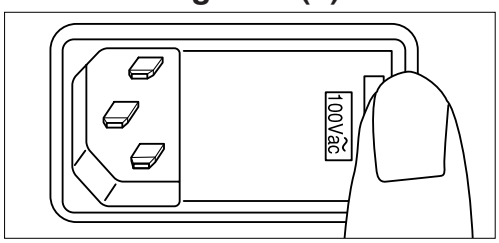


Fig. 3.3 (e)

5) Close the lid of the AC inlet.

Place the interferometer so that the front face is placed toward you after the works above are completed.

3. 5 Installing the IEEE-1394 Interface to Personal Computer

If the IEEE-1394 interface is not provided as standard in the personal computer to be used, separately install it. For the installation procedure, refer to the instruction manuals of the personal computer and the IEEE-1394 interface.

3. 6 Wiring the Cables

1) Connect the connector of the IEEE-1394 interface of the PC to the connector on the rear face of the interferometer unit through the cable.

2) Connect the AC cable of standard accessory. The IRPrestige-21 operates whichever frequency of 50Hz or 60Hz is applied. Confirm that the indicator lamp “Stand By” in front of the equipment lights up if the AC cable is connected.

Refer to each instruction manual for the personal computer and the printer connection.

Warning ELECTRIC SHOCK

Power supply cable of this equipment is 3 wire system containing the grounding wire. Insert it into 3 wire system receptacle and ground is surely. For 2 wire system receptacle, be sure to make grounding from GND terminal of the power supply grounding adapter.

Caution FLUCTUATION OF SUPPLY VOLTAGE AND CAPACITY OF POWER SUPPLY

Fluctuation of supply voltage and capacity of power supply for IRPrestige-21 is 100/120/220/230/240V ± 10%, 240VA, 50-60Hz. Confirm the capacity of power supply, including the power for personal computer. If the supply voltage is unstable or capacity of the power is insufficient, the equipment may not operate correctly. If fluctuation of supply voltage exceeds ± 10%, use the separate stabilization power unit.

Note The dry unit is built in the IRPrestige-21. This dry unit is driven to keep the humidity in the interferometer while the equipment being stopped. Connect the AC cable even if the equipment is not used. Do not turn off the power supply. The consumption power for dry unit is 4.5 VA.

Note The control and calculation in the IRPrestige-21 is performed through the microcomputer. You cannot share the power with the device which generates the spike noise with pulse shape.

3. 7 Installing the Software

When your computer controls the IRPrestige-21/FTIR-8000 series, an instrument driver program must be installed. When the PC is for the data manipulation and/or printing, not for FTIR control, installation of instrument driver is not needed.

3.7.1 Installation of the driver program for the IRPrestige-21

A driver program for the IRPrestige-21 should be installed to control it.

1. Wire the IRPrestige-21 and your PC by refereeing to the section [Wiring the Cabled] of the Instruction Manual - User's System Guide.
2. Turned them ON, and then Windows automatically recognizes the IRPrestige-21 with Plug & Play function.
3. Then Windows requests installation of the driver program. When Windows asks the place to find the driver, check [CD-ROM drive] in the Driver setup wizard dialog box.
4. Insert the [IRsolution] installation CD-ROM into your CD-ROM drive. When the Installation program of IRsolution starts, cancel it by clicking the <Cancel> button.
5. Follow the message on the screen. Then Windows automatically installs necessary drivers.
6. Install IRsolution software in next step.

Note "FTIR-2010", which is displayed on the found hardware wizard dialog box, is a module name of IRPrestige-21.

3.7.2 Installation of the IRsolution software

Install the IRsolution software with the following procedure.

1. When the IRsolution Install CD-ROM is in the CD-ROM drive, Click the <Start> button, and then select the [Run] command.
   Select "setup.exe" on the CD-ROM drive, and then click <Run> button.
   The Install program starts.
2. In another case, prepare the [IRsolution] install CD-ROM.
   Turn on the power of the personal computer to start up the Windows.
   If any software is running, terminate all of them.
   Insert the CD-ROM into the CD-ROM drive.
   The setup program automatically starts up. Execute "setup.exe" if setup program does not run

automatically.

3. Proceed following prompts on the screen. Then the [Select Component] window opens.

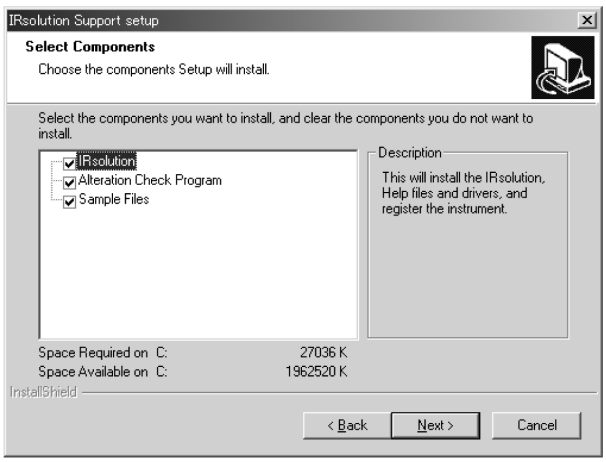


Fig. 3.4 Select Component

4. Select components to be installed. Select all components when the IRsolution is installed newly. Select necessary components when the software is updated. After selection of the components, click the <Next> button.

Table 3.1 Setup Components

Setup	Description
IRsolution	Main Component of the IRsolution software
Alternation Check Program	Alternation Check program to evaluate that the IRsolution software is not altered.
Sample File	Sample files, libraries, print templates, macro programs

5. Install the IRsolution main component..
6. The [Please give in CD key for this product] window opens.

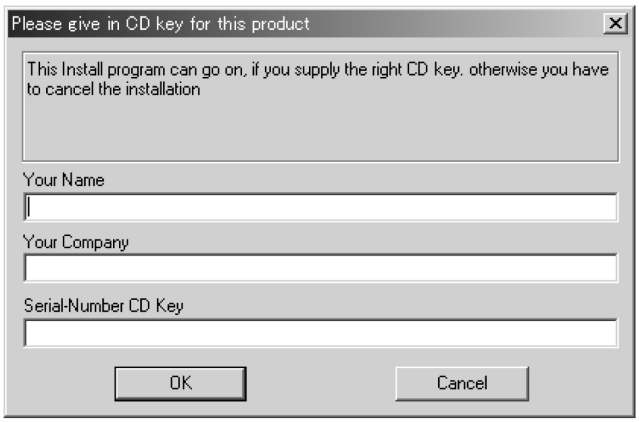


Fig. 3.5 Please give in CD key for this product

7. Input [Your Name], [Your Company]. Input the CD Key written on the CD-ROM package onto the [Serial Number CD Key]. If some of the information is missing or input CD Key is not correct, you cannot proceed to next step. After inputting information, click the <OK> button.
8. Proceed following prompts on the screen. Then the [Chose Destination Location] window opens. Specify the destination folder to be installed. The default folder is used usually. Click the <Browse> button to change the destination.

Fig. 3.6 Chose Destination Location

9. Click the <Next> button to proceed to next step, then the [Backup Replaced File] window opens. Click the <Next> button with the default setting.

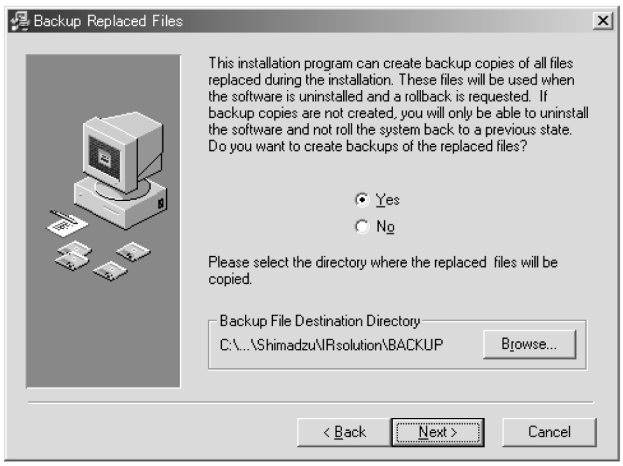


Fig. 3.7 Backup Replaced File

10. The [Select Component] window opens Select components of the IRsolution main components to be installed. Following components can be installed.

Table 3.2 Setup Components (IRsolution)

Setup	Description
Program	The IRsolution main body
Help	Help message file of the IRsolution
GLP mode	Installs the IRsolution on the GLP mode to support the GLP/GMP. Electric Signature function is available on the GLP mode. You cannot switch the GLP/non-GLP mode after installation.
Support for hardlock protected libraries	Installs the hardlock driver to use protected libraries with a protection key (dongle).

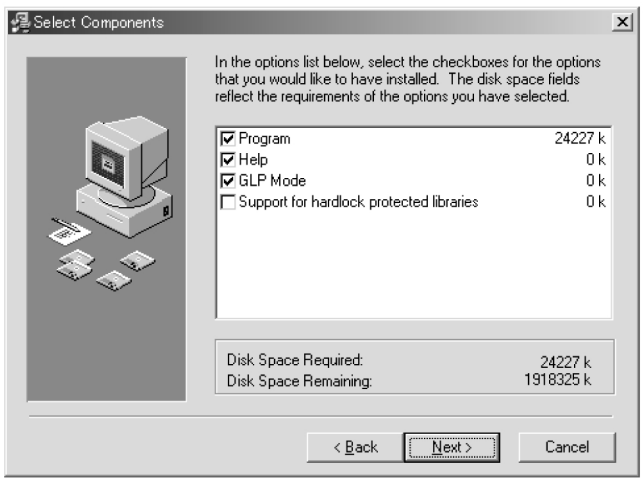


Fig. 3.8 Select Component

11. Put check marks on the necessary components. Click the <Next> button after setting.
12. The [Special Shortcuts] window opens. Put a check mark on the place you want to have short-cut icons. The default setting is usually used. Click the <Next> button.

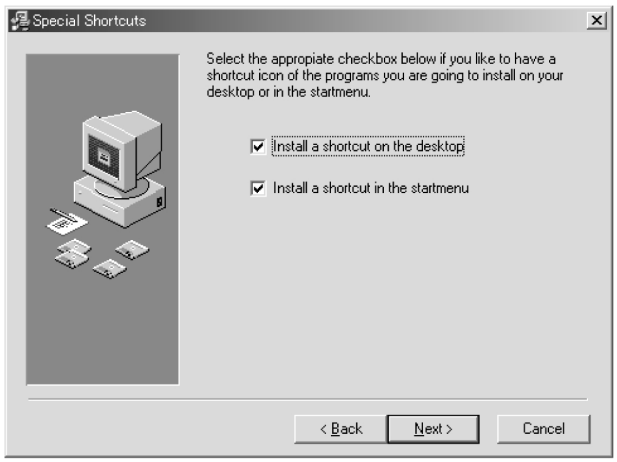


Fig. 3.9 Special Shortcuts

13. Proceed with following the prompts on the screen. The [Installation Completed] window opens when the IRsolution main body is installed correctly.

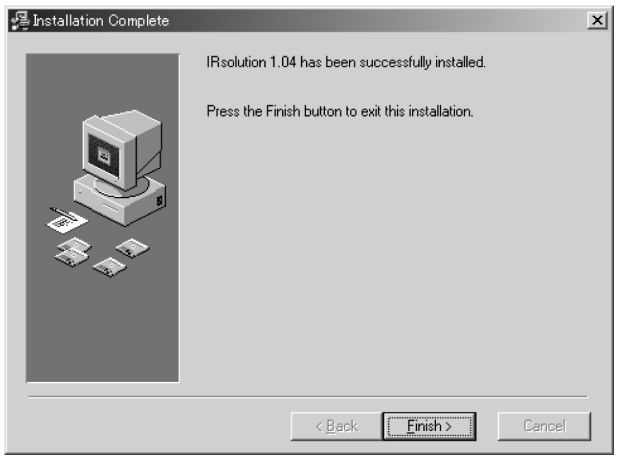


Fig. 3.10 Installation Completed

14. Click the <Finish> button to install the Alternation Check Program and Sample Files.
15. When all selected components are installed, the [Install Shield Wizard Complete] window opens. Click <Finish> button.

Fig. 3.11 Install Shield Wizard Complete

16. Install the Supplemental Disk in the next step.

3.7.3 Installation of the Supplemental Disk

Install the Supplemental Disk to update files and programs for the IRsolution software.

1. Set the supplemental disk in the floppy disk drive in your computer.
2. Click the <Start> button, and then select [Run] command from the menu.
3. Input "a:¥Setup.exe" in the file name and click <Run> button.
4. Run a set-up program, and updated files and programs are installed.

(Note) The contents of files and programs which are updated by a supplemental disk (P/N 206-72407-91) are;.

- Bug fixing of the EP/JP validation program
- Bug fixing (printing) of the ASTM validation program
- Updating the Alteration Check Program because of updating the EP/JP/ASTM validation programs.

3.7.4 Selecting an Instrument

Setup the model of Instrument to be connected.

1. Activate the IRsolution software. Double click the IRsolution icon on the desktop or select the IRsolution menu on the Start menu.

Fig. 3.12 IRsolution icon

2. Set up the model of instrument to connect with the IRsolution. Select the [Environment]-[Instrument Preferences]-[Instruments] menu before initializing the FTIR. Select [IRPrestige-21] as the Scanning FTIR Module. If you are using FTIR-8000 series, It's not necessary to change the setting.

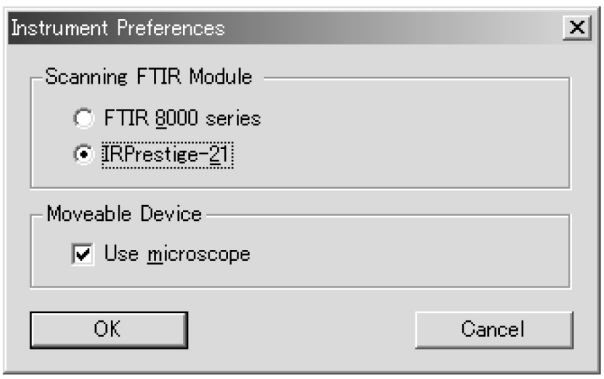


Fig. 3.13 [Instrument Preferences] Dialog box

FTIR 8000series	Connects to the FTIR-8000 series.
IRPrestige-21	Connects to the IRPrestige-21.

3. 8 User Management

IRsolution has a security function by management of users with User ID and Password. Administrator should activate the security function by User ID and Password after installation of IRsolution by use of the [Admin]-[Security] command. Put a check mark on the "Password Restrictions" on the [Security] dialog box.

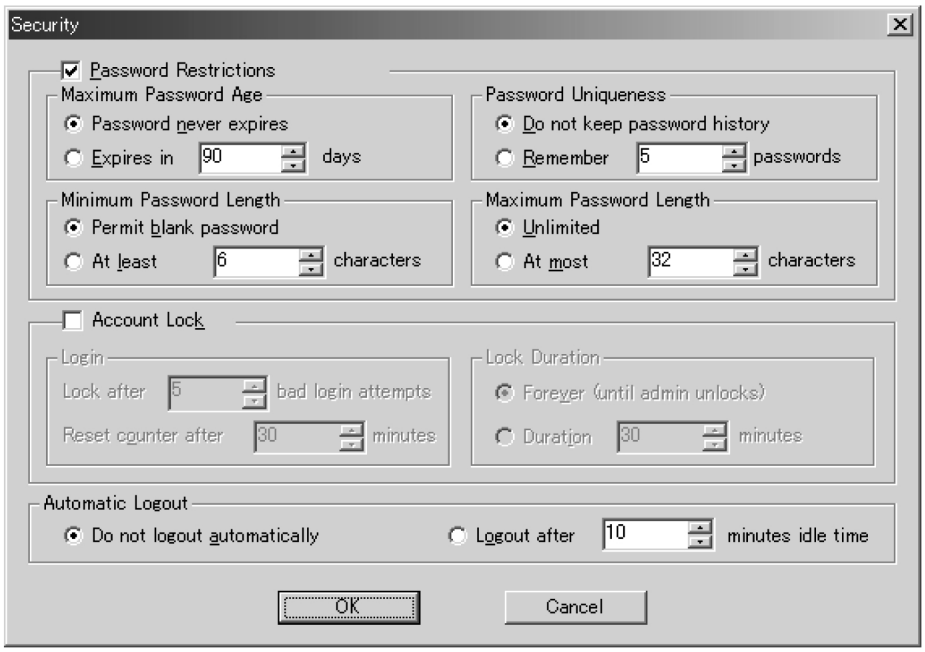


Fig. 3.14 [Security] dialog box

Clicking the <OK> button to open the message [There is no active user "xxxxxx". The application has to be closed. Do you want to continue and close the application?]. Click the <Yes> button to close IRsolution once. The dialog box shown in Fig.3.15 is displayed when IRsolution is run again. Select "Administrator" as User name and nothing is input on the "Password" section, then click the <OK> button.

Fig. 3.15 [Log On] dialog box

Change the password for the Administrator by the [Admin]-[Security] command. Then manage the User and his/her rights of operations.

3. 9 Uninstallation of the IRsolution

Follow the steps to uninstall the IRsolution software.

Note If you re-install IRsolution of install new version of it, it is strongly recommended that you uninstall the old software by the following procedure before installing the new software.

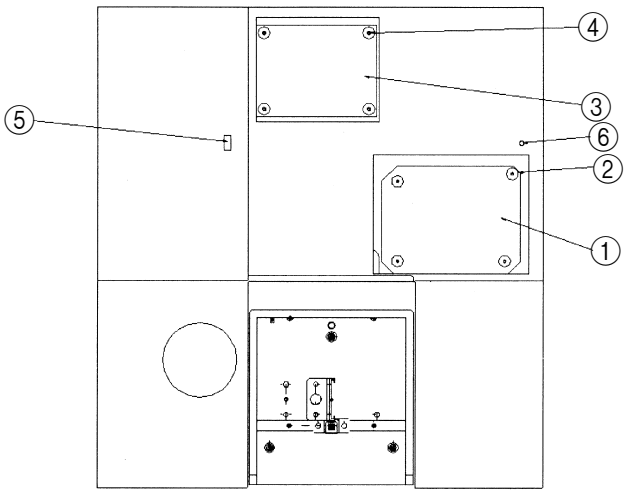
1. Select the Control Panel on the Start menu of the Windows.
2. Select [Add / Remove Programs].
3. There are [IRsolution], [IRsolution x.xx] and [IRsolution Supplemental] on the window.
4. First, select [IRsolution Supplemental] then click the <Modify / Remove> button. Select [Remove] on the window then follow the prompts on the screen.
5. Next, select [IRsolution x.xx] then click the <Modify / Remove> button. Select [Automatic] on the window then follow the prompts on the screen.
6. Finally, select [IRsolution] then click the <Modify / Remove> button. Select [Remove] on the window then follow the prompts on the screen.
7. After uninstallation, close the [Add / Remove Programs] window and the Control Panel.

3. 10 Replacing the Silica Gel and Installing the Beam Splitter Unit

Though the auto dry unit is built in the IRPrestige-21, silica gel is used also to cope with failure of the dry unit and power interruption.

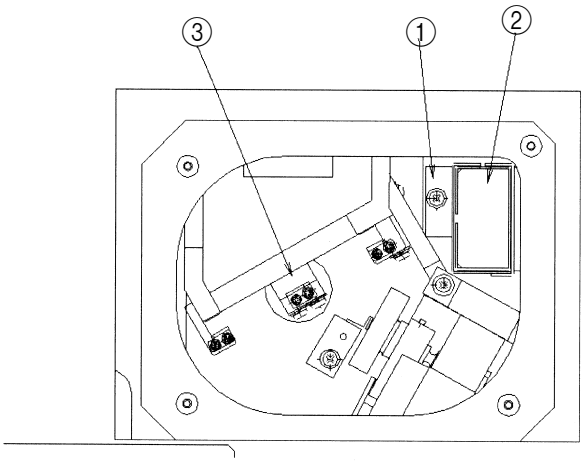
Caution	To install the beam splitter unit, make sure to confirm that the humidity around the IRPrestige-21 is 60% or less.

1) Remove the top cover by lifting it from the right side.



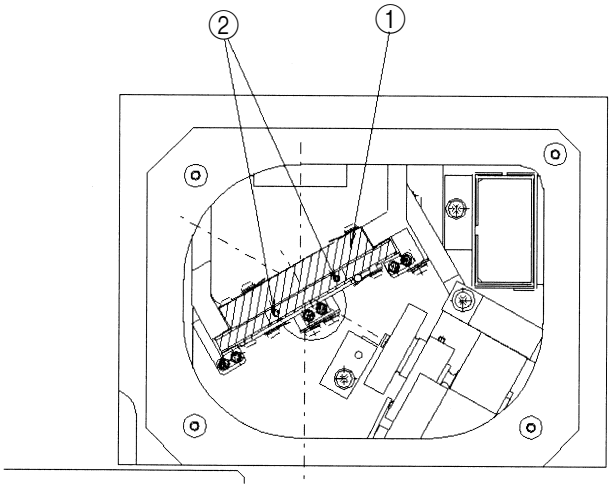
2) When the top cover is removed, the interferometer case cover can be seen. The lid on the right side (① in the figure) is provided for replacing the beam splitter. Remove the four screws which fix this lid (② in the figure), then open the lid.

3) When the lid for replacing the beam splitter is opened, the silica gel case (② in the figure) and the beam splitter installation position (③ in the figure) can be seen.



4) At first, pull upward the silica gel case to remove it, replace the entire silica gel inside it with new one, then install it again.

5) Next, unpack the beam splitter unit, and completely insert it into the installation position so that the wider side is located near you. (Figure in which the beam splitter unit (shaded portion) is installed)



6) Close the lid for replacing the beam splitter and fighten 4 screws.

7) Close the top cover. Insert the top cover so that its left claw is engaged with the square hole (⑤ in the figure) of the outer cover, then put the top cover on the outer cover.

3. 11 Trial Run

After completing the installation work described so far, start up the IRPrestige-21 in conformance to “1. Startup of System” of the Instruction Manual (Basic Operation). Execute “Auto Adjust (cource)” from the IRsolution initial window, measure the power spectrum, then confirm that the intensity of the power spectrum satisfies the standard value shown in “4. Maintenance and Inspection”.

Chapter 4 Maintenance and Inspection

CONTENTS

4. 1 Dry Unit

The IRPrestige-21 keeps the inside of the interferometer at low humidity by driving the dry unit even while the IRPrestige-21 is not used. Accordingly, always let the power plug of the IRPrestige-21 be connected to the AC power supply to keep the power supply. Confirm that the orange LED (standby power indicator lamp) in the lower right portion of the front face is lit. If it is expected that the main power supply will be OFF for a long time, remove the beam splitter unit and individually store it in the desiccator, or put new silica gel into the silica gel case of the main unit. While the main power supply is OFF, silica gel should be replaced once in approximately two weeks. For the silica gel replacement method, refer to 3.8.

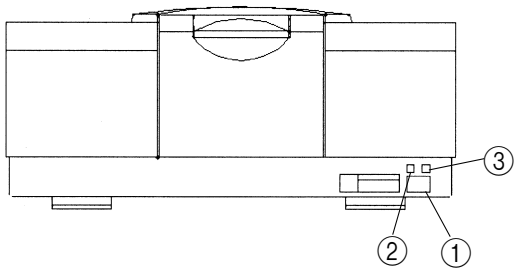


Fig. 4.1 Stand-by lamp

4. 2 Self-diagnosis Function

The IRPrestige-21 has the self-diagnosis function. The IRPrestige-21 automatically checks its own status during operation or startup. If all items are judged as OK, the IRPrestige-21 can be used normally. The contents of the self-diagnosis are described below.

Items checked when the IRPrestige-21 starts up or when "Diagnostics" is executed from the menu:

1. Laser lighting
2. Light source lighting
3. Beam splitter type
4. Fixed mirror piezo actuator voltage
5. Infrared power spectrum shape

Items always checked while the IRPrestige-21 is operating:

1. Laser lighting
2. Light source lighting
3. Beam splitter type

If "1. Laser lighting" or "2. Light source lighting" is judged as NG, the corresponding part should be replaced. Contact our sales or service section. "3. Beam splitter type" indicate beam splitter type, which is currently installed.

"4. Fixed mirror piezo actuator voltage" checks whether or not the voltage at the piezo actuator used for auto alignment of the fixed mirror is located within the correct range. If this item is judged as NG, the fixed mirror adjustment mode starts consecutively. In accordance with displayed messages, adjust the fixed mirror. When adjustment is completed, the fine adjustment mode starts consecutively.

"5. Infrared power spectrum shape" measures the infrared energy in the blank status (with no sample). At startup (or when diagnostics started), let nothing be present inside the sample compartment. Even if this item is judged as NG because the beam was cut in the sample compartment, you can execute the self-diagnosis at any time from the Pull-down menu of the IRsolution. For the details, refer to the Help.

If this item is judged as NG while nothing is present inside the sample compartment, at first, check measurement parameter is set correctly. if OK, execute "Measurement" – "Auto Adjustment". If this item is judged as NG again even after "Auto Adjustment" is executed, the beam splitter may be deteriorated or there may be some other abnormality. Refer "troubleshooting" or contact us.

4. 3 EP2000 and The first Supplement to the Japanese Pharmacopeia Fourteenth Edition Validation

The IRPrestige-21 can automatically execute the inspection in conformance to the EP2000 and the Japanese Pharmacopoeia ; Revised Edition 14. This inspection evaluates the measurement data acquired by using polystyrene as sample. If the result of this inspection is all right, the IRPrestige-21 can be usually used without any problem. In this inspection, use polystyrene whose thickness is approximately 40μm. When the traceability is required in the inspection result, separately purchase the standard sample supplied by NIST, and use it in the inspection.

The validation executed by this validation software conforms to the EP2000 and the Japanese Pharmacopoeia; Revised Edition 14. There are five validation items; power spectrum, resolution, wavenumber accuracy, wavenumber reproducibility and transmittance reproducibility. The performance of the IRPrestige-21 is validated through comparison between the measurement result and the standard value. The validation contents are same in the EP2000 and the Japanese Pharmacopoeia; Revised Edition 14 (plan). The points changed from the Japanese Pharmacopoeia; Revised Edition 13 are “2. Resolution” and “3. Wavenumber accuracy”.

4.3.1 Power spectrum

The most basic performance evaluation of the FTIR can be executed by using the power spectrum size. If the measured power spectrum is equivalent to or more than the standard value at every specified wavenumber, it is judged as OK.

The table below shows the standard values for reference. These standard values are not specified by the EP2000 and the Japanese Pharmacopoeia ; Revised Edition 14.

Wavenumber (cm^{-1})	Standard value
4600 cm^{-1}	10% or more of Max.
4000 cm^{-1}	25% or more of Max.
3000 cm^{-1}	50% or more of Max.
Maximum value	50 or more
700 cm^{-1}	10% or more of Max.
500 cm^{-1}	2% or more of Max.
403 cm^{-1}	0.5% or more of Max.
351 cm^{-1}	0.01% or more of Max.

4.3.2 Resolution

Measure the absorption spectrum of a polystyrene film whose thickness is approximately 0.04mm. If the difference in the %T of the measured absorption spectrum is 18% or more between the minimum around 2,870cm^{-1} and the maximum around 2,850cm^{-1} and if the difference in the %T of the measured absorption spectrum is 12% or more between the minimum around 1,589cm^{-1} and the maximum around 1,583cm^{-1}, it is judged as OK.

4.3.3 Wavenumber accuracy

The EP2000 and the Japanese Pharmacopoeia ; Revised Edition 14 describe the performance evaluation of the wavelength accuracy as follows.

"The wavenumber scale is usually corrected by using some of the following absorption bands of polystyrene film. The values in the parentheses show the accuracy tolerance."

3060.0 (± 1.5) cm^{-1}
2849.5 (± 1.5) cm^{-1}
1942.9 (± 1.5) cm^{-1}
1601.2 (± 1.0) cm^{-1}
1583.0 (± 1.0) cm^{-1}
1154.5 (± 1.0) cm^{-1}
1028.3 (± 1.0) cm^{-1}

In this program, seven wavenumbers above to be used in judgement are specified, the peak wavenumber of the measured spectrum of a polystyrene film is acquired at each specified wavenumber, then it is judged whether or not the measured value is located within the allowable range separately specified. If the peak wavenumber is located within the allowable range at every specified wavenumber, it is judged as OK.

4.3.4 Wavenumber reproducibility

The Japanese Pharmacopoeia ; Revised Edition 14 describe the wavenumber reproducibility as follows.

"The wavenumber reproducibility should satisfy ± 5cm^{-1} around 3000cm^{-1} and ± 1cm^{-1} around 1000cm^{-1}."

In this software, three peak wavenumbers are specified, the actual peak wavenumber at each point is acquired by measurement of a polystyrene film twice, then it is judged whether or not the error is located within the allowable range. If the peak wavenumber is located within the allowable range at every specified wavenumber, it is judged as OK.

The EP 2000 does not describe about wavenumber reproducibility, but this software judge using same criteria as Japanese pharmacopoeia.

4.3.5 transmittance reproducibility

The EP2000 and the Japanese Pharmacopoeia ; Revised Edition 14 describe the transmittance repeatability as follows.

"The transmittance reproducibility should satisfy 0.5%T when the several points of polystyrene absorption from 3000cm^{-1} to 1000cm^{-1} are measured twice."

In this software, three peak wavenumbers are specified, the transmittance at each point is acquired by measurement of a polystyrene film twice, then it is judged whether or not the error is located within the allowable range. If the difference in the transmittance is located within the allowable range at every specified wavenumber, it is judged as OK.

4. 4 Validation in Conformance to ASTM

The IRPrestige-21 can automatically execute the inspection in conformance to the ASTM E1421-94 (level zero) in addition to the inspections in conformance to the Japanese Pharmacopoeia and the EP2000. Use a polystyrene film in conformance to the Japanese Pharmacopoeia whose thickness is approximately 40μm. When the traceability is required in the inspection result, separately purchase the standard sample supplied by NIST, and use it in the inspection.

Though the ASTM specifies the inspection technique and the contents, it does not specify the standard values. The initial standard values are specified by Shimadzu. For more detail please refer to "Validation" manual.

Brief explanation of the ASTM E1421-94 (level zero):

This is a simple check, and completed in several minutes. The measurement result acquired at this time is compared with the result acquired in the previous inspection, then it is checked whether or not malfunction or considerable changes are present in the IRPrestige-21. This inspection does not execute strict quantitative evaluation.

Measurement parameters are "4cm^{-1}" and "approximately 30 sec". Other parameters should be recorded.

Evaluation data

Reference1 : Power spectrum in the blank status acquired in the previous inspection

Reference2 : Spectrum of polystyrene acquired in the previous inspection

Spectrum1 : Power spectrum in the blank status

Spectrum2 : Power spectrum in the blank status or 100% line just after "Spectrum1" was measured

Spectrum3 : Spectrum of polystyrene acquired by using "Spectrum2" or "Spectrum1" as the background

Contents of evaluation

1. "Reference1" and "Spectrum1" are overlayed and displayed, or the ratio (100% line) between "Spectrum1" and "Reference1" is obtained, then the variation is evaluated.

   Report formats

   (1) "Reference1" and "Spectrum1" overlayed printout

   (2) 100% line (full scale: 95 to 105%) obtained as the result of "Spectrum1/Reference1"

   (3) "Spectrum1" evaluated with respect to the following values

   R4000/2000 = Energy intensity at 4,000cm^{-1}/Energy intensity at 2,000cm^{-1}

   R2000/1000 = Energy intensity at 2,000cm^{-1}/Energy intensity at 1,000cm^{-1}

   (R nonphysical = Energy intensity at cutoff (150cm^{-1}) or less/Maximum energy intensity)

Measurement parameters which should be recorded together with the acquired data: Date of data acquisition and number of scans.

2. The 100% line is evaluated for a short time (ratio between "Spectrum1" and "Spectrum2").

Report formats

(1) "Spectrum1" and "Spectrum2" overlayed printout

(2) 100% line (full scale: 99 to 101% or 90 to 110%) obtained as the result of "Spectrum1 /Spectrum2"

(3) Noise quantity (RMS or P-P) within the 100cm^{-1} range whose center is 4,000, 2,000, 1,000 or 500cm^{-1} in the 100% line above

3. The polystyrene measurement data acquired at this time is compared with the measurement data acquired in the previous inspection. The difference between the polystyrene spectrum acquired by "Spectrum1/Spectrum2" at this time and the polystyrene spectrum acquired in the previous inspection, then evaluated.

Report formats

(1) Polystyrene spectrum (full scale: 0 to 100%)

(2) Difference between data at this time and data at the previous time (full scale: −1 to +1%)

4. 5 Replacement Procedure of Light Source

When the light source lighting confirmation indicator ("Lamp" in the figure below) is red on the IRsolution main window, it indicates that wire breakage has occurred in the light source. In this case, the power spectrum must be 0 even if measurement is started. In this case, replace the light source with a new one by using the following procedure.

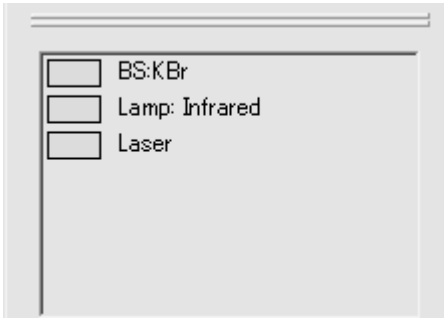


Fig. 4.2 Statns Indicate window

Caution	1	Turn off the power of the IRPrestige-21, wait for 2 hours or more, then replace the light source.

Caution	2	To replace the light source, make sure to confirm that the humidity around the IRPrestige-21 is 60% or less.

1) Remove the top cover by lifting it from the right side.

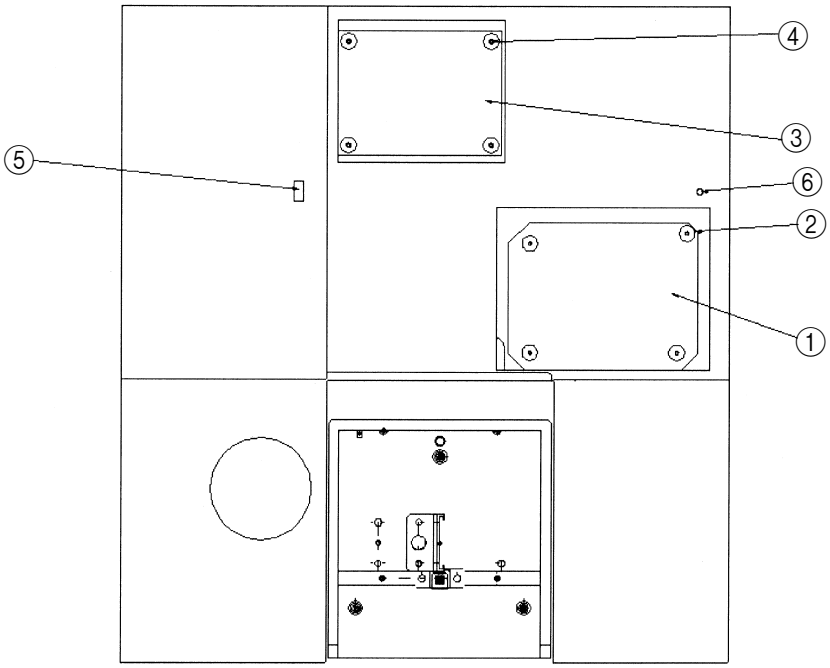


Fig. 4.3 Top Cover is opened

2) When the top cover is removed, the lid for replacing the light source (③ in the figure 4.3) can be seen. Remove the four screws (④ in the figure 4.3) which fix this lid, then open the cover.

3) When the lid for replacing the light source is opened, the infrared light source assembly (① in the figure 4.4) can be seen. Loosen the long screw (② in the figure 4.4) which fixes the infrared light source assembly until the infrared light source assembly can be moved. (Do not remove only this long screw.)

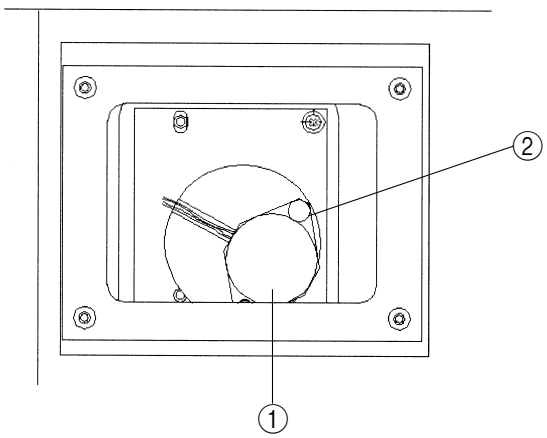


Fig. 4.4 Light Source

4) Hold by hand the cylindrical main part of the light source assembly, and pull upward the light source assembly to remove it.

5) Install a new light source assembly along the guide pin of the interferometer. At this time, make sure that the opening on the side of the light source ASSY is located on the right side of the interferometer. When installing a light source ASSY, make sure to put it downward straight from the just above. If the light source ASSY is installed diagonally, the electrodes of the light source may be imperfectly contacted. The figure above shows the correct installation status.

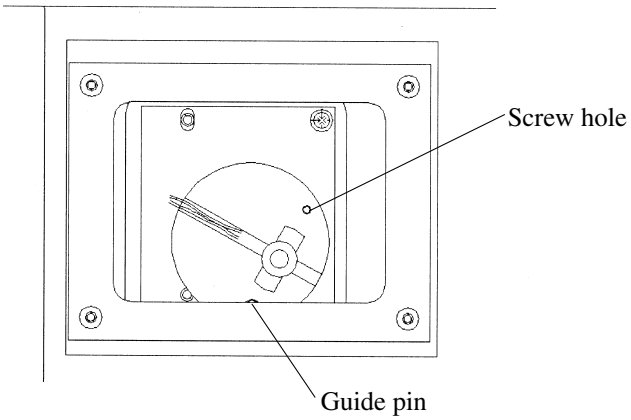


Fig. 4.5 Light Source is removed

4. 6 Maintenance Part and Consumables

	Part name	P/N
1	Beam splitter ASSY	206-71721-91
2	IRsolution (Software CD-R)	206-72328-91
3	Polystyrene film	202-30689-01
4	AC cable (for 100/120V)	071-60814-01
5	Grounding adapter	071-60813
6	AC cable (for 220/230/240V)	071-60814-06
7	Fuse 6.3A (100/120V)	072-02004-24
8	Fuse 4.0A (220/230/240V)	072-02004-22
9	Silica gel	200-53655
10	Cassette	206-70001
11	Infrared light source ASSY	206-71628-91
12	Laser ASSY (with power supply)	206-71580-91
13	PCB ASSY, laser detector	206-71684-91
14	PCB ASSY, POWER (power board)	206-71588-95
15	PCB ASSY, NINJA (CPU board)	206-71555-91
16	Infrared detector MTG-21	206-72234
17	DriCabi TS-51 D.U.S	206-71946
18	Supplemental Disk	206-72407-91

Note He-Ne laser has the structure that seals the gas in the glass tube. If the sealed gas gradually leaked, FTIR may not light up in several years after purchased.
As the result of this, measurement will not be performed. In this case, contact our sales office.
Period of guaranty for the laser is 30 months after installation whether the system is used or not.
If the system cannot be used within 30 months after installation, we can replace it free of charge. Contact our sales office at your earliest opportunity.

4.7 Cleaning the System

If the outside of the interferometer becomes dirty, wipe it clean with a soft cloth or tissue; soak the cloth in water or detergent, and wring it out. Do not use organic solvents, such as thinner or benzene, and avoid contact with mirrors and other internal components.

Caution	Do not spill water or solvents on the system; spills may result in system damage, fire or electric shock.

4. 8 Transporting the System

Caution The interferometer weighs approximately 55 kg. To carry the system, two or more people should grip the instrument at the corners, as shown in Figure 4.6. A strong impact (drop, collision, etc.) may damage the system.

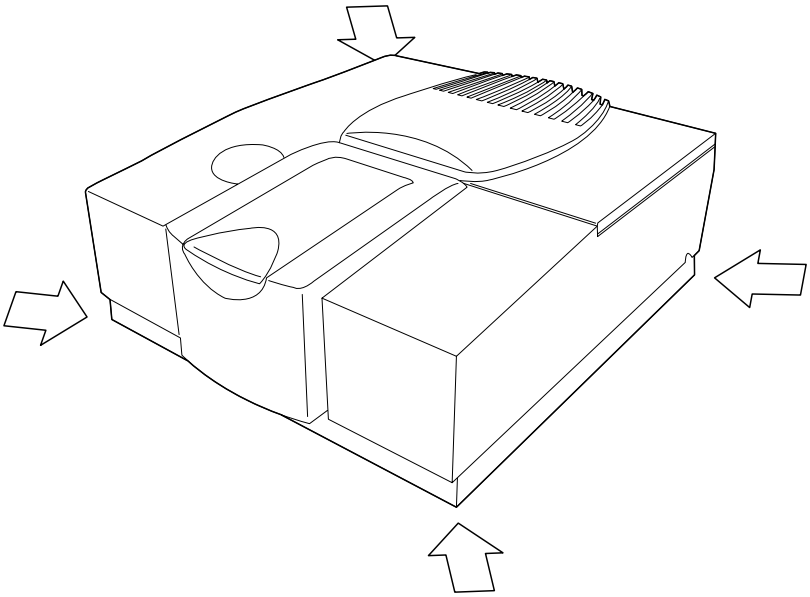


Fig. 4.6

4.9 Appendix: Automatic Recognition Function of Accessory

When an accessory is installed in the sample compartment, IRPrestige-21 can automatically recognize the type of the accessory, and execute the method (macro program) or validation assigned to the accessory (as far as the accessory has the recognition function).

When an accessory having the recognition function is installed in the sample compartment, the accessory name is displayed on the status window of the IRsolution software and set parameters suitable for the accessory automatically. After that, execute the automatic validation to confirm the performance including the accessory. The contents of the automatic validation are determined for each accessory. Execute the performance inspection in accordance with messages displayed while the validation program is executed. Then, the IRsolution judges the final result as OK or NG. The result is recorded in the operation log, and recorded also together with the accessory name and the date and time in all measurement data acquired with the accessory.

On the other hand, instead of Validation program, user programed macro program can also be executed automatically when installing these attachment. (macro program is option)

At the time of delivery, the contents of the automatic validation are set as reference in accordance with the Shimadzu standards. They can be changed using optional macro program and “Environment” menu. For the details, refer to the “Help document” included in the software.

Chapter 5 Troubleshooting

CONTENTS

5. 1 Error Message Table

When measurement parameters have some mismatch or the instrument has some adjustment error, these error messages are indicated on the Pop-up window.

This table shows Error message Meanings and How to operate. So refer this contents and operate again.

Error Message	Meanings and Operation
None of the available background matches the sample parameters.	There is no background data stored which matches the sample measurement (%T or Abs) When you change parameter such as "Resolution", background data must be measured then sample measurement becomes available.
Can't open the File	File to be loaded might be set as "Read only"? If so , file can not be open. If not, the contents of the file may be broken.
XXX(File name) already exist. Please choose a different file name!	When GLP mode, File overwriting is prohibited. Change file name and save again.
XXX to XXXX wavenumber should be inputed.	Wavenumber range value in measurement parameter is out of the range which is set to the beam splitter used. Input correct value.
For NIR scan OPTION detector must be used. Continue?	To execute NIR measurement ,optional InGaAs detector is necessary. Confirm "Detector" parameter is set to "Option1"when you measure NIR measurement. Note that you can "continue" but data quality is not satisfied the specification.
Note! XXX beam splitter does not match selected NIR range, Continue?	To execute NIR measurement ,optional CaF_2 beam splitter is necessary. Confirm "CaF_2" beam splitter is mounted when you measure NIR measurement. . Note that you can "continue" but data quality is not satisfied the specification

5. 2 Error Message shown in the "Status Window"

When measurement parameters have some mismatch or your instrument has some adjustment error, these error messages are indicated in the "Status Window".

This table shows Error message Meanings and How to operate. Please read the message and refer to operate. If no improvement is obtained in spite of this operation, your instrument may be broken. Please call Shimadzu branch.

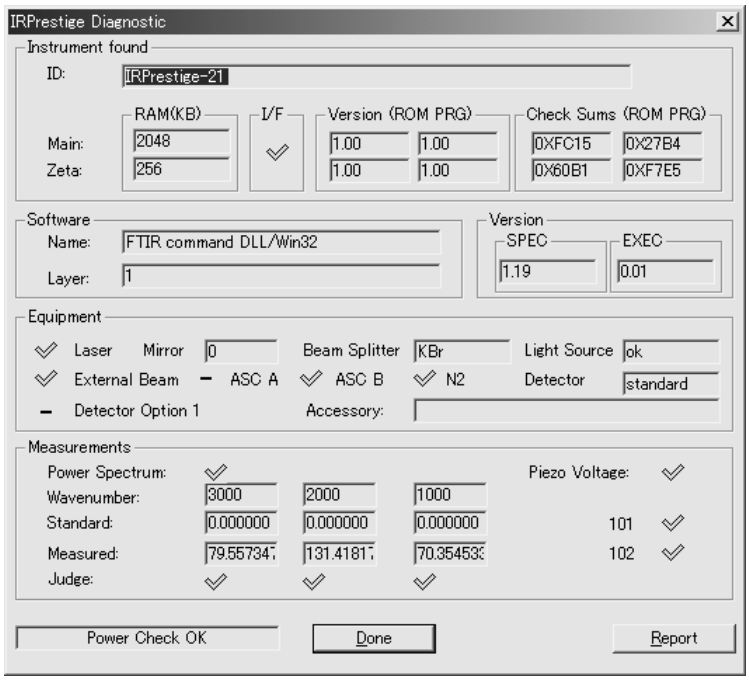
Error Message	Meanings and Operation
NoBackground spectrum!¥r¥nMeasurement aborted.	There is no background data stored which matches the sample measurement (%T or Abs) When you change parameter such as "Resolution", background data must be measured then sample measurement becomes available.
No AIM device on %s	When mapping measurement, AIM microscope is not connected or just operating other task. Confirm Mapping measurement is finished then operate again.
Option Detector is not mounted	When Option detector is not mounted and "Option1" detector is selected. Confirm the measurement parameters.
Parameter check Error.	There are some mismatch in the measurement parameters. Confirm the measurement parameters.
No detector or no liquid N	When detector parameter is set to "Option1 or Option2", liquid nitrogen sensor is active and if there is no liq N2 in the MCT dewer, this error message is shown. Confirm that MCT dewer is fulfilled with liq N2 and cable connection.
Diagnostic Power measurement failed	Power spectrum shape check in diagnostics is failed. Execute [Measure]-[Auto adjust(fine)] and try again.
Could not retrieve diagnostic power results.	Power spectrum shape check in diagnostics can not be completed. Execute [Measure]-[Auto adjust(Course)] and try again.
Piezo voltage is out of range	Piezo voltage check in in diagnostics is failed. Execute [Measure]-[Auto adjust(Course)] and try again.
Piezo voltage can not be obtained	Piezo voltage check in in diagnostics can not be completed. Execute [Measure]-[Auto adjust(Course)] and try again.
Not enough memory available ! Out of memory	The rest of memory in your PC becomes little. If you use other application on the PC, terminate other application and restart the PC.
Failure of mirror drive in the interferometer.	Moving mirror movement is failed. Execute [Measure]-[Auto adjust(Course)] and try again
Moving Mirror Error X	Moving mirror movement is failed. Execute [Measure]-[Auto adjust(Course)] and try again
A/D out of range	Measured data beyond the A/D converter range limit. When using standard detector, check if transmittance of the sample is changed, or when MCT detector, reduce the light intensity using the aperture, etc.
Interferogram beyond A/D converter limit	Measured data beyond the A/D converter range limit. When using standard detector, check if transmittance of the sample is changed, or when MCT detector, reduce the light intensity using the aperture, etc.

Error Message	Meanings and Operation
Offset value beyond A/D converter limit	Measured data beyond the A/D converter range limit. When using standard detector, check if transmittance of the sample is changed, or when MCT detector, reduce the light intensity using the aperture, etc.
No centerburst detected	Centerburst of measured interferogram can not be detected. Execute [Measure]-[Auto adjust(Fine)] .
Vertical value beyond the limit	The parameters of fixed mirror beyond the software limit. Execute [Measure]-[Auto adjust(Course)]
Horizontal value beyond the limit	The parameters of fixed mirror beyond the software limit. Execute [Measure]-[Auto adjust(Course)]
Optim. vertical value beyond the limit after AutoAdjust	The parameters of fixed mirror adjustment beyond the software limit. Execute [Measure]-[Auto adjust(Course)]
Optim. horizontal value beyond the limit after AutoAdjust	The parameters of fixed mirror adjustment beyond the software limit. Execute [Measure]-[Auto adjust(Course)]
Fixed mirror adjustment failed.	Fixed mirror adjustment falied. Execute [Measure]-[Auto adjust(Course)]
No interferogram	FFT in manipulation must be executed to IFG data.
Recalculation can not be performed (no data)	There is no data for recalculate. Load again the data to be recalculated.
ASC-A initialization error	Error is occurred when initializing Auto sample changer connected to the connector A. Confirm the connection of ASC.
ASC-B initialization error	Error is occurred when initializing Auto sample changer connected to the connector B. Confirm the connection of ASC.
Laser Failure	If the laser indicator of status window becomes red, laser is broken. Call Shimadzu branch.
No beamsplitter	Beamsplitter is not mounted or not mounted correctly. Please check .
Lamp offline. Please change it	If the lamp indicator of status window becomes red, selected lamp is disconnected. Call Shimadzu branch
Timeout on initialization	When initialization, communication between interferometer and PC is not active. Check if interferometer power is not ON or IEEE1394 cable is disconnected.
Instrument Timeout Error	Communication between interferometer and PC is not active. Check if interferometer power is not ON or IEEE1394 cable is disconnected.
No valid range object	Wavenumber range set file (*.rng) may be broken. Please delete the .rng file and make a new range set file.

There are more error messages but in normal use seldom appears. If undefined errors in the table above frequently occur, the instrument may have software or hardware problem. Please contact Shimadzu branch.

5. 3 Describing the Diagnostic Screen

Inspect the equipment status using the Diagnostic command. Select this command to display the following screen. This section describes this screen.



[Unit connected]

ID	Equipment name
RAM (KB)	RAM size of Main/Zeta CPU
I/F	Operating status of interface
Version	ROM/PRG version No. of Main/Zeta CPU
Check Sums	Check sums of Main/Zeta CPU

[Software]

Name	Name of the software bult in the equipment transferred from PC
Layer	Layer No. of the software

[Version]

SPEC/EXEC	Version No. of each program

[Equipment]

Laser	Laser lighting
Mirror	Mirror stability
Beam Splitter	Beam splitter type
Light Source	Light source lighting

External Beam	Status of external beam (exist/ not exist)
ASC A/ASC B	Connection status of autosample changer A/B
N_2	Present/absent of liquid nitrogen
Detector	Condition of detector
Accessory	Name of connected accessory

[Measurements]

Power Spectrum	Power spectrum inspection (executed/not executed)
Wavenumber	Wavenumber to check intensity
Standard	Judgement reference intensity in each wavenumber (variable)
Measured	Actual measured intensity
Judge	OK/NG in each wavenumber
Piezo Voltage	Piezo voltage (inspected or not)
101/102	Results of Piezo voltage inspection of each code No. (OK/NG)

(Status column)	Displays the inspection content which is running
[Done]	Click this button to close the screen.
[Report]	Click this button to output results to the text file.

5. 4 Power Indicator Lamp

IRPrestige-21 has two Power Indicators - the Main power indicator (green) and the Standby power indicator (orange) - on the front panel. The Main power indicator lights up when the main power is turned on. The Standby power indicator lights up when AC cable is connected to power source correctly to have standby power.

As described on the section 4.1, the IRPrestige-21 keeps the inside of the interferometer at low humidity by driving the dry unit even while the IRPrestige-21 is not used. Accordingly, always let the power plug of the IRPrestige-21 be connected to the AC power supply to keep the power supply. Confirm that the orange standby power indicator is lit. If the AC power line may be cut out for long time for weekend, vacation or facility maintenance, remove the beam splitter unit and store it in the Beam splitter container with new silica gels. Refer to the section 3.8 to remove the Beam splitter unit.

If the standby power indicator is not lighting, please confirm following checkpoints.

1. AC for IRPrestige-21 is correctly the connected to AC line.
2. The AC line is correctly alive.

If the standby power indicator is not lighting even if above points are not troubled, it may cause by hardware trouble on the IRPrestige-21. Remove the beam splitter unit and store it in the Beam splitter container with new silica gels immediately, and then contact to your SHIMADZU representatives.

5. 5 What's happening?

This section lists up troubles that you will meet during operating the IRPrestige-21 and describes their reasons and solutions. Refer to the Chapter 5 to solve your troubles. If the trouble may not be solved, please contact to your SHIMADZU representatives.

5.5.1 Incorrect Beam splitter status is displayed on the Status Monitor.

Phenomena

- Incorrect Beam splitter status was displayed on the Status Monitor.
- An error was displayed and NIR mode was set, even if the KBr Beam splitter was installed.

Reason

- Beam splitter was not installed correctly.

Solution

When the Beam splitter was installed first, or the Beam splitter was replaced, it was not inserted towards the end. Open the top cover and the interferometer cover referring to the section 3.9, then confirm that the Beam splitter is installed facing to correct surface and towards the end.

If this error comes again even if the Beam splitter is correctly installed, shut down the FTIR and turn it on again, close the IRsolution and activate it again, and then, initialize again.

5.5.2 Abnormal behavior during Initialization

Phenomena

- The message "Power diagnostic Failed" was displayed at the Initialization.
- "Auto Adjustment" was executed during Initialization.

Reason

- Initialization was executed when any accessory or sample is set on the sample compartment, or when the "beam" was set to [External].

Solution

1. Check following items.
   - No accessory or no sample is set on the sample compartment.
   - Set the "beam" to the [Internal] when the optional Beam Switching Kit was installed.
2. Execute the [Measurement]-[Autoadjust (Coarse)].
3. Turn off the FTIR once, and then turn it on again. Execute [Measurement]-[Initialize] again.
4. If the trouble may not be solved, please contact to your SHIMADZU representatives.

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