

# FTIR Series and Infrared/Raman Microscope Accessories



## Selection of FTIR/Raman and Optional Accessories

FTIR is a method of measuring the light that is transmitted or reflected from a sample when it is irradiated with infrared light. In comparison with conventional dispersive IR, this method is in principle superior as it has advantages in terms of multiplex measurements, solid angles, and wavenumber accuracy. Utilizing these advantages, new accessories capable of achieving what conventional dispersive IR cannot are being developed in succession.

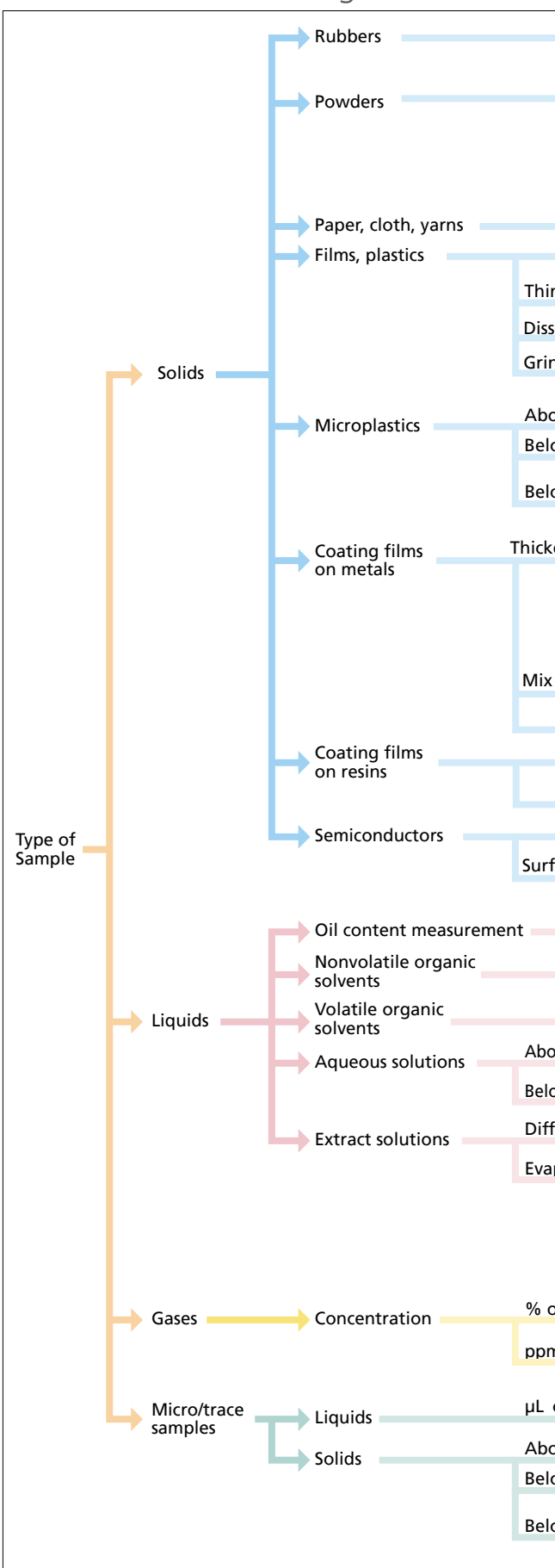
On the other hand, Raman is a method of measuring Raman light scattered from samples when they are irradiated with laser light. This method can detect C-C, S-S, and other structurally derived peaks not caused by changes in the dipole moment, which are difficult to detect with FTIR, and can perform a qualitative analysis of inorganic compounds. A laser is used as the light source, so the measurement position can be determined in 3D. Also, the focus size can be changed depending on the accessory.

The table at right shows a flow chart for the selection of FTIR and Raman accessories. In FTIR, the selection of infrared analysis method can be said to be synonymous with the selection of the accessories. In FTIR, analysis, the analysis method is basically determined by the physical form (liquid, solid, and so on) of the sample. This could be said to be a feature of infrared analysis, and a significant difference from other instrument types such as ultraviolet/visible light spectrophotometers (UV-Vis) and gas chromatographs (GC).

Refer to this flow chart when selecting the optimal accessories.

Contact your Shimadzu representative regarding special accessories and systems not indicated in this catalog.

## Flow Chart for Selecting Attachments



# and Accessories

Pyrolysis	Total reflectance method	ATR accessories (Black rubbers requires Ge prism)
	Liquid film method	Demountable cell
	Nujol method	Demountable cell
	KBr pellet method	KBr die + hand press + vacuum pump, or mini hand press
	Total reflectance method	Single-reflection ATR
	Diffuse reflectance method	DRS-8000A ..... Mix with KBr powder
	Total reflectance method	ATR accessories
	Total reflectance method	ATR accessories
Thinner than 100 $\mu\text{m}$	Transmission method	Film holder ..... Use grid polarizer for study of molecular orientation
Dissolve in solvent	Film method	Demountable cell ..... Evaporate the solvent to obtain the film
and	SiC sampler	DRS-8000A + SiC sampler
Thicker than several hundreds of $\mu\text{m}$	Total reflectance method	Single-reflection ATR
Thinner than several hundreds of $\mu\text{m}$	Infrared microscopy	AIMsight, AIM-9000, Particle filter holder (transmission, reflection), Particle analysis program
Thinner than 10 $\mu\text{m}$	Infrared/Raman microscope	AIRsight, Particle filter holder (transmission, reflection), Particle analysis program
Thinner than 1 $\mu\text{m}$	Total reflectance method	Single-reflection ATR ..... Measurement to a depth of 1/5 of the wavelength with a KRS-5 prism and to 1/15 with a Ge prism
	Specular reflectance method	SRM-8000A
Thinner than 1 $\mu\text{m}$	Reflection absorption spectrometry	RAS-8000A ..... Use of a grid polarizer enhances sensitivity about two times
Mix with KBr powder	KBr pellet method	KBr die + hand press + vacuum pump, or mini hand press
	Diffuse reflectance method	DRS-8000A
	Total reflectance method	ATR accessories ..... Measurement to a depth of 1/5 of the wavelength with a KRS-5 prism and to 1/10 with a Ge prism
	Specular reflectance method	SRM-8000A ..... Convert a reflection spectrum into the absorption spectrum by the Kramers-Kronig method
	Film holder	
Surface measurement	Total reflectance method	Single-reflection ATR (Ge prism)
	Quartz cell	..... Detection limit is 1 ppm level with 10 mm optical path
	Liquid film method	Demountable cell
Rapid measurement	Solution method	Fixed thickness cell, sealed liquid cell
Decrease 10% in concentration	Total reflectance method	Horizontal ATR, Single-reflection ATR
Decrease 10% in concentration	Liquid film method	Demountable cell with KRS-5 window
Difference spectrometry	Solution method	Fixed thickness cell
Evaporate solvent	Total reflectance method	Horizontal ATR, Single-reflection ATR ..... The sample solution is supplied dropwise on prism and measured after evaporating the solvent
	Diffuse reflectance method	DRS-8000A ..... The sample solution is supplied dropwise on KBr powder and measured after evaporating the solvent
Order		5 cm/10 cm gas cell
Order		Gas cell with long pathlength
Order	Total reflectance method	Single-reflection ATR
Thicker than several hundreds of $\mu\text{m}$	Total reflectance method	Single-reflection ATR
Thinner than several hundreds of $\mu\text{m}$	Infrared microscopy	AIMsight, AIM-9000 ..... Applicable to transmission, reflection, and ATR methods
Thinner than 10 $\mu\text{m}$	Infrared/Raman microscope	AIRsight ..... Objective lenses are selectable based on the focus size, with two types available.

# Shimadzu Accessory Line-up

These attachments and accessories are ideal for the IRTracer-100, IRPrestige-21, IRXcross, IRAffinity-1 series, IRSpirit series or FTIR-8000 series systems, which have been developed and manufactured using state-of-the-art optical and precision machining technologies. Models are available for a variety of liquid, gas, and solid samples. Refer the following table and detailed descriptions for each accessory. For information about the options and consumables that can be used with respective accessories, see the details for each accessory.

	Description		P/N	Compatible Instrument Model						Remarks	Page
				IRTracer	IRPrestige	IRXcross	IRAffinity	FTIR-8000	IRSpirit		
Attenuated Total Reflectance Measurement	Single Reflection Type Attenuated Total Reflection Attachment Integral with Sample Compartment	QATR 10	227-38001-XX	✓		✓	✓			with Diamond, ZnSe, Ge prism	7
		QATR-S	227-38004-XX						✓		
	Single Reflection Type Attenuated Total Reflection Attachment Integral	MicromATR	206-36177-01	✓	✓	✓	✓	✓	✓	with Diamond prism	8
		MicromATR Vision	206-36177-02	✓	✓	✓	✓	✓	✓		
	Single Reflection Type Attenuated Total Reflection Attachment Integral with Sample Compartment	MIRacle 10	206-74127-XX	✓		✓	✓			with Diamond, ZnSe, Ge prism	9
		GladiATR 10	206-74128-XX	✓		✓	✓				
	Horizontal Type Attenuated Total Reflection Attachment Integral with Sample Compartment	HATR 10	206-74126-91	✓		✓	✓			with ZnSe prism	11
	Attenuated Total Reflection Attachment	ATR-8000A	206-62303-58	✓	✓	✓	✓			with KRS-5 prism	12
		ATR-8000	206-62303-51	✓	✓	✓	✓	✓			
Horizontal Type Attenuated Total Reflection Attachment	ATR-8200HA	208-97240-92	✓	✓	✓	✓		✓ <sup>*1</sup>	with ZnSe prism	13	
	ATR-8200H	208-97240		✓		✓	✓	✓ <sup>*1</sup>			
Reflectance Measurement	Specular Reflectance Attachment	SRM-8000A	206-62304-58	✓	✓	✓	✓		✓ <sup>*1</sup>	Incident Angle: 10°	15
		SRM-8000	206-62304-51	✓	✓	✓	✓	✓	✓ <sup>*1</sup>		
	Reflection Absorption Spectrometry Attachment	RAS-8000A	206-62302-58	✓	✓	✓	✓		✓ <sup>*1</sup>	Incident Angle: 70° to 75°	16
		RAS-8000	206-62302-51	✓	✓	✓	✓	✓	✓ <sup>*1</sup>		
	Grid Polarizer	GPR-8000	206-61550-58	✓	✓	✓	✓	✓			17
Diffuse Reflectance Measurement	Diffuse Reflectance Attachment	DRS-8000A	206-62301-58	✓	✓	✓	✓		✓ <sup>*1</sup>		19
		DRS-8000	206-62301-51	✓	✓	✓	✓	✓	✓ <sup>*1</sup>		
	SiC Sampler		200-66750-01	✓	✓	✓	✓	✓	✓		20
	Automatic Diffuse Reflectance Attachment	DRS-8010ASC	206-62308-91	✓	✓	✓	✓	✓			21
Infrared Microscope	AIMsight	206-33000-58	✓		✓	✓				23	
Trace Sample Measurement (FTIR)	ATR Objective Mirror		206-32600-41	Accessory for AIRsight, AIMsight and AIM-9000						with Ge prism	24
	Micro Vise Holder		206-33293	Accessory for AIRsight, AIMsight and AIM-9000							
			208-97202	Accessory for AIM-8800							
	ATR Pressure Sensor		206-32603-42	Accessory for AIRsight and AIMsight							
			206-32603-41	Accessory for AIM-9000							
	Grazing Angle Objective	GAO	206-32602-41	Accessory for AIRsight, AIMsight and AIM-9000							25
	TEC MCT Detector		206-36820-41	Accessory for AIRsight and AIMsight							
	Room Temperature Detector	DLATGS	206-32580-42	Accessory for AIRsight and AIMsight							
			206-32580-41	Accessory for AIM-9000							
	Particle Filter (PF) Holder	For 13 mm dia.	206-36610-41	Accessory for AIRsight, AIMsight and AIM-9000							26
		For 25 mm dia.	206-36610-42								
	Diamond Cell C II		208-92289-01	Accessories for AIMsight and AIM-9000/8800							27
	Sampling Kit		208-92171								
Other Microscope Options		See text	Accessory for AIMsight and AIM-9000								
Trace Sample Measurement (Raman)	Infrared/Raman Microscope	AIRsight	206-35000-58	✓		✓	✓				23
	Objective Lens for AIRsight	50x	206-35092-41	Accessories for AIRsight							27
		100x	206-35092-42								
Accessories for Automated Measurement	Automatic Diffuse Reflectance Attachment	DRS-8010ASC	206-62308-91	✓	✓	✓	✓	✓			29
	Auto Sampler for Transmission Measurement	ASC-8000T	206-63900-91	✓	✓	✓	✓	✓			
	Sample Switcher 21		206-63663-9x	✓	✓	✓	✓	✓			
Purge Control Kit	Purge Control Kit	PCK-100	206-74251-41	✓							30
		PCK-21	206-72352-91		✓						
		PCK-X	206-37038-41			✓					
		PCK-8941	206-73512-94				✓	✓			
	Dry Air Generator		—	✓	✓	✓	✓	✓			

	Description		P/N	Compatible Instrument Model						Page
				IRTracer	IRPrestige	IRXross	IRAffinity	FTIR-8000	IRSpirit	
External Detector	External Light Beam Switching Kit		See text	✓	✓	✓	✓	✓		31
Optional Detector	T2SL Kit		See text	✓		✓				
Transmission Measurement	Cassette (Sample Holder)		206-17384	✓	✓	✓	✓	✓	✓	32
	Magnetic-Type Film Sample Holder		200-66754-11	✓	✓	✓	✓	✓	✓ <sup>*1</sup>	
	Universal Clip Holder		208-97207	✓	✓	✓	✓	✓	✓ <sup>*1</sup>	33
	EZ-Clip 13		208-97208	✓	✓	✓	✓	✓	✓ <sup>*1</sup>	
	EZ-Clip 25		208-97209	✓	✓	✓	✓	✓	✓ <sup>*1</sup>	34
	Gas Cell	5 cm Gas Cell	202-32006-XX	✓	✓	✓	✓	✓		
		10 cm Gas Cell	202-32007-XX	✓	✓	✓	✓	✓		
		Long Pathlength Gas Cell	—	✓	✓	✓	✓	✓		
Pellet Measurement	Mini Hand Press		MHP-1	200-66747-91	✓	✓	✓	✓	✓	35
	Evacuatable Die for KBr Pellets		202-32010-58	✓	✓	✓	✓	✓	✓	
	Micro Die for KBr Pellets	ø2 mm	202-32011	✓	✓	✓	✓	✓	✓	36
		ø5 mm	202-32012	✓	✓	✓	✓	✓	✓	
	10-ton Hydraulic Press		206-33547	✓	✓	✓	✓	✓	✓	
	Vacuum Pump	G-20DA	206-36017	✓	✓	✓	✓	✓	✓	
	Magnetic-Type Pellet Holder		200-66753-11	✓	✓	✓	✓	✓	✓	
	Agate Mortar and Pestle		200-93508	✓	✓	✓	✓	✓	✓	
KBr Crystal		202-34141	✓	✓	✓	✓	✓	✓	37	
Cells for Liquid Samples	Demountable Cell		202-32000-XX	✓	✓	✓	✓	✓		✓
	Sealed Liquid Cell		202-32001-XX	✓	✓	✓	✓	✓		✓
	Fixed Thickness Cell		202-32002-XX	✓	✓	✓	✓	✓		✓
	Sample Cell for Oil Content Determination		See text	✓	✓	✓	✓	✓		✓
Crystal Polishing Kit		202-32024	Can be used separately.						38	
Others	Far Infrared Kit		See text	✓	✓					
	KRS-5 Window Set		206-74211-58	✓						
NIR Measurement	NIR Kit		206-74253-58	✓						39
	Topload Type Diffuse Reflectance Attachment		UpIR A	208-97271-92	✓	✓				
	NIR Integrating Sphere		IntegratIR A	208-97272-92	✓	✓				
Optional Software	Rapid Scan		206-30200-91	✓	✓	✓				40
	Time Course Software		206-74558-91	✓	✓	✓	✓	✓	✓	
	Curve-Fitting (Peak Splitting) Program		206-74561-91	✓	✓	✓	✓	✓	✓	
	PLS Quantitation Program		206-74560-91	✓	✓	✓	✓	✓	✓	
	3D Processing Program		206-74563-91	✓	✓	✓	✓	✓	✓	41
	High-Speed Mapping Program		206-36299-41	Software for AIRsight and AIMsight						
	Particle Analysis Program		206-36628-41							
	AIMsolution DB/CS (DI-compatible version of an infrared microscope)		206-33541-41	Software for AIMsight and AIM-9000						
	KnowItAll Bundle		206-36793-41	✓	✓	✓	✓	✓	✓	42
	Macro Platform		206-74562-91	✓	✓	✓	✓	✓	✓	
EDXIR-Analysis Software		206-33175-XX	✓	✓	✓	✓	✓	✓		
Others	EDXIR-Holder Sample Holder/Stocker		212-25890-41	✓	✓	✓	✓	✓	✓	

\*1: For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

# Attenuated Total Reflectance Measurement

## Attenuated Total Reflection Method

Of the many infrared analysis methods available, the attenuated total reflectance (ATR) method is one of the more commonly used methods. It is also frequently used for dispersive infrared spectrophotometers.

The popularity of the ATR method is due to the fact that it does not require any chemical pretreatment of samples in a variety of forms, and that it also satisfies requirements for analyzing samples without any mechanical processing. In other words, it can be used for non-destructive analysis.

Given the high sensitivity of FTIR systems, uses for the ATR method

have expanded into applications that were unthinkable not long ago. Consequently, there have been many new attachments and accessories developed for the ATR method, which continues to expand the range of samples for which it can be used.

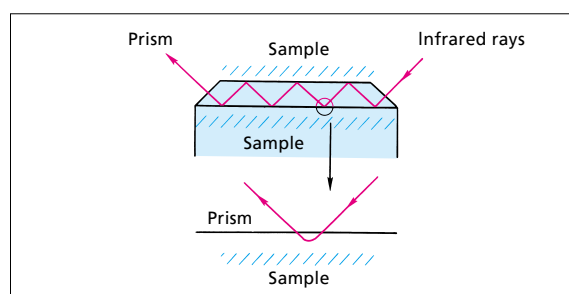
It is also sometimes referred to as the multiple internal reflectance (MIR) method.

A wide variety of ATR attachments and accessories are available to ensure the best possible method can be selected for the given substance being measured using the IRTracer-100, IRPrestige-21, IRXross, IRAffinity-1 series, IRSpirit series or FTIR-8000 series systems.

## Principle

The sample is held in contact with a prism made of highly refractive material, which transmits infrared rays; infrared rays are made incident on this sample at an angle larger than the critical angle (angle that induces total reflection). The light that is totally reflected by the interface between the sample and the prism is measured to obtain an infrared spectrum.

Though it is called "total reflection", the light travels through the thin surface layer of the sample, as shown in the figure on the right, and therefore, the spectrum obtained is similar to that obtained from a very thin slice of the same sample.



## Requirements for Measurements by the ATR Method

The sample must be placed in close contact with the surface of the prism.

This method is applicable to soft rubber or plastic samples, solid samples with a flat surface, liquid samples, and powder samples.

The prism has a higher refractive index than the sample.

It is necessary to use a prism having an appropriate refractive index.

## Penetration Depth of IR Light (Sample thickness)

Infrared light can penetrate to a depth expressed by the next equation:

$$dp = \frac{\lambda_1}{2\pi \sqrt{(\sin^2 \theta - n_{21}^2)}}$$

where,  $\theta$  : Incident angle

$n_{21}$ : (Refractive index of sample) / (Refractive index of prism)

$\lambda_1$  : Wavelength in prism

$\lambda_1 : \frac{\lambda}{n_1}$ ,  $\lambda$  : Wavelength in air,  $n_1$  : Refractive index of prism

## Example of Penetration Depth

Sample refractive index of 1.5

Material	ZnSe/KRS-5/Diamond		
Refractive index (1,000 cm <sup>-1</sup> )	2.4		
Incident angle	45°	60°	
Penetration depth	4,000 cm <sup>-1</sup>	0.5 μm	0.28 μm
	2,000 cm <sup>-1</sup>	1.0 μm	0.55 μm
	1,000 cm <sup>-1</sup>	2.0 μm	1.10 μm
	400 cm <sup>-1</sup>	5.0 μm	2.80 μm

Material	Germanium		
Refractive index (1,000 cm <sup>-1</sup> )	4		
Incident angle	30°	45°	60°
Penetration depth	4,000 cm <sup>-1</sup>	0.3 μm	0.17 μm
	2,000 cm <sup>-1</sup>	0.6 μm	0.33 μm
	1,000 cm <sup>-1</sup>	1.2 μm	0.66 μm
	400 cm <sup>-1</sup>	3.0 μm	1.70 μm

When  $\theta = 45^\circ$  and  $n_{21} = 0.5$ , therefore, 10 μm (1,000 cm<sup>-1</sup>) dp corresponds to 3.18 μm and 5 μm dp (2,000 cm<sup>-1</sup>) to 1.6 mm.

The ATR method provides spectra of surface layers without actually slicing them.

Since the measurable depth (thickness) differs with the wavelength of the light, the ATR method gives spectra of a little different shape though the peak wavenumbers are the same.

The commercial availability of ATR libraries is evidence of this fact.

The software program for correcting for penetration depth, incorporated in the IRTracer-100, IRPrestige-21, IRXross, IRAffinity-1 series, IRSpirit series and FTIR-8000 series further widens the application field of the ATR method.

## Single Reflection Type Attenuated Total Reflection Attachment Integral with Sample Compartment

**QATR 10** (P/N 227-38001-XX) for IRTracer-100/IRXross/IRAffinity-1 series

**QATR-S** (P/N 227-38004-XX) for IRSpirit series

This is a single reflection type horizontal attenuated total reflection attachment. Samples are measured by pressing them against an approximately 1.8 mm diameter prism that is positioned horizontally. Because the prism is made only of diamond (wide-range specifications), it allows for measurements up to 400  $\text{cm}^{-1}$ . This ATR attachment supports the measurement of liquid samples and solid samples such as plastics, fibers, films, and powders. Diamond (high-throughput specifications), Ge, and ZnSe prism plates are also available. Use the Ge prism to measure samples with a high refractive index, such as black rubber.

The clamp, which makes the prism adhere to the sample, is equipped with a built-in torque limiter. It enables reproducible pressure while minimizing the potential of damage to the prism.

Range of measurable wavenumbers:

Diamond (wide-range specifications): Up to 40  $\text{cm}^{-1}$ \*

Diamond (high-throughput specifications): Up to 400  $\text{cm}^{-1}$

ZnSe: Up to 500  $\text{cm}^{-1}$

Ge: Up to 480  $\text{cm}^{-1}$

Accessories are automatically recognized when installed on the main body. Note that QATR 10 is the dedicated accessory for IRTracer-100/IRXross/IRAffinity-1S, and QATR-S is the dedicated accessory for IRSpirit series. The IRAffinity-1 series system with an optional blue ASC connector installed cannot be used.

\*: The actual wavenumber ranges that can be measured will vary depending on the specifications of the FTIR main unit. With the IRAffinity-1 series, IRXross, IRTracer-100 (mid-infrared specifications) or IRSpirit series (except ZX model) the range is up to 400  $\text{cm}^{-1}$ .

### Measurable Samples

- Film
- Paper
- Rubber
- Molded plastic
- Surface coating
- Liquid and gel samples
- Powder

### Notes

- For details about the chemical resistance of the prisms, see the table at the end of this guide.

### QATR 10 Part Names and P/N

Description	P/N
QATR 10 (Wide-range specifications)	227-38001-01
QATR 10 (High-throughput specifications)	227-38001-02
QATR 10 (ZnSe disk specifications)	227-38001-03
QATR 10 (Ge disk specifications)	227-38001-04

### QATR-S Part Names and P/N

Description	Warranty	P/N
QATR-S (Wide-range specifications)	One year	227-38004-01
	Ten years	227-38004-12
QATR-S (High-throughput specifications)	One year	227-38004-02
	Ten years	227-38004-22
QATR-S (ZnSe disk specifications)	One year	227-38004-03
QATR-S (Ge disk specifications)	One year	227-38004-04

### Maintenance Parts

Description	P/N
Stainless-steel flat anvil	227-38002-02
Stainless-steel pellet anvil	227-38002-03
Volatile corrosion inhibiting cover	227-38002-04
Ball driver 3.0 mm (Used for removing the cover plate of optical unit)	227-38002-06
Ball driver 2.5 mm (Used for adjusting the mirror of optical unit)	227-38002-07
Purge sponge set (for QATR 10)	227-38002-11
Cover plate for FTIR (for QATR 10)	227-38002-10



QATR 10

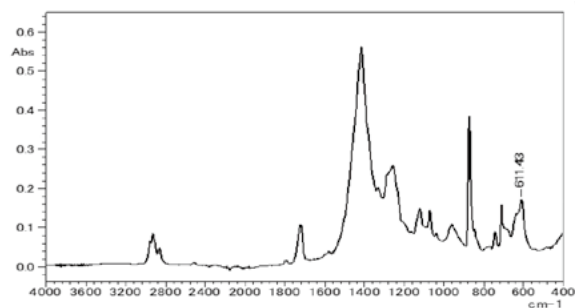
QATR-S



IRXross + QATR 10



IRSpirit-X + QATR-S



Infrared Spectrum of PVC Resin Piece

### Options

Description	P/N
Diamond disk (Wide-range specifications)	227-38002-05
Diamond disk (High-throughput specifications)	227-38003-01
ZnSe disk	227-38003-02
Ge disk	227-38003-03
Specular reflection disk	227-38003-04



## Single Reflection Type Attenuated Total Reflection Attachment Integral

**MicromATR (P/N 206-36177-01)**

**MicromATR Vision (P/N 206-36177-02)**

These are single reflection type horizontal attenuated total reflection attachment. MicromATR Vision has a visual image viewing function. Samples are measured by pressing them against an approximately 2 mm diameter prism that is positioned horizontally. Because the prism is made only of diamond, it allows for measurements up to 400  $\text{cm}^{-1}$ . This ATR attachment supports the measurement of liquid samples and solid samples such as plastics, fibers, films, and powders. Images can be displayed and saved on PC by USB connection. ATR measurement can be performed while observing the sample. It can be available 3- and 9-reflection diamond and Ge prism as option (In the case of Ge prism, visual observation is not possible). Use the Ge prism to measure samples with a high refractive index, such as black rubber. The clamp, which makes the prism adhere to the sample, is equipped with a built-in torque limiter. It enables reproducible pressure while minimizing the potential of damage to the prism.



MicromATR Vision

Range of measurable wavenumbers:

Single reflection diamond: Up to 400  $\text{cm}^{-1}$

3- and 9-reflection diamond: Up to 650  $\text{cm}^{-1}$

Ge: Up to 500  $\text{cm}^{-1}$

Video capture software e-Spot is included as standard.

An optional pressure sensor can be installed.

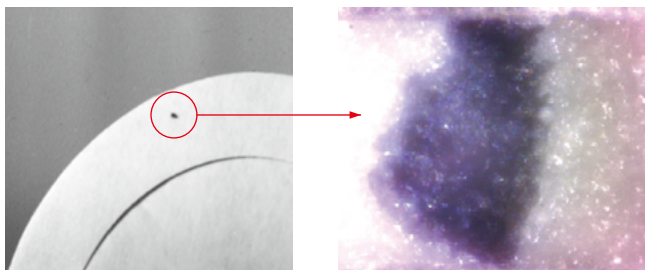
Accessory recognition function is not Included.

### Measurable Samples

- Film
- Paper
- Rubber
- Molded plastic
- Surface coating
- Liquid and gel samples
- Powder

### Notes

- For details about the chemical resistance of the prisms, see the table at the end of this guide.
- Since the metal part of the diamond plate is made of stainless steel, it cannot be used with strong acid. However, if the plate is replaced with a Hastelloy one, it can be used for measuring samples with strong acid.
- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.



In the case of contaminant adhering to the resin, by observing the image, the sample can be contacted with ATR prism.



Observation image of a 50  $\mu\text{m}$  thick fiber  
The illumination enables clear image observation.

### Options

Description	P/N
Single reflection diamond disk (Wide-range specifications)	100-00-0025
Ge disk	100-00-0026
3 reflection diamond disk	
9 reflection diamond disk	
Hastelloy plate	



## Single Reflection Type Attenuated Total Reflection Attachment Integral with Sample Compartment

### MIRacle 10 (P/N 206-74127-XX)

This is a single reflection type horizontal attenuated total reflection attachment.

Samples are measured by pressing them against an approximately 1.5 mm diameter prism that is positioned horizontally. The prism materials available are diamond (with ZnSe support element), ZnSe, and Ge.

This ATR attachment supports the measurement of liquid samples and solid samples such as plastics, fibers, films, and powders.

Use the diamond or Ge prism to measure acidic or alkaline samples. Use the Ge prism to measure samples with a high refractive index, such as black rubber.

The measurement wavenumber range is 4,600 - 600  $\text{cm}^{-1}$  for diamond and ZnSe and 4,600 - 700  $\text{cm}^{-1}$  for Ge.

MIRacle 10 is a dedicated accessory for IRTracer-100, IRXross and IRAffinity-1 series that incorporates an automatic accessory recognition function. It cannot be used with IRPrestige-21, IRSpirit series or the FTIR-8000 series.



### Measurable Samples

- Film
- Paper
- Rubber
- Molded plastic
- Surface coating
- Liquid and gel samples
- Powder

### Notes

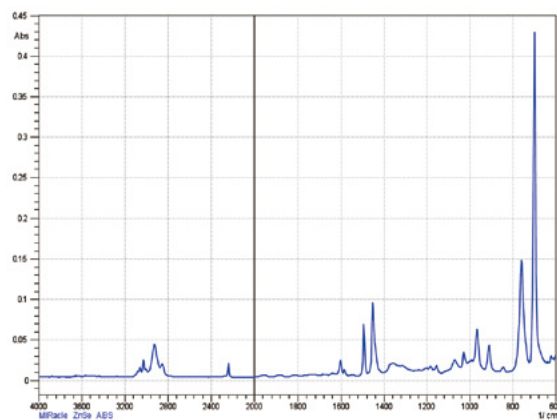
- Toxic hydrogen selenide may be generated if strongly acidic samples are measured using the ZnSe prism. Measure samples between pH5 and 9. Use the diamond or Ge prism to measure acidic samples to approximately pH2. Note, however, that measuring samples more acidic than this may result in corrosion of the prism or prism plate. Consult your Shimadzu representative.
- For details about the chemical resistance of the prisms, see the table at the end of this guide.
- The following power supply is required if a pressure sensor is attached:  
90 to 264 V AC adaptor, 0.5 VA power consumption

### MIRacle 10 Part Names and P/N

Description	P/N
MIRacle 10 diamond prism	206-74127-93
MIRacle 10 diamond prism with pressure sensor	206-74127-96
MIRacle 10 ZnSe prism	206-74127-91
MIRacle 10 ZnSe prism with pressure sensor	206-74127-94
MIRacle 10 Ge prism	206-74127-92
MIRacle 10 Ge prism with pressure sensor	206-74127-95

### Standard Content

Description	Quantity
MIRacle 10 main unit	1
Prism plate (Select diamond, ZnSe, or Ge.)	1
Sample clamp (Select clamp with or without pressure sensor.)	1
Adaptor for liquid samples	1



IR Spectrum of ABS Resin

### Options and Maintenance Parts

Description	P/N
ZnSe prism plate for MIRacle 10	208-97320-44
Ge prism plate for MIRacle 10	208-97320-45
Diamond prism plate for MIRacle 10	208-97320-46
Pressure sensor for MIRacle 10	208-97320-62

## Single Reflection Type Attenuated Total Reflection Attachment Integral with Sample Compartment

### GladiATR 10 (P/N 206-74128-XX)

This is a single reflection type horizontal attenuated total reflection attachment.

Samples are measured by pressing them against a 2.2 × 3 mm diamond prism that is positioned horizontally. An optional Ge prism is available. This ATR attachment supports the measurement of liquid samples and solid samples such as plastics, fibers, films, and powders. Use the optional Ge prism to measure samples with a high refractive index, such as black rubber.

As the prism is made of diamond only, the measurement wavenumber range is 4,600 - 400 cm<sup>-1</sup> and 4,600 - 700 cm<sup>-1</sup> for the Ge prism. GladiATR 10 is a dedicated accessory for IRTracer-100, IRXross and IRAffinity-1 series that incorporates an automatic accessory recognition function. It cannot be used with IRPrestige-21, IRSpirit series or the FTIR-8000 series.



### Measurable Samples

- Film
- Paper
- Rubber
- Molded plastic
- Surface coating
- Liquid and gel samples
- Powder

### Notes

- Measuring strongly acidic samples below pH3 may result in corrosion of the prism or prism plate. Consult your Shimadzu representative.
- For details about the chemical resistance of the prisms, see the table at the end of this guide.
- The following power supply is required if a pressure sensor is attached:  
90 to 264 V AC adaptor, 0.5 VA power consumption

### GladiATR 10 Part Names and P/N

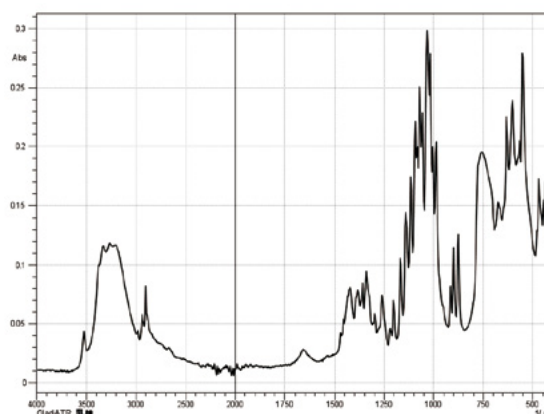
Description	P/N
GladiATR 10 diamond prism	206-74128-91
GladiATR 10 diamond prism with pressure sensor	206-74128-92

### Standard Content

Description	Quantity
GladiATR 10 main unit	1
Diamond prism plate	1
Sample clamp (Select clamp with or without pressure sensor.)	1
Adaptor for liquid samples	1

### Options and Maintenance Parts

Description	P/N
Ge prism plate for GladiATR 10	208-97321-44
Diamond prism plate for GladiATR 10	208-97321-42
Pressure sensor for GladiATR 10	208-97321-62



IR Spectrum of Lactose Powder

## Horizontal Type Attenuated Total Reflection Attachment Integral with Sample Compartment HATR 10 (P/N 206-74126-91)

Samples are measured by pressing them against a prism that is positioned horizontally. The prism is made of ZnSe, and an optional Ge prism is also available. This ATR attachment supports the measurement of liquid samples and flat solid samples such as films, rubbers, and flat plastics. It is not suitable for powder samples or very small samples. Use the optional Ge prism to measure samples with a high refractive index, such as black rubber.

HATR 10 is a dedicated accessory for IRTracer-100, IRXross and IRAffinity-1 series that incorporates an automatic accessory recognition function. It can not be used with IRPrestige-21, IRSpirit series or the FTIR-8000 series.



### Features

- Two separate prisms for solid and liquid samples are supplied as standard.
- The prism is easy to install and remove, making cleaning and replacement of the prism simple.
- The measurement wavenumber range is 4,600 - 700  $\text{cm}^{-1}$  for the ZnSe prism. It supports the measurement of liquid samples between pH5 and 9.
- The measurement wavenumber range is 4,600 - 700  $\text{cm}^{-1}$  for the Ge prism. It supports the measurement of samples with a high refractive index and acidic or alkaline samples. Note, however, that measuring strongly acidic samples below pH3 may result in corrosion of the prism or prism plate. Consult your Shimadzu representative.
- Number of reflections: 10
- Prism dimensions: 80 mm  $\times$  10 mm
- For details about the chemical resistance of the prisms, see the table at the end of this guide.

### Measurable Samples

- Film
- Flat plastic
- Paper
- Surface coating on flat metal
- Rubber
- Liquid and gel samples

### Notes

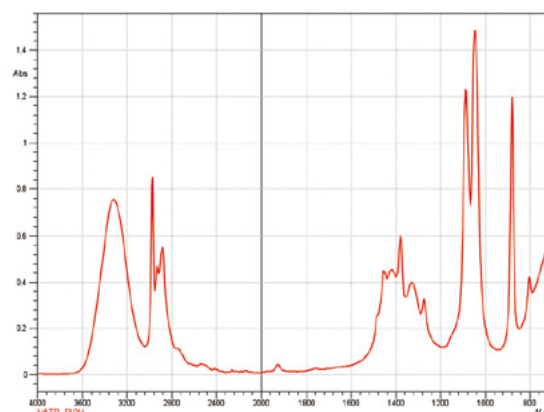
- Toxic hydrogen selenide may be generated if strongly acidic samples are measured using the ZnSe prism. Measure samples between pH5 and 9. Use the Ge prism to measure acidic samples to approximately pH2. Note, however, that measuring samples more acidic than this may result in corrosion of the prism or prism plate. Consult your Shimadzu representative.
- For details about the chemical resistance of the prisms, see the table at the end of this guide.

### Standard Content

Description	Quantity
HATR 10 main unit	1
ZnSe prism for solid samples, 45° incident angle	1
ZnSe prism for liquid samples, 45° incident angle	1
Sample clamp	1

### Options and Maintenance Parts

Description	P/N
ZnSe prism plate for solid samples, 45° incident angle, for HATR 10	208-97319-44
Ge prism plate for solid samples, 45° incident angle, for HATR 10	208-97319-48
ZnSe prism plate for liquid samples, 45° incident angle, for HATR 10	208-97319-43
Ge prism plate for liquid samples, 45° incident angle, for HATR 10	208-97319-47



IR Spectrum of Ethanol

## Attenuated Total Reflection Attachment

**ATR-8000A** (P/N 206-62303-58)

**ATR-8000** (P/N 206-62303-51)

In the ATR-8000 series, the incident angle is changeable in three steps of 30°, 45°, and 60°, so that measurement can be made to different depths. Combined with the program to correct for the penetrating depth of the infrared rays (which is a weak point of the ATR method because it differs depending on the wavenumber), this feature provides spectra that are highly comparable to those given by another method. A KRS-5 prism is provided standard. An optional Ge prism is used to measure samples with a high refractive index. ATR-8000A includes the automatic accessory recognition function.

### Features

- It is not necessary to adjust the position of the prism when a new sample is set.
- The sample holder is held at one point; hence, the prism is under minimized force.
- 25 times reflection (with an incident angle of 45°) ensures high sensitivity.
- Maximum sample size: 40 mm × 15 mm, 10 mm thick
- The measurement wavenumber range is 4,600 - 400 cm<sup>-1</sup> for the KRS-5 prism.
- The measurement wavenumber range is 4,600 - 700 cm<sup>-1</sup> for the Ge prism. It supports the measurement of samples with a high refractive index and strongly acidic or alkaline samples. Note, however, that measuring strongly acidic samples below pH3 may result in corrosion of the prism or prism holder. Consult your Shimadzu representative.
- For details about the chemical resistance of the prisms, see the table at the end of this guide.

### Measurable Samples

- Film
- Rubber
- Surface coating on flat metal
- Paper
- Flat plastic

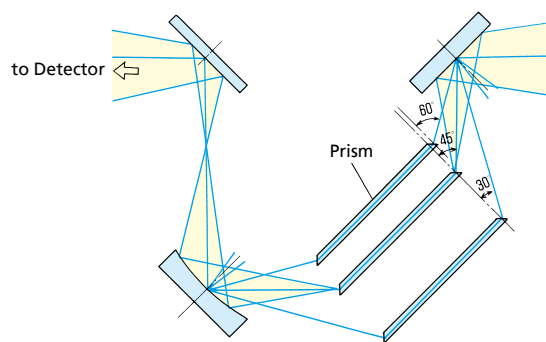
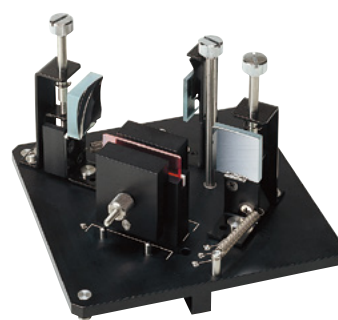
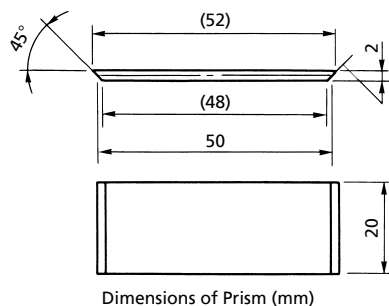
### Standard Content

Description	Quantity
Attenuated Total Reflection Attachment main unit	1
ATR prism (KRS-5)	1
Sample holder	1 set
Hex key wrench	1
Phillips screwdriver	1

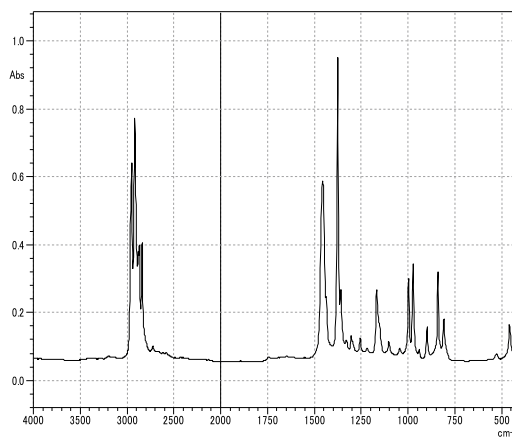
### Options and Maintenance Parts

Material	With holder (P/N)	Without holder (P/N)
KRS-5	206-61560-01	200-66125-01
Ge	206-61560-02	200-66125-02

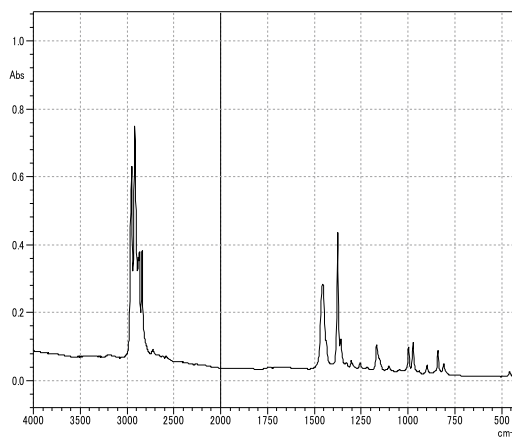
Note: Prisms without a holder are recommended as supplies, while those with a holder are recommended when prisms of different materials are purchased.



Optics of ATR-8000



IR Spectrum of PET (KRS-5 prism)



IR Spectrum of PET, Corrected for Penetration Depth

## Horizontal Type Attenuated Total Reflection Attachment

**ATR-8200HA** (P/N 208-97240-92)

**ATR-8200H** (P/N 208-97240 except IRTracer-100, IRXcross)

The principle is the same as the ATR-8000. Since the prism can be placed horizontally, liquid or gel samples, which cannot be analyzed with the ordinary ATR-8000/8000A can be readily measured.

ZnSe prisms are provided standard. An optional Ge prism is used to measure samples with a high refractive index or highly acidic or alkaline samples.

ATR-8200HA includes the automatic accessory recognition function.

### Features

- Prisms for liquid samples and for solid samples are provided as standard.
- The prism is mounted and dismounted by one-touch operation, which ensures easy exchange of samples and cleaning of prism.
- The measurement wavenumber range is 4,600 - 700  $\text{cm}^{-1}$  for the ZnSe prism. It supports the measurement of samples between pH5 and 9.
- The measurement wavenumber range is 4,600 - 700  $\text{cm}^{-1}$  for the Ge prism. It supports the measurement of samples with a high refractive index and strongly acidic or alkaline samples. Note, however, that measuring strongly acidic samples below pH3 may result in corrosion of the prism or prism plate. Consult your Shimadzu representative.
- Number of reflections: 10
- Prism dimensions: 80 mm  $\times$  10 mm
- For details about the chemical resistance of the prisms, see the table at the end of this guide.

### Measurable Samples

- Film
- Paper
- Rubber
- Flat plastic
- Surface coating on flat metal
- Liquid and gel samples

### Notes

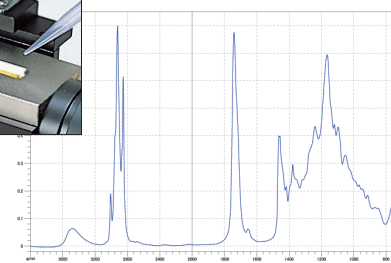
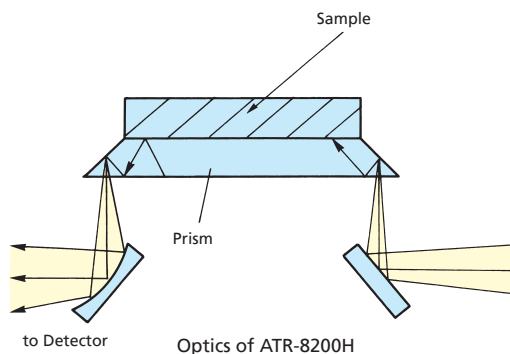
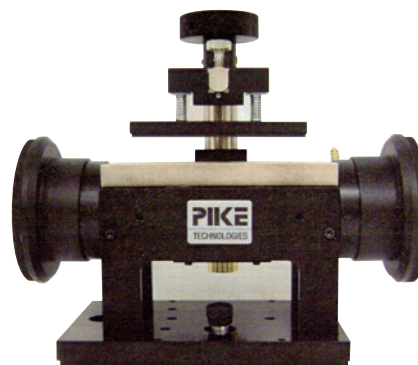
- Toxic hydrogen selenide may be generated if strongly acidic samples are measured using the ZnSe prism. Measure samples between pH5 and 9.
- Use the Ge prism to measure acidic samples to approximately pH2. Note, however, that measuring samples more acidic than this may result in corrosion of the prism or prism plate. Consult your Shimadzu representative.
- For details about the chemical resistance of the prisms, see the table at the end of this guide.
- When ATR-8200HA (P/N 208-97240/97240-91) is used on IRTracer-100, IRXcross or IRSpirit series the Purge tube (P/N 208-97240-36) is required.
- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

### Standard Content

Description	Quantity
Horizontal Type Attenuated Total Reflection Attachment main unit	1
ZnSe prism for solid samples, 45° incident angle	1
ZnSe prism for liquid samples, 45° incident angle	1
Gripper (P/N 208-97240-25)	1

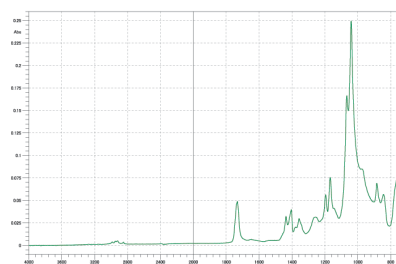
### Maintenance Parts

Description	P/N
ZnSe prism for solid samples, 45° incident angle	208-97240-03
ZnSe prism for liquid samples, 45° incident angle	208-97240-01
Ge prism for solid samples, 45° incident angle	208-97240-13
Ge prism for liquid samples, 45° incident angle	208-97240-10
Purge tube	208-97240-36



FTIR Spectrum of Edible Oil

The prism for liquid samples is fixed in the bottom of a boat-shaped groove, as shown in the above figure, so that liquid, powder or gel samples can be easily measured. The indentation to accept the sample is accessible from above to ensure ease when replacing samples and cleaning the prism.



FTIR Spectrum of PVDC Sheet

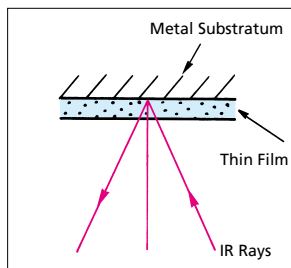
The prism for solid samples permits easy measurement of film and other solid samples, with operation being the same as that for the regular ATR. A gripper is fixed to hold the sample in close contact with the prism surface, which enables highly reliable spectra.

# Reflectance Measurement

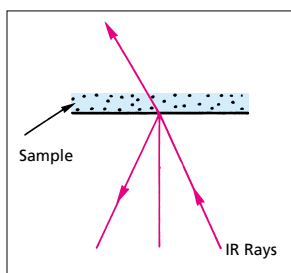
## Specular Reflectance Method

FTIR measurement by the specular reflectance method provides three types of information shown below:

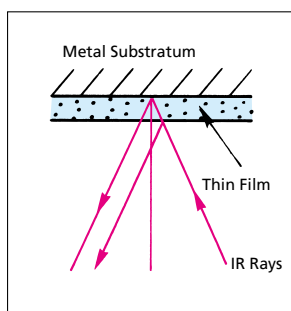
① The incident light passes through the sample layer and is reflected by the substrate: the spectrum given is similar to that obtained by the transmission method. Measurement of thin film on a metal plate is a typical example of this method.



② The incident light is reflected by the surface of the sample: the reflection spectrum is obtained, which can be converted into absorption spectrum through the use of the Kramers-Kronig analysis method. Transmitted light cannot be detected.



③ The above mentioned two types of information are mixed: the spectrum given is the sum of the transmission spectrum and the reflection spectrum. When the sample has a uniform thickness, the two reflection light beams interfere with each other, and the sample thickness can be obtained from the interference pattern. The measurement of an epitaxial layer of a semi-conductor sample is a typical application of this method.



1. In perpendicular polarization, the vectors of the polarized light are opposite to each other. Therefore, no stationary waves are produced on the substrate, and interaction with the film material
2. is not detected.

In parallel polarization, the vectors of the polarized light meet at a point to produce stationary waves, which interact with the film and are absorbed. The intensity of this absorption is dependent on the incident angle: the larger the incident angle, the higher the intensity of absorption. The optimum incident angle is different with the type of sample and the wavelength of the peak under study. In many cases, an incident angle between 70° and 80° is used.

## 2. Conversion of Reflection Spectra into Absorption Spectra

A reflection spectrum, which provides information on the optical properties of the sample, must be converted into the absorption spectrum to be informative about the chemical structure of the sample. The Kramers-Kronig analysis method is quite convenient in that it is useful to convert a reflection spectrum into an absorption spectrum: it is not necessary to shave or slice the sample. In the example (2) shown on the left, when the  $\theta$  is sufficiently small, each element of the complex refractive index of a material may be expressed as:

$$\text{Reflectance value} \quad n = \frac{1-R}{1+R-2\sqrt{R}\cos\theta} \quad \text{----- (1)}$$

$$\text{Absorption coefficient} \quad k = \frac{-2\sqrt{R}\sin\theta}{1+R-2\sqrt{R}\cos\theta} \quad \text{----- (2)}$$

where, R: Reflectance value

$\theta$ : phase shift when the light is reflected.

The  $\theta$  for the wavenumber  $\nu_g$  may be calculated from the following Kramers-Kronig equation:

$$\theta(\nu_g) = \frac{2\nu_g}{\pi} \int_0^\infty \frac{\ln\sqrt{R}(\nu)}{\nu^2 - \nu_g^2} d\nu \quad \text{----- (3)}$$

The  $\theta$  can be obtained from the reflectance value R, and substituting that  $\theta$  in the equation (2) gives the absorption coefficient k.

Performing this calculation for all the wavenumbers will give the absorption spectrum.

## Examples of Applications

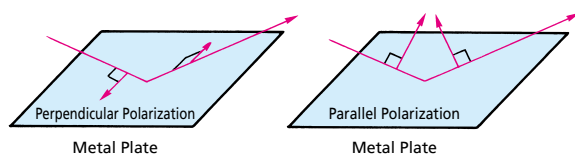
Since a reflection spectrum can be converted into the absorption spectrum through Kramers-Kronig analysis,

- ① Absorption spectrum can be obtained without shaving or slicing the sample, provided that the sample has a smooth surface. It is not necessary to use an ATR prism or a costly attachment.
- ② Kramers-Kronig analysis method is especially effective for infrared microscopy, where it is virtually impossible to slice the sample.

## 1. Reflection Absorption Spectroscopy

The Reflection Absorption Spectroscopy (RAS) method permits high-sensitivity measurement of a thin film sample on a metal substrate. This method has recently come to be applied to the measurement of very thin (a few tens of angstroms thick) samples and to the determination of molecular orientation.

When a polarized light beam is made incident on a metal substrate, as shown below, it is changed in phase when reflected by the metal surface.



Reflection of Light on Metal Substratum

## Specular Reflectance Attachment

**SRM-8000A** (P/N 206-62304-58)

**SRM-8000** (P/N 206-62304-51)

The specular reflectance measurement method is an old method to obtain reflection IR spectra.

The SRM-8000 series permits not only measurement of reflection spectra, but also measurement of absorption spectra through the combined use of the Kramers-Kronig analysis method.

This attachment provides absorption spectra of solids, such as high polymers, without using a prism, which is required in the ATR method.

QuickStart SRM-8000A includes the automatic accessory recognition function.

### Features

- Easy sample setting.
- Kramers-Kronig conversion software provides IR spectra without sample preparation.
- The incident angle is 10° on average.

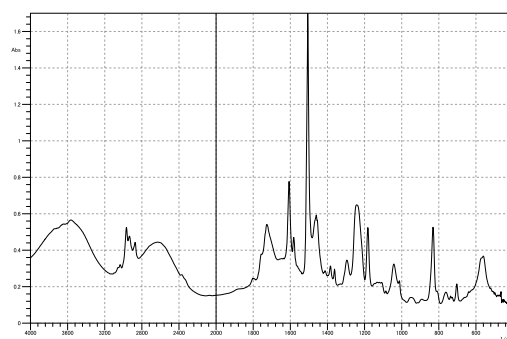
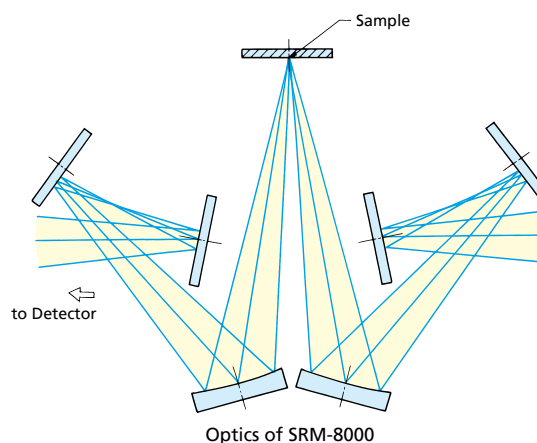
### Measurable Samples

- Coatings on flat metal surfaces with  $\mu\text{m}$  order.
- Flat plastic sheet.

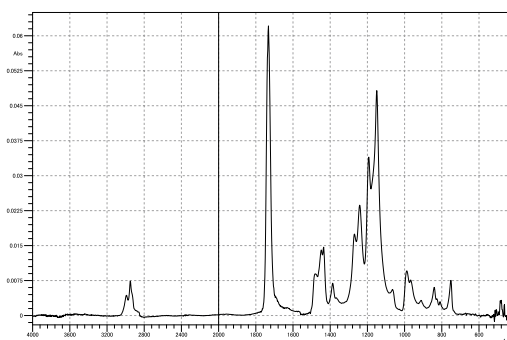
### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

Description	P/N	Quantity
Specular reflectance attachment main unit		1
Standard mirror	200-66123	1
Sample mask, 15 mm dia.	206-18752-02	1
Hex key wrench		1
Phillips screwdriver		1



Specular Reflectance Spectrum of the Inner Wall of Aluminum Can



Specular Reflectance Spectrum of PMMA after Kramers-Kronig Conversion



## Reflection Absorption Spectrometry Attachment

**RAS-8000A** (P/N 206-62302-58)

**RAS-8000** (P/N 206-62302-51)

The reflection absorption spectrometry method is used only in FTIR. When a perpendicularly polarized light and a horizontally polarized light are made incident on a metal substrate, the lights are changed in the respective phase.

In the case of perpendicularly polarized light, the phase change is  $\pi$  about , irrespective of the incident angle, and, hence, the vectors of the reflected light interact destructively with each other; the stationary waves produced have almost zero amplitude - no absorption of the sample is detected.

In the case of horizontally polarized light, the amount of phase change varies continuously from zero (for  $0^\circ$  incident angle) to  $\pi$  (for  $90^\circ$ ). The amplitude of the stationary waves produced also changes with the incident angle: when a high incident angle is selected, the stationary waves will have a high amplitude and the interaction of the light beam and the sample will be high, resulting in a high detecting sensitivity. This method permits high-sensitivity measurement of thin films on metals having a high reflectance. Combined use of a grid polarizer further enhances the sensitivity. A grid polarizer (P/N 206-61550-58) is not included in the standard content of the RAS-8000 series but is available as an option.

QuickStart RAS-8000A includes the automatic accessory recognition function.

### Features

- Easy sample setting.
- The incident angle is selectable between  $70^\circ$  and  $75^\circ$ .

### Measurable Samples

- Coatings on flat metal surfaces with a thickness in the nanometer range
- Flat plastic sheet

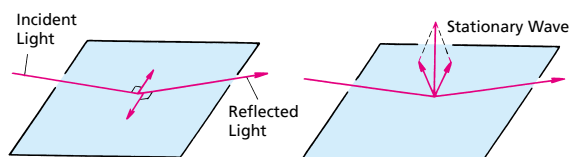
### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

### Standard Content

Description	P/N	Quantity
Reflection absorption spectrometry attachment		1
Standard mirror	200-66123	1
Sample mask, 8 mm dia.	206-18752-01	1
Sample mask, 15 mm dia.	206-18752-02	1
Sample mask, 25 mm dia.	206-18752-03	1
Light beam mask, 3 × 3 mm	206-18608-01	1
Light beam mask, 5 × 5 mm	206-18608-02	1
Light shielding plate*		1
Hex key wrench		1
Phillips screwdriver		1

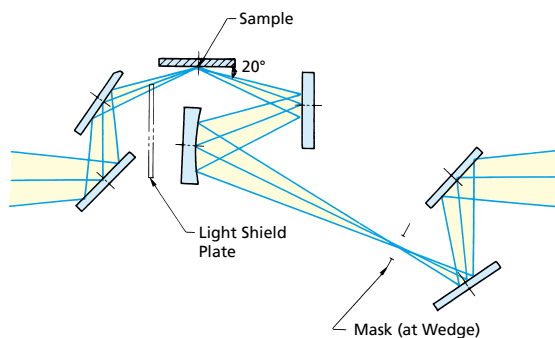
\* Attaching the light shielding plate raises the mean incident angle of the light beam from  $70^\circ$  to  $75^\circ$ .



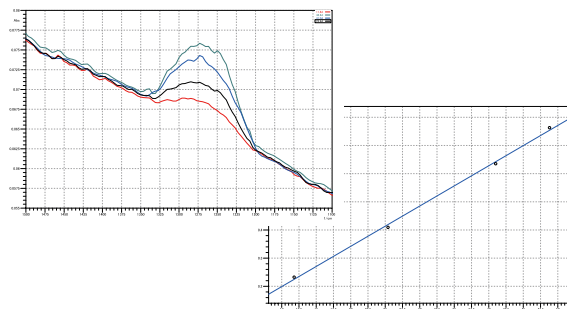
Perpendicular Polarization

Parallel Polarization

Principle of Reflection Absorption Spectrometry



Optics of RAS-8000



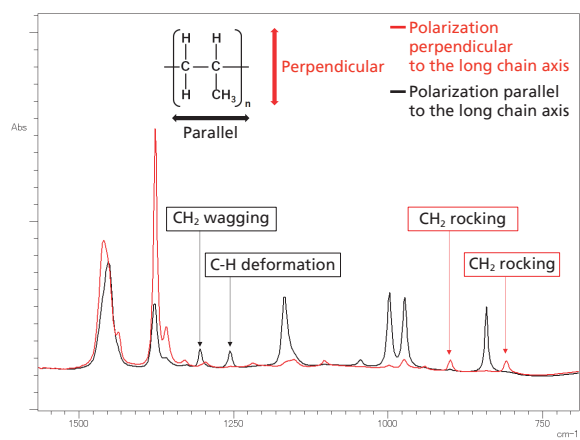
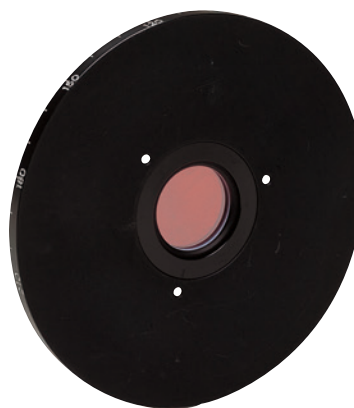
Relationship between Spectrum of Fluorine Film on Hard Disk, Peak Area and Film Thickness (Calibration Curve)

## Grid Polarizer

**GPR-8000** (P/N 206-61550-58)

A grid is precisely produced on the substrate by the photographic technique. The grid polarizer enhances the sensitivity of the RAS-8000 Reflection Absorption Spectroscopy Attachment.

Degree of polarization: 99% (at 10  $\mu\text{m}$ ), 95% (at 3  $\mu\text{m}$ )  
Quenching ratio: 148:1 (at 10  $\mu\text{m}$ ), 23:1 (at 3  $\mu\text{m}$ )  
Effective area: 25 mm dia.  
Angle scale: 360°, 10° increments  
Material of substrate: KRS-5, 2 mm thick  
Measurement wavenumber range: 5,000 to 350  $\text{cm}^{-1}$

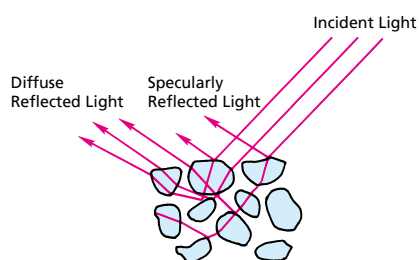


# Diffuse Reflectance Measurement

## Diffuse Reflectance Spectroscopy

In measurement of powder samples by the dispersive IR method, the KBr pellet method is often used. The powder sample is mixed with alkali halide powder, such as KBr, and briquetted into a pellet, which is then measured by the transmission method. This KBr pellet method is also used in FTIR, but the diffuse reflection spectroscopic method is easier to perform.

As shown in the figure below, when a light beam is made incident on a powder sample, some part of the light is specularly reflected by the surface of the powder. The other part penetrates into the sample and is transmitted and reflected repeatedly, and then emerges out of the sample as a diffuse reflected (scattered) light. This diffuse reflected light is informative of the IR spectrum of the powder sample.



Reflection within Powder Sample

Diffuse reflected light, which has been repeatedly transmitted within the powder sample, gives a spectrum similar to ordinary transmission spectrum. The spectral intensity is not completely proportional to the concentration of the compounds under study: those components which are detected as rather low intensity absorption bands are detected at higher intensity because the light beam is transmitted repeatedly in the sample. It is necessary, therefore, to compare diffuse reflected spectra with ordinary transmission spectra or to convert them with the Kubelka-Munk equation.

$$f = (1 - R)^2 / 2R = K/S$$

where, K: absorption coefficient

S: scattering coefficient

R: reflection index

(sample power spectrum/dilution power spectrum)

Since it is very difficult to measure absolute reflection indices, diffuse reflection indices, which are the values relative to the reflection of KBr or KCl powder having no absorption in the IR region, are generally used.

The spectra thus obtained are Kubelka-Munk converted to have intensities proportional to concentration. The result is spectra useful for quantitative determination. LabSolutions IR which control FTIR incorporates the Kubelka-Munk conversion function as a standard feature.

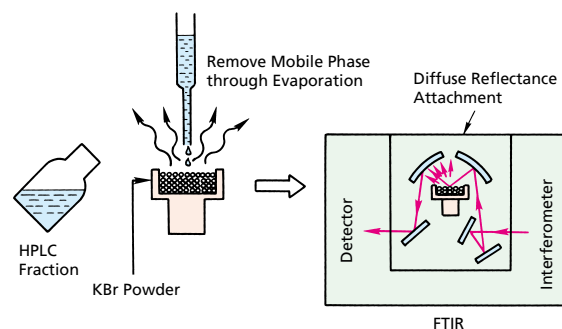
## Application 1

The diffuse reflectance spectroscopic method is applicable to any sample that can be pulverized. It also permits using, as the diluting substance, diamond powder or the like, which is not applicable to the KBr pellet method.

## Application 2

### LC Effluent Measurement

This method is also applicable to detection of substances dissolved in a volatile solvent, such as fractions of liquid chromatography. LC effluent is made to drop on KBr powder, the mobile phase is removed by evaporation, and then the fraction is analyzed with the FTIR instrument equipped with a diffuse reflectance attachment.



FTIR Analysis of HPLC Fractions

## Application 3

### Diffuse Reflectance Measurement in a Heated Vacuum

This can be used to measure samples in a high-temperature, vacuum, or reaction gas environment, which is useful for researching catalytic mechanisms, temperature dependency, zeolite, and so on. The measurement requires using a dedicated heated vacuum diffuse reflectance attachment. For information about heated vacuum diffuse reflectance attachments, contact your Shimadzu sales representative.

## Diffuse Reflectance Attachment

**DRS-8000A** (P/N 206-62301-58)

**DRS-8000** (P/N 206-62301-51)

The method of diffuse reflectance spectrometry is one of the most popular FTIR application methods of application of FTIR. It features high-energy throughput and simple operation.

The Shimadzu FTIR series incorporates, as standard, the Kubelka-Munk conversion functions, essential to diffuse reflectance spectrometry for correcting the light scattering by the KBr powder. LabSolutions IR which control FTIR incorporates the Kubelka-Munk conversion function as a standard feature.

DRS-8000A includes the automatic accessory recognition function.

### Features

- The small measuring light beam ( $1.8 \times 1.8$  mm) ensures reliable analysis of small samples.
- The attachment is a drawer type, which ensures easy replacing.
- The standard data processing functions include the Kubelka-Munk conversion functions as standard.

### Measurement Sample

- Powder

### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

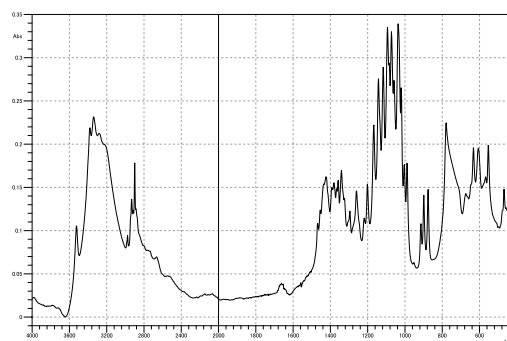
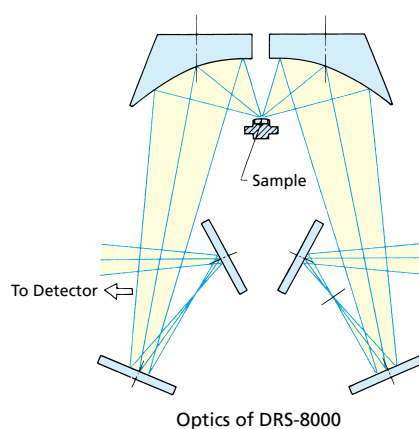
### Standard Content

Description	P/N	Quantity
Diffuse reflectance attachment main unit		1
Sample holder 2 mm ID cup		1
Sample holder 4 mm ID cup		1
Aluminum cup holder*		1
Standard mirror	206-62232-01	1
Ground glass mirror	206-62232-02	1
Sample holding rod		1
Hex key wrench		1
Phillips screwdriver		1

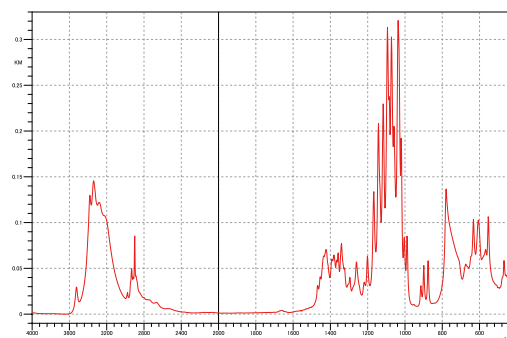
\* Holder for disposable sample cup. Disposable sample cups are available as extra.

### Options

Description	P/N
Sample cup, 50 pieces per set, aluminum, 6 dia. $\times$ 1.5 deep (mm)	201-52943
Sample die for aluminum cup	206-63950
SiC sampler	200-66750-01



Diffuse Reflectance Spectrum of Lactose



Diffuse Reflectance Spectrum of Lactose after Kubelka-Munk Conversion

## SiC Sampler

(P/N 200-66750-01)

In diffuse reflectance spectrometry, it is necessary to pulverize the sample and mix the powder with KBr powder.  
When the SiC sampler is used, the operation is simplified as follows:

### Features

- Diluent such as KBr powder is not required.
- The solid sample is ground with SiC emery paper and the sample powder on the emery paper is directly analyzed with the DRS-8000. (The SiC has a hardness of 9.0 and is quite chemically stable.)
- Samples are measured left clinging to emery paper in a holder that is attached directly to the DRS-8000 series attachment.
- New emery paper is used as reference.

### Measurement Samples

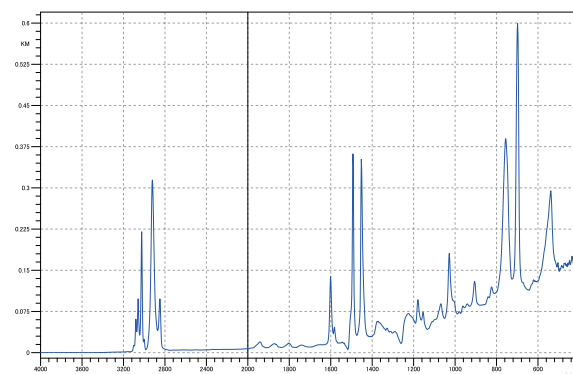
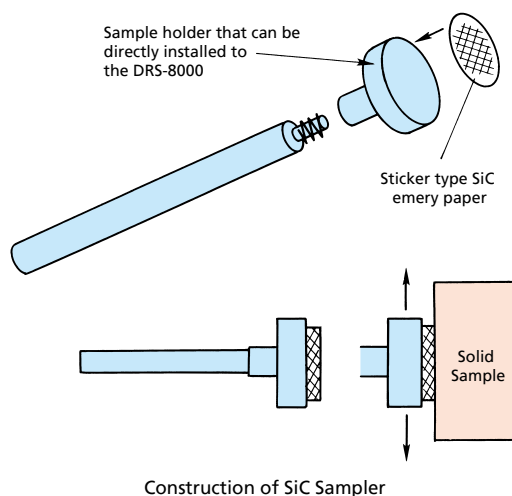
- Plastic molded parts

### Standard Content

Description	P/N	Quantity
Holding rod		1
Sample holder	208-92176	2
SiC emery paper (#320)		100 sheets
SiC emery paper (#400)		100 sheets

### Supplies

Description	P/N
SiC emery paper (#320), 100 sheets	200-66751-03
SiC emery paper (#400), 100 sheets	200-66751-02



Diffuse Reflectance Spectrum of Plastic Products Obtained with SiC Sampler

## Automatic Diffuse Reflectance Attachment DRS-8010ASC (P/N 206-62308-91)

Having the same optics as the DRS-8000, the DRS-8010ASC accepts 24 samples to permit automated measurement.

The IRTracer-100, IRPrestige-21, IRXross, IRAffinity-1 series and FTIR-8000 series systems incorporate as standard a control output capability that eliminates the need for a special controller and enables a simpler system configuration.

### Features

- One-touch connection to the main unit, which has the control capability as standard.
- With no external control unit required, the DRS-8010ASC is very compact.
- Controlled by Labsolutions IR software.
- Manual control to reduce the frequency of opening the lid of the sample compartment is possible, resulting in higher analytical productivity.
- Use of the disposable sample cups ensures easy exchange of samples.

### Notes

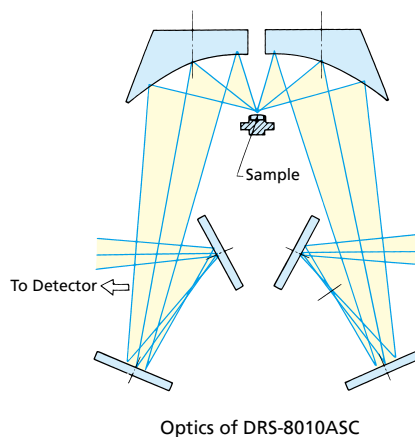
- When this attachment is used on IRAffinity-1S, the ASC cable (P/N 206-73433-41) is required.
- When this attachment is used on IRPrestige-21, the power unit (P/N 206-72018-91) is required.
- When this attachment is used on IRAffinity-1, the ASC cable (P/N 206-73433-91) is required.
- The BASIC software is required separately for the HYPER-IR model.
- When old version of DRS-8010ASC (P/N 206-62308) is used on IRTracer-100 and IRAffinity-1S, the ASC conversion connector (P/N 206-74385-41) is required.

### Standard Content

Description	Quantity
Automatic diffuse reflectance attachment main unit	1
Sample holder, 24-sample type	2
Standard mirror	1 set
Sample cup	200
Die	1
Tweezers	1 pair
Sample handling rod	1
Hex key wrench	1
Phillips screwdriver	1

### Options and Supplies

Description	P/N
Sample holder, 24-sample type	206-65234
Sample cup, aluminum, 6 dia. x 1.5 deep (mm)	201-52943



Sample stage of DRS-8010ASC

# Trace Sample Measurement

## Measurement Methods for Trace Samples

Methods (accessories) used for trace sample measurement include the single reflection ATR method, the infrared microscopy, and the Raman microscopy. Additionally, the infrared microscopy can be broadly separated into three measurement methods: transmission, reflection, and ATR. Select the optimal accessory depending on the size of the measured object.

### Single Reflection ATR Method

In this method, an accessory is attached to the sample compartment of the FTIR unit, and a signal is detected using the detector in the FTIR unit. Samples are pressed tightly to prisms with a diameter between approximately 1.5 and 2.0 mm. With the diamond ATR, an accessory with a built-in CCD camera, the sample can be checked through the prism, so the measured part can be configured at the level of a few mm.

### Infrared Microscopy

Measurements are performed by incorporating the infrared light source from an FTIR unit in a microscope. The measurement size can be freely configured via the aperture inside the microscope. However, when the aperture is reduced to 10  $\mu\text{m}$  or less, the correct spectrum might not be obtained due to the impact of diffraction of the infrared light.

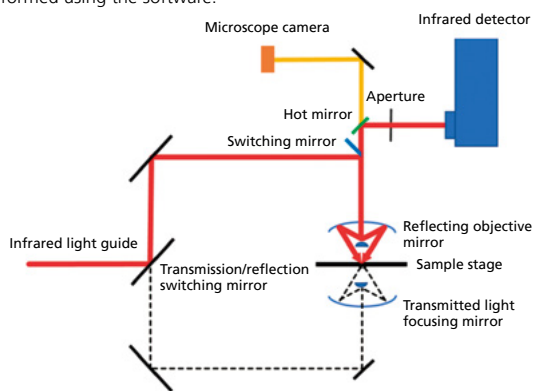
### Raman Microscopy

The sample is irradiated by laser light within the microscope, and the light scattered from the surface of the sample is detected by a CCD detector. A laser is used as the light source, so there is no need to stop down the light with an aperture as in infrared microscopy. The laser can irradiate samples as small as 3  $\mu\text{m}$  in diameter depending on the objective lens used.

	Single Reflection ATR Method	Infrared Microscopy	Raman Microscopy
Measurement Mode	ATR	Transmission/reflection/ATR	Scattering
Selection of the Measured Part	Possible in part	Possible Selection by aperture	Possible
Minimum Measurement Size	On the order of several hundred $\mu\text{m}$	10 $\mu\text{m}$	3 $\mu\text{m}$
Detector	FTIR unit detector	T2SL	CCD
Installation Method	FTIR unit sample compartment	Installed to the exterior of the FTIR unit	Installed to the exterior of the FTIR unit

## Notes Related to Measurement

The optical system of the infrared microscope is shown below. Using the transmission/reflection switching mirror, the mode can be switched between transmission and reflection/ATR mode. Switching is performed using the software.



### Infrared Microscopy (Transmission Mode)

The infrared light introduced from the FTIR unit interferometer is collected by a condenser mirror and then irradiates the sample. The infrared light that penetrates the sample is collected once again by the reflecting objective mirror, and is led to the infrared detector. One point that should be considered when performing the measurement is the sample thickness. The thicker the sample, the more saturated the infrared spectrum obtained, which can make it impossible to confirm the peak positions accurately, worsening the qualitative accuracy with respect to the object. In such cases, use a diamond cell to compress the sample, and obtain the optimal sample thickness before performing the measurement. Note that the optimal thickness is generally said to be on the order of 10  $\mu\text{m}$ .

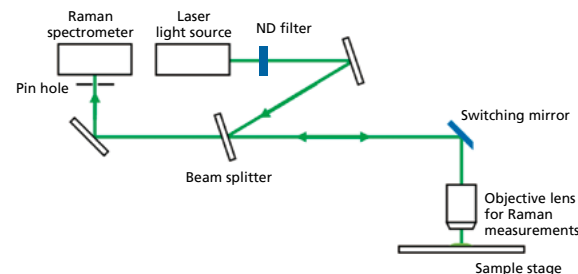
### Infrared Microscopy (Reflection Mode)

The infrared light introduced from the FTIR unit interferometer is collected by a reflecting objective mirror and then irradiates the sample. The infrared light that penetrates the sample is collected once again by the reflecting objective mirror, and is led to the infrared detector. The incident light path to the sample and the reflection light path are basically the same. One point that should be considered when performing the measurement is the form of the sample. As the name of the measurement mode implies, in this method, the light reflected from the sample is detected. Accordingly, if the reflectance for the object is low, the light led to the infrared detector will be very weak. As a result, the data will be noisy, and it might not be possible to detect the spectrum of the object. In such cases, perform sampling with the sample on an aluminum mirror or other substrate with a high reflectance before performing the measurements.

### Infrared Microscopy (ATR Mode)

The ATR method has been widely used in recent years because it is effective for samples with poor infrared light transmission. This method demonstrates its efficacy in the measurement of trace samples using an infrared microscope. Just as in reflection mode, a point that should be considered when performing the measurement is the form of the sample. In the ATR method, the infrared spectrum is obtained by pressing the sample tightly against an ATR prism, so a tight fit against the prism is important. Samples with slanting or irregular surfaces can be difficult to press tightly against the prism, so before performing the measurements, it might be necessary to pretreat the sample in order to flatten the surface.

The optical system of the infrared microscope in Raman mode is shown below.



### Raman Microscopy

In Raman measurements, a confocal optical system is used, enabling measurements with high spatial resolution. Additionally, in the case of transparent resin or glass where the laser light can penetrate into the sample, information on the interior can be obtained by condensing the laser light in the interior. Note that the focal size will differ depending on the objective lens used. Points that should be considered when performing the measurement are the laser intensity and fluorescence from the sample. If the sample is irradiated with high-intensity laser light, the object could become scorched if it contains organic compounds. To avoid this, reduce the intensity of the laser light irradiating the sample by using an ND filter before performing the measurements. In addition, the sample might produce fluorescent light depending on the wavelength of the laser light source. If this occurs, change the oscillation wavelength of the laser used before performing the measurements. With the 532 nm lasers that are generally used, the Raman scattered light is strong, so the peaks for the object are easy to detect. However, many samples produce fluorescence when irradiated by a laser at this wavelength. If the fluorescence has an impact, it raises the baseline of the Raman spectrum, which impedes peak detection. In this case, the impact of the fluorescence can be lessened by irradiating the object with a different laser with an oscillation wavelength longer than 532 nm.



## Infrared Microscope **AIMsight** (P/N 206-33000-58) Infrared/Raman Microscope **AIRsight** (P/N 206-35000-58)

These automatic analysis systems can be used with ease even by users new to analysis work. They are equipped with standard with a variety of enhanced functions that support analysis work.

### Features

#### AIMsight/AIRsight Infrared Mode

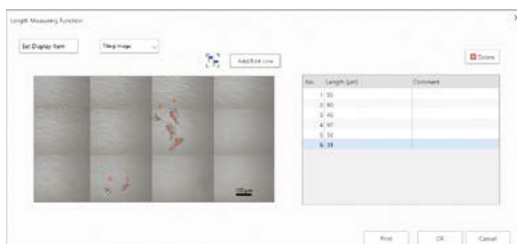
- This system is equipped with a bright theoretical optical system and a high-sensitivity, environmentally friendly, mercury-free T2SL detector, which provides an S/N ratio of 30,000:1, the highest level in this class.
- Reflection/ATR measurements can be performed with samples up to 40 mm in thickness.
- Equipped as standard with up to 330 magnification zoom using a wide field-of-view camera and a microscope camera. The measurement values can be determined quickly.
- Equipped as standard with an automatic contaminant recognition system that automatically determines the measurement position.
- Capable of recording up to 60 measurement positions.
- Equipped as standard with a contaminant analysis program for specifying the object.
- Equipped as standard with a length measurement function capable of measuring the length of the object.
- Equipped as standard with a spectral adviser function that provides troubleshooting for the operations and accessories characteristic of an infrared microscope.

#### AIRsight

- Capable of Raman measurements of samples up to 40 mm in thickness.
- Both infrared and Raman spectra can be obtained from the same location in an extremely small area without moving the sample.
- Equipped as standard with up to 1,330 magnification zoom thanks to a wide field-of-view camera and an objective lens for Raman measurements. The measurement values can be determined quickly.
- A single software program switches between infrared measurements and Raman measurements. Also, both spectra can be overlaid, and a variety of data analyses can be performed.
- Both organic and inorganic compounds can be analyzed with one microscope.
- Equipped with both infrared microscope and Raman microscope functions, substantially reducing the installation space required.

### Notes

- The following parts are required in order to use this accessory.  
When connected to the IRTracer-100:  
External light beam switching kit (P/N 206-32570-41)  
Microscope connection kit (P/N 206-35091-41)  
When connected to the IRXross:  
External light beam switching kit (P/N 206-37033-41)  
Microscope connection kit (P/N 206-37030-41)  
When connected to the IRAffinity-1 series:  
External light beam switching kit (P/N 206-32570-42)  
Microscope connection kit (P/N 206-35091-42)
- To perform mapping measurements, purchase the separately available High-Speed Mapping Program (P/N 206-36299-41).



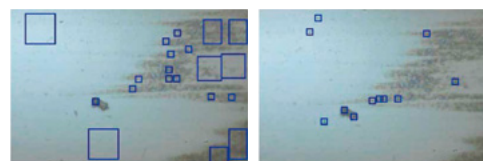
Length Measurement Function



IRXross + AIMsight  
Infrared Microscope System

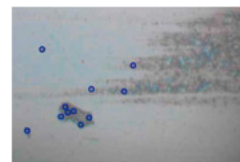


IRXross + AIRsight  
Infrared Raman Microscope System



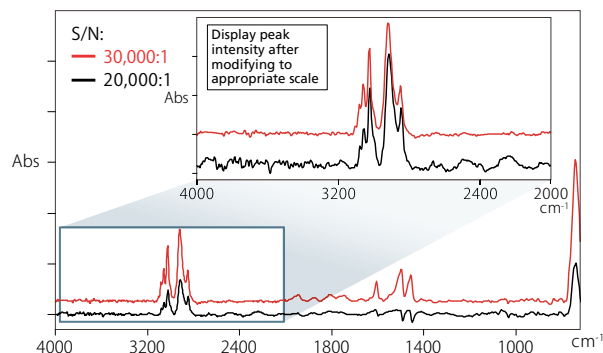
Infrared (Standard Mode)

Infrared (Micro Mode)



Raman

Automatic Contaminant Recognition System



Transmission Spectra of 10 µm Diameter Polystyrene Bead Obtained by Two Infrared Microscopes AIMsight with Different Noise Levels

### ATR Objective Mirror

(P/N 206-32600-41 for AIRsight, AIMsight and AIM-9000)

Using a cone-type Ge prism, this single reflection objective mirror features 15x magnification and a 45-degree mean incident angle. The slide-on type prism makes it easy to switch back and forth between visible observation and infrared measurement. This ATR objective is especially effective in analyzing samples that do not transmit or reflect infrared light easily, such as paper and plastics, or extremely thin areas, such as stains.



### Micro Vise Holder

(P/N 206-33293 for AIRsight, AIMsight and AIM-9000)

(P/N 208-97202 for AIM-8800)

This holds various types of samples for microscopy. It ensures positive holding of samples of a difficult shape or measurement of a sample at a user-selectable angle. Measurement with a polarizer, with the sample under tensile load, provides information on the molecular orientation.

#### Sizes of Storable Samples

- Tensile load Within approx. width of 20 mm  
Film of length 14 to 54 mm (excluding grip allowance)
- Gripped load Max. approx. length 40 mm  
Approx. width 40 mm

#### Standard Content

Description	Quantity
Micro vise holder main unit	1
Holding fixture	2



Micro Vise Holder

### ATR Pressure Sensor

(P/N 206-32603-42 for AIRsight and AIMsight)

(P/N 206-32603-41 for AIM-9000)

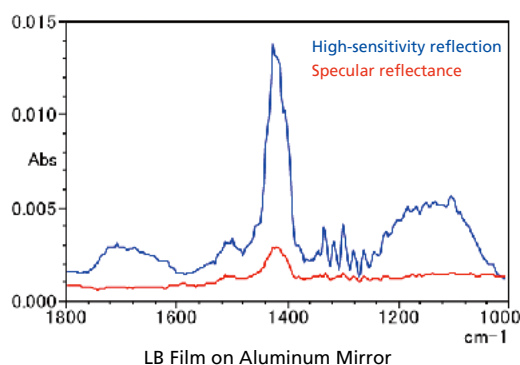
This pressure sensor prevents prism damage due to excessive pressures applied during ATR measurements using an ATR objective. It can also be used to automatically measure how tightly the sample is pressed against the prism.



## Grazing Angle Objective (GAO)

(P/N 206-32602-41 for AIRsight, AIMsight and AIM-9000)

This high-sensitivity objective mirror is useful for measuring samples with concave surfaces that cannot be pressed tightly against the ATR prism or samples that must be measured without contacting them. It is particularly beneficial for failure analysis of stains on circuit boards or extremely thin films on mirrors.



## TEC MCT Detector

(P/N 206-36820-41 for AIRsight and AIMsight)

## Room Temperature Detector (DLATGS)

(P/N 206-32580-42 for AIRsight and AIMsight)

(P/N 206-32580-41 for AIM-9000)

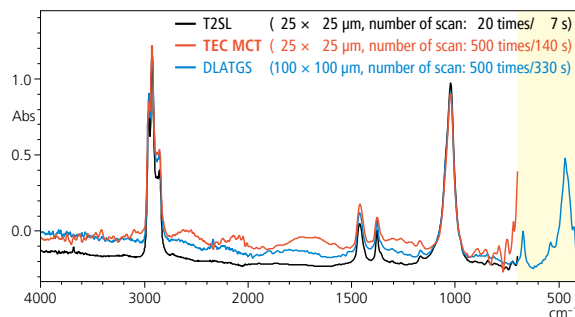
Equipping the AIMsight Infrared Microscope or the AIRsight Infrared/Raman Microscope with the TEC MCT (peltier cooled MCT) detector<sup>\*1, \*2</sup> makes it possible to obtain infrared spectra without using liquid nitrogen. If more sensitivity is required, simply switch to the standard T2SL detector<sup>\*3</sup> in the software.

\*1 A TEC MCT and DLATGS cannot be installed at the same time.

\*2 The DLATGS can measure across a wide wave-number range.

However, its sensitivity is substantially lower than the T2SL and TEC MCT.

\*3 Liquid nitrogen is required when using the T2SL.



Infrared spectra of polypropylene-based (containing TALC) resin for automotive bumpers using the three different detectors

## Particle Filter (PF) Holder

For 13 mm dia. (P/N 206-36610-41)

For 25 mm dia. (P/N 206-36610-42)

The PF holder fastens the Membrane Filter (PTFE or stainless steel (SUS)) used in microplastics analysis by gripping it. This prevents the Membrane Filter from sagging during drying, which keeps the surface flat and enables more accurate measurements.

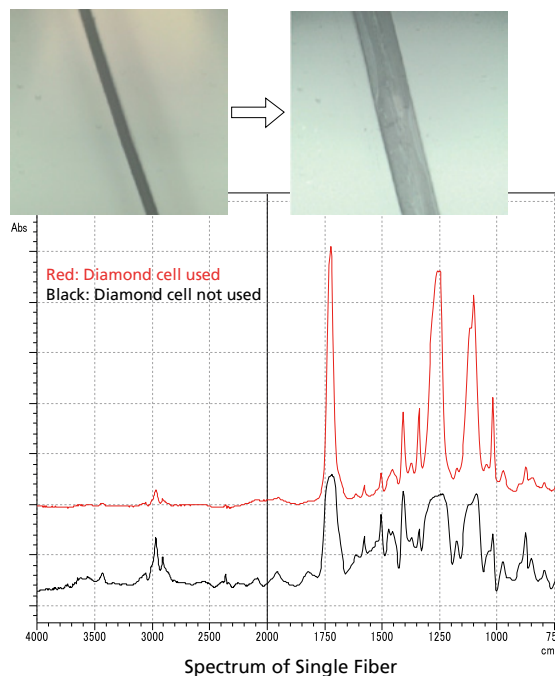
- Quantity: two each



## Diamond Cell

This pressurized cell thinly compresses samples with a certain degree of thickness or minute samples placed on a microscope's stage to perform transmission measurement as they are. This cell is applicable to a variety of samples including drugs, rubber and plastic.

- Notes
- Diamonds exhibit slight absorption in the range 3,000 to 1,500  $\text{cm}^{-1}$ .
  - Diamonds are hard but brittle and may crack depending on the sample and method of use.



## Diamond Cell C II (P/N 208-92289-01)

### Features

- Artificial diamond used
- Large-size diamond provides 1.6 mm diameter window

### Standard Content

Description	Quantity
C II plate	1
C II screws	3
Holder with diamond window for C II	2
Case	1

### Options and Maintenance Parts

Description	P/N
C II plate	208-92289-13
C II screws (pack of 3)	208-92289-14
Holder with diamond window for C II	208-92289-11



Diamond Cell C II

## Sampling Kit (P/N 208-92171)

This kit is for pretreating samples for microscope measurement. It comprises a set of tweezers, roller knife, needles, scissors, replacement blades and replacement needles.

### Standard Content

Description	Quantity
Tweezers (straight)	1
Tweezers (curved)	1
Roller knife	1
Needle (straight)	1
Needle (bent)	1
Needle holder	1
Scissors	1
Replacement blades (pack of 5)	1
Replacement needles (pack of 5)	1
Exclusive case	1



Sampling Kit

## Options for Infrared Microscope AIRsight and AIM-9000

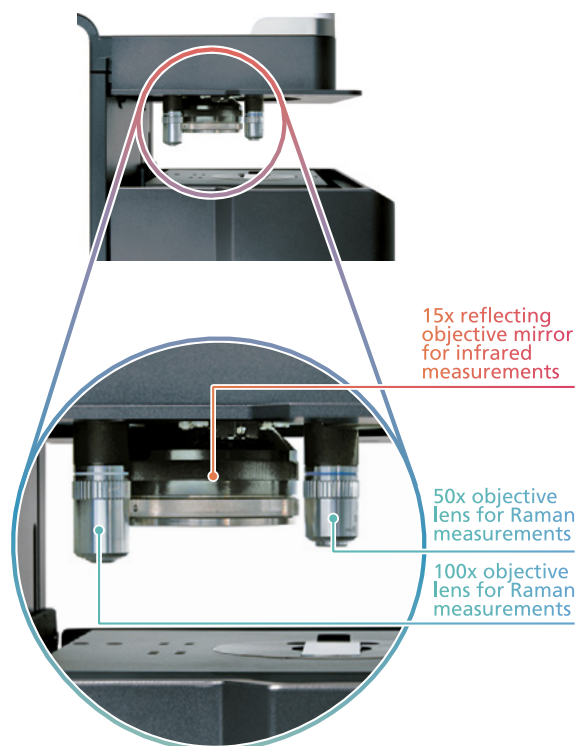
Description	P/N	Remarks
Aluminum reference mirror	206-90104	13 mm dia.
KBr window	—	13 mm dia. × 2 mm thick
CaF <sub>2</sub> window	—	
Infrared polarizer	206-32605-41	
Visible polarizer	206-32540-41	

## Objective Lens for AIRsight

50x (P/N 206-35092-41)

100x (P/N 206-35092-42)

There are two objective lenses available: a standard 50x objective lens that allows observation within a range of  $200 \times 150 \mu\text{m}$ , and a high-magnification 100x objective lens (for fine observation) that allows observation within a range of  $100 \times 75 \mu\text{m}$ . It is also possible to simultaneously mount both objective lenses on the revolver. Each objective lens can be switched using the rotation of the revolver. The spatial resolution is  $5 \mu\text{m}$  or less for the 50x objective lens and  $3 \mu\text{m}$  or less for the 100x objective lens.



# Accessories for Automated Measurement

## Automating the Operation

The technique of Fourier Transform Infrared Spectrophotometry (FTIR) is now extensively used in various fields for R&D and industrial purposes.

Since samples measured by infrared spectrophotometry are mostly chemically stable and can be measured without pretreatment, it is fairly easy to automate the measurement of many samples.

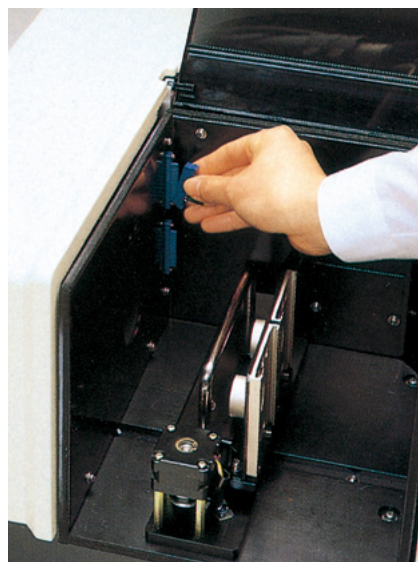
Automating the measurement saves labor and ensures high analytical productivity.

## Automating the FTIR Measurement

One of the most important methods to automate the operation of the FTIR main is to utilize a computer system.

Combination of a computer and the program, described below, provides automation of sample loading and unloading, measurement, data processing, and presentation of the analytical results.

The photo to the right shows the ASC connector equipped in the sample compartment of FTIR-8000 series (supplied as standard), which is used to export the control signals to an automatic sample changer. The software incorporated in the FTIR can control the automatic sample changer via a pair of the ASC connectors.



ASC Connector

## Operation by Automated Sequence

The operation must be carried out in the sequence programmed to be most appropriate for the particular type of samples under study.

The Shimadzu FTIR-8000 series instruments incorporate, as standard, the SPECTROMACRO software, which permits flexible programming through simple procedures.

As for the FTIR-8200PC/8300/8400/8600PC/8700/8900 (HYPER-IR model) the optional BASIC software has the same functions as SPECTROMACRO.

IRTracer-100, IRPrestige-21, IRXross, IRAffinity-1 series and FTIR-8400S which can be controlled by LabSolutions IR can also be controlled from the software.



## Automatic Diffuse Reflectance Attachment

### DRS-8010ASC (P/N 206-62308-91)

This attachment automates measurement of up to 24 samples.  
For details, refer to page 20.

## Auto Sampler for Transmission Measurement

### ASC-8000T (P/N 206-63900-91)

This attachment accepts up to 18 samples for measurement in the transmission mode.

#### Features

- The control is made by the standard control signals from the FTIR main unit, meaning no external controller is required.
- External control unit is not required.
- The attachment is easily installed in the standard sample compartment.
- A holder for a 13 mm dia. pellet is provided.
- Use of the KRS-5 window set enables measurement in the Nujol method.

#### Notes

- When this attachment is used on IRAffinity-1S, the ASC cable (P/N 206-73433-41) is required.
- When this attachment is used on IRPrestige-21, the power supply (P/N 206-72018-91) is required.
- When this attachment is used on IRAffinity-1, the ASC cable (P/N 206-73433-91) is required.
- The BASIC software is required separately for the HYPER-IR model.
- When old version of ASC-8000T (P/N 206-63900) is used on IRTracer-100, IRXross or IRAffinity-1S, the ASC Conversion Connector (P/N 206-74385-41) is required.

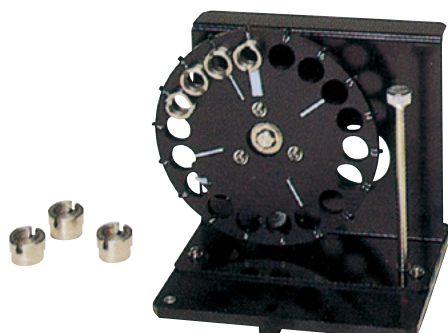
#### Standard Content

Description	P/N	Quantity
ASC-8000T main unit		1
Pellet holder	206-63917	20
Fixing spring	206-63951-01	20
Tweezers		1 pair

#### Options

Description	P/N
Film holder (9 pcs. as a set)*	206-81522

\* Up to nine film holders can be installed on the ASC-8000T unit.



## Sample Switcher 21

### (P/N 206-63663-91)

(P/N 206-63663-92 except IRTracer-100 and IRAffinity-1S)

All the Shimadzu FTIR series spectrophotometers are single-beam type.

This attachment allows any one of them to be operated in the "quasi double-beam mode" by switching two samples during measurement.

#### Features

- Two cassettes for liquid cells or pellet holders are provided.
- A built-in quasi double-beam mode is used, which eliminates the need for any special program.

#### Accessories That Can Be Used

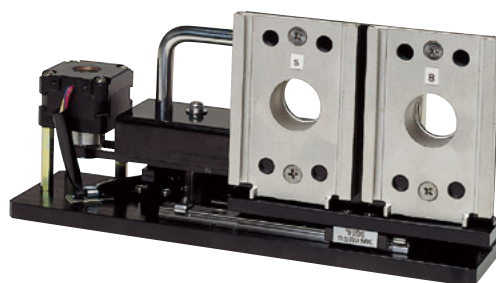
- Evacuatable die for KBr pellets
- Sealed liquid cell
- Magnetic pellet holder
- Diamond cell
- Sample holder for MHP-1 Mini Hand Press
- Fixed thickness cell
- Magnetic film holder
- 5 cm gas cell

#### Accessories That Cannot Be Used

- 10 cm gas cell

#### Notes

- When this attachment is used on IRAffinity-1S, the ASC cable (P/N 206-73433-41) is required.
- When this attachment is used on IRPrestige-21, the Power unit (P/N 206-72018-91) is required.
- When this attachment is used on IRAffinity-1, the ASC cable (P/N 206-73433-91) is required.
- The BASIC software is required separately for the HYPER-IR model.
- When Sample Switcher 21 (P/N 206-63663-92) is used on IRTracer-100, IRXross or IRAffinity-1S, the ASC Conversion Connector (P/N 206-74385-41) is required.





# Purge Control Kit

The FTIR series uses a sealed interferometer to ensure high sensitivity and stability during measurement without using dry air. To eliminate the interference of carbon dioxide and water vapor, it is recommended to purge the interferometer, the sample compartment, the second sample compartment, etc. through a combined use of the purge control unit and the dry air supply unit or nitrogen gas.

## Purge Control Kit

This kit is for adjusting the piping between the FTIR and purge gas source, piping sections along which purge gas flows and the purge gas flow rate.

Description	P/N	Compatible Models
PCK-100	206-74251-41	IRTracer-100
PCK-21	206-72352-91	IRPrestige-21
PCK-X	206-37038-41	IRXross
PCK-8941	206-73512-94	IRAffinity-1 series, FTIR-8400/8400S/8900

This kit contains the following parts:

- Flow path and flow rate controller
- Purge tube (10 m, 7 mm I.D., 10 mm O.D.)
- Exhaust parts

### Note

- Ventilate the site when purging with nitrogen gas.



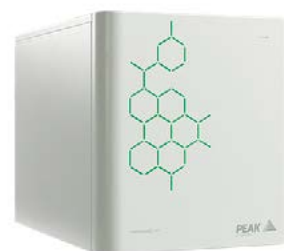
PCK-21

## Dry Air Supply Unit

Interference of moisture in the FTIR body can be reduced with dry air supply unit. By combining a dry air generator with CO<sub>2</sub>-free gas purification unit, it enables to supply gases with a CO<sub>2</sub> content of less than 1 ppm and a dew point of -70 °C.

### Specifications

Flowrate of purge gas:	30 L/min Max. (14 L/min when using CO <sub>2</sub> -free gas purification unit)
Content quantity of CO <sub>2</sub> :	No provisions (less than 1 ppm when using CO <sub>2</sub> -free gas purification unit)
Environment temp.:	5 to 35 °C
Power supply:	110 VAC 50/60 Hz 11A
Dimension:	
(W) 380 x (D) 540 x (H) 405 mm	(Dry Air Supply Unit)
(W) 250 x (D) 160 x (H) 660 mm	(CO <sub>2</sub> -free Gas Purification Unit)



Dry Air Supply Unit



CO<sub>2</sub>-free Gas Purification Unit

# External Detector / Optional Detector

A room temperature detector (DLATGS) is mounted as standard on the IRTracer-100, IRPrestige-21, IRXross and IRAffinity-1 series. Some applications require use of a high-sensitivity T2SL detector or external installation of a special optical system.

## Required Parts

	When Using the T2SL Detector	When Using an External Optical System
IRTracer-100	T2SL Kit	External Light Beam Switching Kit
IRXross		
IRAffinity-1 series	–	

## External Light Beam Switching Kit

(P/N 206-32570-41 for IRTracer-100+AIRsight, AIMsight and AIM-9000)

(P/N 206-37033-41 for IRXross+AIRsight, AIMsight and AIM-9000)

(P/N 206-32570-42 for IRAffinity-1 series+AIRsight, AIMsight and AIM-9000)

(P/N 206-74250-41 for IRTracer-100+AIM-8800)

(P/N 206-70125-41 for FTIR+AIM-8800 except IRTracer-100)

This kit extracts infrared light from the right side of the IRTracer-100, IRPrestige-21, IRXross, IRAffinity-1 series and FTIR-8000 series, and switches the light to externally installed accessories such as an infrared microscope.

Also attached is a polystyrene film about 50 µm thick so that instrument validation can be fully automated based upon Japanese, European, US, Chinese Pharmacopoeia or ASTM. Note, however, this polystyrene film doesn't have a traceability, so that a separate standard sample must be prepared if traceability is required.

## Standard Content

Description	Quantity
Switching mirror main unit (with polystyrene film)	1
External input signal connector	1set

## Notes

- Traceability is not provided for the polystyrene film.
- This kit cannot be used on the FTIR-8100/8100M/8100A/8200/8200D/8200A/8500/8600 and FTIR-8200PC/8600PC.

## T2SL Kit

(P/N 206-38200-41 for IRTracer-100)

(P/N 206-38200-42 for IRXross)

A high-sensitivity T2SL detector is used when analyzing minute or dark samples, or performing measurement using a long pathlength gas cell. This kit is an T2SL detector unit for switching between the standard room temperature detector (DLATGS). Switching of detectors is performed automatically from LabSolutions IR. It has a built-in liquid nitrogen monitor to cut off current flow when the detector element is not being cooled, thus protecting the T2SL detector. The liquid nitrogen dewar is made of glass and does not require reevacuation.

## Specifications

Detector	Liquid nitrogen cooled T2SL detector With glass dewar (approx. 300 mL) With liquid nitrogen monitor
Wavelength Range	5,000 to 700 cm <sup>-1</sup>
Liquid Nitrogen Retention Time	8 hours (when liquid nitrogen is newly purchased)

## Notes

- This kit cannot be mounted at the same time as the NIR Kit (see page 41).
- Liquid nitrogen is required when using the T2SL detector.

# Transmission Measurement

## Accessories for Transmission Measurement

Film samples can be measured easily if they are attached to the standard cassette or optional film holder.

### Cassette (Sample Holder) (P/N 206-17384)

A cassette (sample holder) provided as standard on the FTIR can be used for options for attaching to cassettes for liquid and gas cells. However, with some accessories, there may be clearance between the cell and the cassette, which sometimes results in poor attachment reproducibility.

Also, bending sometimes occurs when heavy accessories such as the 10 cm gas cell are attached. Use this optional cassette when performing measurement with such accessories with better reproducibility.

This attachment cannot be used on the FTIR-8100/8100M/8100A/8200/8200D/8200A/8500/8600 and FTIR-8200PC/8600PC.

#### Features

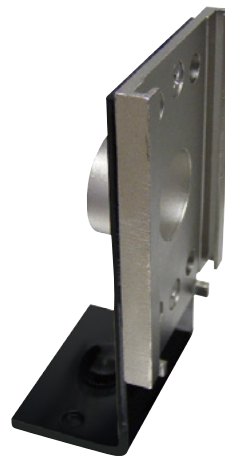
- Little clearance
- Rigid

#### Standard Content

Description	Quantity
Cassette ASSY	1

#### Maintenance Parts

Description	P/N
Cassette mounting screws	037-02820-18



### Magnetic-Type Film Sample Holder

(P/N 200-66754-11)

This holder holds films up to 0.5 mm thick. Film samples are held between the stainless backplate (SUS 430) and rubber magnet for direct analysis.

#### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

#### Standard Content

Description	Quantity
Backplate (SUS430)	1
Magnet sheet without hole	1
Magnet sheet with 13 mm dia. hole	1
Magnet sheet with 7 × 13 mm hole	1
Magnet sheet with 7 × 19 mm hole	1
Magnet sheet with 10 × 23 mm hole	1



### Universal Clip Holder (P/N 208-97207)

This holds a sample by one-touch operation through the use of a clip. A silicone rubber o-ring is used for positive contact and sample protection.

#### Features

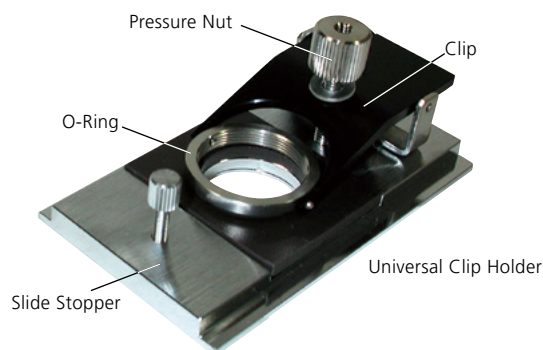
- Applicable sample sizes range from 13 to 40 mm in diameter, and up to 13 mm thick.
- The pressure nut ensures easy measurement of mull samples.
- Thick samples (max. thickness 13 mm) also can be held.
- The rubber magnet and o-ring are used for positive holding of samples.
- Diameter of light passage hole: 10 mm

#### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

#### Standard Content

Description	Quantity
Universal clip holder	1
Magnet base, 22 mm dia.	1
Magnet base, 10 × 14 mm hole	1
Spare o-ring	1



### EZ-Clip13 (P/N 208-97208)

This one-touch sample holder uses a clip exclusive for 13 mm dia. samples. An o-ring is located on the surface of the holder that contacts the sample to prevent damage to the sample.

#### Features

- Thick samples (max. thickness 13 mm) also can be held.
- Diameter of light passage hole: 10 mm

#### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

#### Standard Content

Description	Quantity
EZ-Clip13	1



### EZ-Clip25 (P/N 208-97209)

This one-touch sample holder uses a clip exclusive for 25 mm dia. samples. An o-ring is located on the surface of the holder that contacts the sample to prevent damage to the sample.

#### Features

- Thick samples (max. thickness 13 mm) also can be held.
- Diameter of light passage hole: 10 mm

#### Note

- For IRSpirit series, due to interference with the sample chamber cover and front panel, and accessories, please remove the sample chamber cover and front panel when using.

#### Standard Content

Description	Quantity
EZ-Clip25	1



## Gas Cell

Gas cells are used when measuring gas samples. Select the optical pathlength to suit the concentration of the component.

### Short Pathlength Gas Cells

**5 cm Gas Cell** (P/N 202-32006-XX)

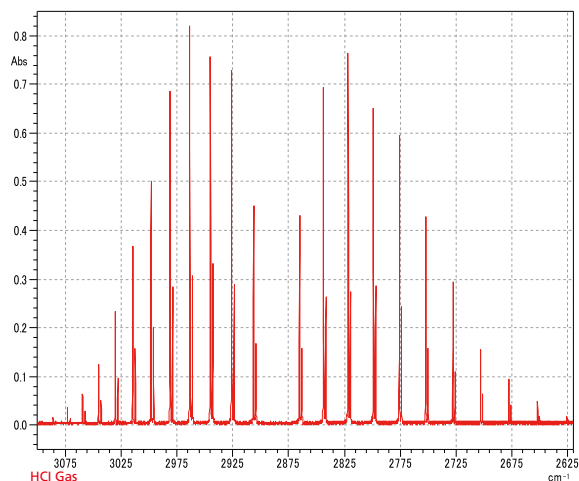
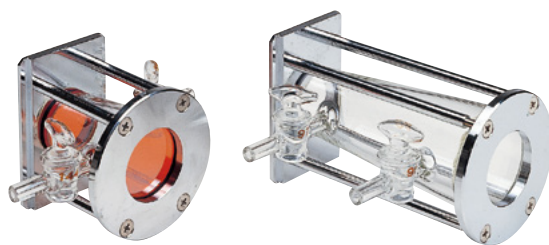
**10 cm Gas Cell** (P/N 202-32007-XX)

Used for measurement of gas samples or liquid samples of low boiling points. The cells are designed conic to make the inner volume smaller.

The inner volumes of the 5 cm and 10 cm gas cells are 42 mL and 98mL, respectively. The last two digits of the catalog numbers show the material of the window plate, as listed below.

#### Cell Window Plates

Type of Window Plate	NaCl	KBr	KRS-5
Last two digits of P/N	-10	-20	-30



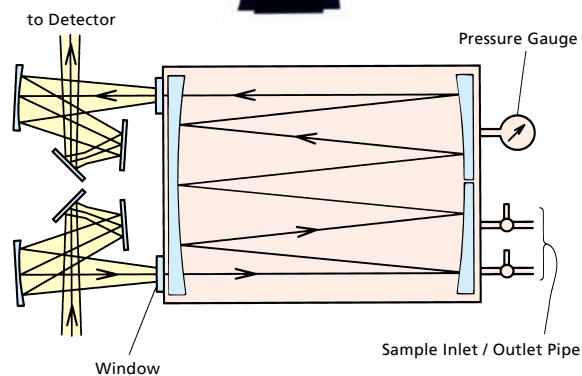
Spectrum of HCl Gas

### Long Pathlength Gas Cell

A gas cell with a long pathlength is used when measuring low concentration gas samples. Inside a long pathlength gas cell, light repeatedly doubles back, which results in a long pathlength.

There are two types of long pathlength gas cells, one with a sample compartment and the other with a second sample compartment. A regular T2SL detector is used as the detector.

The pathlength of long pathlength gas cells, gas cell material, window plate material, and detector must be selected according to the gas component, concentration, temperature, capacity, and other factors to be measured. When selecting a long pathlength gas cell, contact us so that you can select the appropriate cell.



Optics of Long Path Cell

# Pellet Measurement

## KBr Pellet Method

With this method, powder samples are diluted with KBr powder to produce pellets for transmission measurement. On the FTIR, the light intensity is large, so measurement is possible using pellets made easily with the Mini Hand Press. When making regular 13 mm dia. pellets, the evacuable die for KBr pellets, hydraulic press and vacuum pump are used.

### Mini Hand Press

#### MHP-1 (P/N 200-66747-91)

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; this ensures exceptional simplicity of operation. No dies or vacuum pump are required.

#### Standard Content

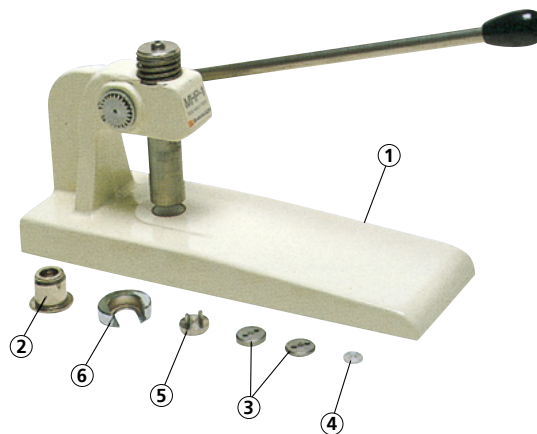
Description	P/N	Quantity
① Mini hand press		1
② Pellet holder	202-35258	1
③ Upper and lower cylinder	206-73717-91	1 set
④ Briquetting frame, 4 mm dia.		10
⑤ Pellet remover	200-66747-03	1
⑥ Pellet remover base	200-66747-04	1

\* Parts other than ① Mini Hand Press are provided as maintenance parts.

②, ⑤ and ⑥ are shared for 4 and 3 mm dia. parts.

#### Options and Maintenance Parts

Description	P/N
4 mm dia. briquetting frame, 20 pieces	206-73718-91
3 mm dia. briquetting frame, 10 pieces	200-66748
Upper/lower cylinder set	
3 mm dia. briquetting frame, 20 pieces	200-66749-01



The following items are recommended for using MHP-1

Description	Quantity
KBr crystal	100 g
Agate mortar and pestle	1 each
Micro spatula	1

### Evacuatable Die for KBr Pellets (P/N 202-32010-58)

Used to prepare KBr pellets, 13 mm dia. The amount of KBr crystal necessary for one pellet is about 200 mg and the sample 1 to 2 mg.

#### Standard Content

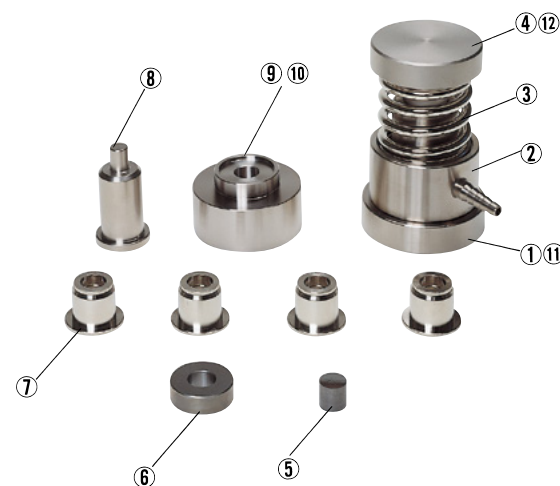
Description	P/N	Quantity
① Base*	202-35247	1
② Plunger guide	206-33129-58	1
③ Spring	202-35252	1
④ Plunger*	204-21049	1
⑤ Mandrel	206-73889**	2
⑥ Die frame	202-35250**	4
⑦ Pellet holder	202-35258**	4
⑧ Punching rod	202-35256	1
⑨ Punching base	202-35255	1
⑩ Plug	202-35257	1
⑪ O ring for base	036-10229	1
⑫ O ring for plunger	036-11025	1

\* Order by this P/N doesn't have a O ring with. If you need it, please order ⑪ or ⑫.

\*\* Packet of one when ordering by this P/N.

#### Notes

- The diameter of ①Base and ④Plunger are each 70 and 60 mm. If you would like to use another Hand Press, please check whether it can be set ①Base with 70 mm dia.
- The total height from ①to ④is about 120 mm. If you would like to use another Hand Press, please check whether it can be set Shimadzu's Evacuatable Die with 120 mm height. The situation is the same when it is used Evacuatable Die with Micro Die for 2/5 mm dia. KBr Pellets.



The following items are recommended for producing pellets of high transmittance:

Description	Quantity
10 tons hydraulic press	1
G-20DA vacuum pump	1
KBr crystal	100 g
Agate mortar and pestle	1 each
Micro spatula	1

## Micro Die for KBr Pellets

2 mm dia. (P/N 202-32011)

5 mm dia. (P/N 202-32012)

Used in combination with the KBr die (P/N 202-32010-58), which is for 13 mm dia. pellets, to produce smaller pellets, 5 mm or 2 mm in diameter. Specify the diameter you require or the Cat. No. when placing an order.

### Standard Content

Description	P/N	Quantity
① Mandrel for 2 mm dia. pellets	202-35262	2
Mandrel for 5 mm dia. pellets	202-35264	
② Die frame for 2 mm dia. pellets	202-35263	4
Die frame for 5 mm dia. pellets	202-35265	
③ Tool	202-35266	2
④ Pellet holder	202-35258	4

Note: Orders for the above P/N are for a quantity of one.



## 10-tons Hydraulic Press

(P/N 206-33547)

Used for producing KBr pellets. The maximum pressure is 10 tf/cm<sup>2</sup>. A high-precision pressure gauge is provided.

### Specifications

Max. pressure capacity: 10 tons (at 700 kg/cm<sup>2</sup>)

Total weight: 21.9 kg



## Vacuum Pump

**G-20DA** (P/N 206-36017)

This is a compact rotary vacuum pump used for vacuum dehydration in production of KBr pellets.

### Specifications

Exhaust velocity: 20/24 L/min (50/60Hz)

Ultimate pressure: 1.3 Pa

Size: 156.0 × 295.5 × 199.5 mm



## Magnetic-Type Pellet Holder

(P/N 200-66753-11)

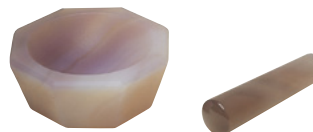
13 mm diameter pellets are held between the stainless backplate (SUS430) and rubber magnet for direct analysis.



## Agate Mortar and Pestle (P/N 200-93508)

Used to mix sample with KBr or Nujol using the KBr pellet method, diffuse reflection method, or Nujol method.

Size: 60 mm



## KBr Crystal (100 g) (P/N 202-34141)

Used to prepare KBr pellets. Features a long storage life, thanks to its low hygroscopicity.





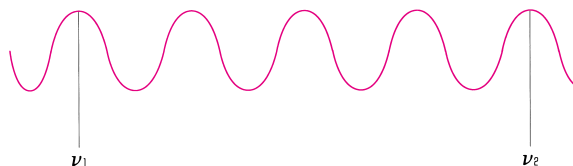
# Cells for Liquid Samples

## Measurement Using Demountable Cells

Demountable cells, sealed liquid cells, fixed thickness cells, etc. are useful for measurement of liquid samples. In quantitative analyses, it is necessary to know the thickness of the cell accurately. Interference patterns are often used for the thickness measurement.

In transmission/reflection FTIR of thin films, an interference pattern as shown above is overlaid on the spectrum. The film thickness,  $t$ , is given by the next equation:

$$t = \frac{M}{2\nu\bar{n}^2 \sin^2\theta(\nu_1 - \nu_2)}$$

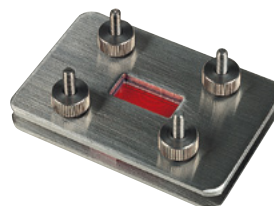


where  $\nu_1$  and  $\nu_2$  are the wavelengths of peaks or valleys,  $M$  is the degree of interference (number of the waves) between  $\nu_1$  and  $\nu_2$ .

When the refractive index ( $n$ ) of the film is known and is uniform between the  $\nu_1$  and  $\nu_2$ , the cell thickness may be obtained from the above equation. In practice, the cell is measured without any sample in it, and its thickness is obtained by substituting  $n = 1$  and  $\theta = 0^\circ$ .

### Demountable Cell (P/N 202-32000-XX)

This type of cell is used for qualitative analysis of less volatile liquid samples, Nujol mulls, or film samples. The cell is assembled and disassembled in each analysis run.



P/N	202-32000-10	202-32000-20	202-32000-30
Type	NaCl Demountable Cell	KBr Demountable Cell	KRS-5 Demountable Cell
Contents	A pair of NaCl plates (201-97942)	A pair of KBr plates (201-97977)	A pair of KRS-5 plates (201-97943)
	Metal holder (201-77662)	1 set	0.025 mm lead spacer (204-04900-13) 10 sheets
	0.05 mm lead spacer (204-04900-14) 10 sheets	0.1 mm lead spacer (204-04900-15) 10 sheets	

### Sealed Liquid Cell (P/N 202-32001-XX)

This type of cell is used for measurement of volatile liquid samples. The cell is assembled sandwiching a spacer of the desired thickness, a sample is injected into the cell, and then drawn out with a syringe.

When it is necessary to prevent leaks of samples, the use of the fixed thickness cell is recommended.



P/N	202-32001-10	202-32001-20	202-32001-30
Type	NaCl Sealed Liquid Cell	KBr Sealed Liquid Cell	KRS-5 Sealed Liquid Cell
Contents	A pair of NaCl plates, with and without hole (201-77160-10)	A pair of KBr plates, with and without hole (201-77160-20)	A pair of KRS-5 plates, with and without hole (201-77160-30)
	Metal holder (201-77661)	1 set.	0.025 mm lead spacer (204-04901-13) 10 sheets*
	Gasket (202-35425)	2 pcs.	0.05 mm lead spacer (204-04901-14) 10 sheets*
	Lead cushion (202-35426)	2 pcs.	(204-04901-34) for KRS-5
	Rubber cushion (202-35427)	2 pcs.	0.1 mm lead spacer (204-04901-15) 10 sheets*
	PTFE stopper (201-75546)	2 pcs.	(204-04901-35) for KRS-5
	Syringe (200-34835)	1 pc.	0.5 mm lead spacer (204-04901-18) 10 sheets* (204-04901-38) for KRS-5

\* Four spacers are included if the corresponding sealed liquid cell is purchased. Ten sheets are included if the spacers are ordered separately with the above P/N.

### Fixed Thickness Cell (P/N 202-32002-XX)

This type of cell is used for quantitative measurement of liquid or volatile samples. The cell is assembled in the Shimadzu factory to have the customer-specified cell thickness.

The last two digits of catalog numbers indicate the type of cell window plates, as shown in the table below:

Example: The catalog number of the fixed thickness cell, 0.1 mm in thickness, KBr window plate, is 202-32002-25

### Cell Window and Thickness

Thickness \ Type	NaCl	KBr	KRS-5
0.025 mm	-13	-23	Not available
0.05 mm	-14	-24	-34
0.1 mm	-15	-25	-35
0.2 mm	-16	-26	-36
0.5 mm	-18	-28	-38
1.0 mm	-19	-29	-39
2.0 mm	-11	-21	-31
5.0 mm	-12	-22	-32

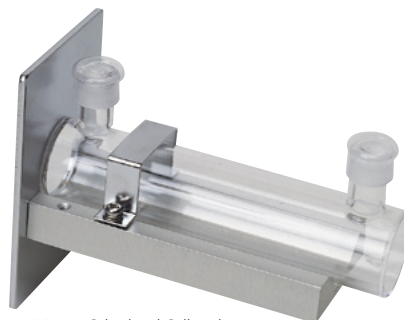
### Sample Cell for Oil Content Determination

Optional path length	P/N	Capacity	Quantity	Type of cell
100 mm	200-34473-02	38 mL	1	Oil content cell holder
50 mm	200-34473-01	19 mL	1	Type 1 (P/N 202-39897)
10 mm	201-98716 200-34442	4 mL	a set of 2 1	Square cell holder (P/N 204-51216)
5 mm	200-34449	2 mL	1 Spacer (204-21473-02) is required	
2 mm	200-34655	0.8 mL	1 Spacer (204-21473-01) is required	
1 mm	200-34660-01	0.4 mL	1 Spacer (204-21473-03) is required	

### Crystal Polishing Kit (P/N 202-32024)

This kit is used for polishing an NaCl and KBr window plate. The kit contains a polishing plate, abrasive, chamois and rubber gloves.

Note: Do not polish KRS-5 window plate.



100 mm Cylindrical Cell and  
Oil Content Cell Holder



Square Cell Holder



# Others

## Far Infrared Kit

(P/N 206-30616-58 for IRTracer-100)

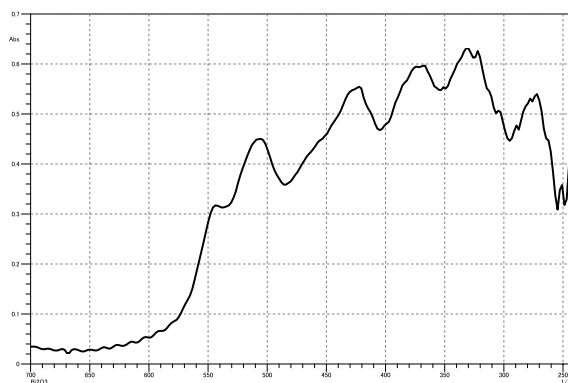
(P/N 206-30069-58 for IRPrestige-21)

In the far infrared region up to  $240\text{ cm}^{-1}$ , peaks of inorganic compounds and organometallic complexes are observed. The Far Infrared Kit is a CsI beam splitter for measuring spectra in the far infrared region. Using the CsI beam splitter enables spectra in the far infrared region up to  $240\text{ cm}^{-1}$  to be measured.

A standard light source and detector are used.

Since the  $500\text{ cm}^{-1}$  to  $240\text{ cm}^{-1}$  region absorbs lots of moisture in air, purge the instrument with dry air or dry nitrogen gas, for example, before performing measurement. Also, store the CsI beam splitter in a desiccator when it is not in use since it is extremely sensitive to moisture.

Window on the sample compartment should be replaced to KRS-5 window to use on IRTracer-100.



Far Infrared Spectrum of Bismuth Oxide

## Feature

- Measurement wavelength range  $5000\text{ cm}^{-1}$  to  $240\text{ cm}^{-1}$

## Standard Content

Description	Quantity	
	for IRTracer-100	for IRPrestige-21
CsI beam splitter	1	1
KRS window	1	0

## KRS-5 Window Set (P/N 206-74211-58)

The IRTracer-100 uses a KBr window with moisture-resistant coating for infrared light entering the sample compartment from the interferometer. When the window is replaced with a KRS-5 window, the system can be used in higher humidity environments with confidence. And this is used with Far Infrared kit to obtain spectra between  $350$  and  $240\text{ cm}^{-1}$ .

KBr beam splitter took out must be stored in a dedicator or dedicated storage box.

## Standard Content

Description	Quantity
KRS-5 window	1

# NIR Measurement

## NIR Measurement Accessories for the IRTracer-100 and IRPrestige-21

Accessories are available for easier and higher-sensitivity NIR measurement of a wide range of samples. Each accessory is equipped with the Automatic Accessory Recognition function. When the accessory is fitted to the sample compartment, the accessory type and its serial number are recognized automatically and the optimal measurement parameters are set.

## Introduction to Near-Infrared (NIR) Analysis

In the near IR regions, absorption due to molecular vibration appears. Therefore, substances can be identified by comparing spectral patterns, and quantitatively determined from the peak intensity.

Absorbance is lower in the near IR region than in the mid IR region, so samples can be measured without dilution. The IRTracer-100 and IRPrestige-21, which employs the Fourier transform method and offers spectra with high wavelength precision, is optimal for identifying substances by comparing spectral patterns. Samples contained in glass or thin plastic containers can be measured directly. It is also possible to analyze a sample using a probe. Thus, sample pretreatment is easy, and the near IR measurement is also suitable for measuring samples that cannot be easily unpacked. Note that the IRXross, IRAffinity-1 series, IRSpirit series and FTIR-8000 series systems cannot be used for near-infrared measurements.

## Near-Infrared Applications

Near-Infrared is used for qualitative and quantitative analysis, just as with the mid-infrared. Its applications include quality inspections of raw materials received, and endpoint quantitations for reaction processes.

## Applications and Accessories

### Multicomponent Quantitation of Liquid Samples

The quantities of various components in liquid pharmaceuticals and foods are measured and controlled. For example, quantitation can be made of the quantities of components such as sugar and proteins when manufacturing soft drinks. In this case, the location and shape of each component peak will depend on temperature. Therefore, measurement is conducted at a constant temperature using a heating transmission cell system. Here, the LabSolutions IR PLS Quantitation Program will be required to create the calibration curves.

### Acceptance Inspections for Raw Materials (Qualitative)

When determining whether the correct raw materials have been delivered based on the spectral shape, select accessories in accordance with the form of the raw materials. After measurement, pass/fail determinations and library searches can be conducted using the PharmaReport program.

If the sample is a powder, use either diffuse reflection equipment UpIR A, near-infrared integrating sphere IntegratIR A, or a reflection-type fiber probe.

For liquid samples, pastes, pellets, and cloths, use near-infrared integrating sphere IntegratIR A.

For tablet samples (pharmaceuticals), use either near-infrared integrating sphere IntegratIR A or a reflection-type fiber probe.

For diffuse reflection equipment UpIR A and near-infrared integrating sphere IntegratIR A, the sample is prepared, and the prepared sample is then placed in the measurement window for measurement. Measurement can be conducted as is with the sample placed in the test tube included, or left in a plastic bag. In the latter case, however, there may be a significant impact from the bag's interference fringe.

If the reflection-type fiber probe is used, measurement is possible without sampling. The probe can be inserted directly into the sample, or measurement can be taken directly of a sample placed in a glass bottle or plastic bag. In the latter case, however, there may be a significant impact from the bag's interference fringe.

### Difference Between UpIR A and IntegratIR A

Diffuse reflection equipment UpIR A and near-infrared integrating sphere IntegratIR A differ as shown below. The selection should be made on the basis of the experimental objective.

### Benefits of IntegratIR A

1. The peak strength is several times stronger than for UpIR A, and the obtained spectrum has a superior S/N ratio.
2. Good data is obtained when measuring powdered samples in plastic bags.
3. Measurements can be conducted of pellets, pastes, tablets, liquids and cloth samples.

### Benefits of UpIR A

1. Cost
2. Specialized for powdered sample analysis.

### NIR Kit (P/N 206-74253-58)

An option for the IRTracer-100 that allows near-infrared measurement. Experiments are conducted via software that switches between the mid-infrared and the near-infrared.

#### Specifications

Measurement Range: 12,500 to 3,800  $\text{cm}^{-1}$

Beam Splitter: Silicon-coated  $\text{CaF}_2$

Light Source: Tungsten iodine lamp

Detector: InGaAs detector

#### Standard Contents

Description	Quantity
Beam splitter storage box	1
$\text{CaF}_2$ beam splitter	1

### Topload Type Diffuse Reflectance Attachment UpIR A (P/N 208-97271-92)

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

#### Specifications

Measurement range: 10,000 to 3,800  $\text{cm}^{-1}$

Accessory recognition function: Included

#### Standard Accessories

Description	P/N	Quantity
UpIR A main unit		1
Gold-coated mirror for reference	208-97271-41	1
Solid sample holder	208-97271-42	1
Powder sample holder	208-97271-43	1

#### Options

Description	P/N
Test tube with screw cap (pack of 200)	208-97271-20
Sapphire window	208-97271-21
Purge tube for IRTracer-100	208-97271-25



### NIR Integrating Sphere

#### IntegratIR A (P/N 208-97272-92)

- Pretreatment such as KBr dilution is unnecessary. Samples contained in a plastic bag or glass bottle can be measured.
- Applications include qualitative or verification tests in acceptance inspections and quantitative analysis of components contained within samples.  
Powders, tablets, liquids, pastes, fibers, plastic pellets and molded samples can be placed on the sample stage for measurement (reflectance measurement).
- A highly sensitive InGaAs detector is built-in.

#### Specifications

Measurement range: 10,000 to 3,800  $\text{cm}^{-1}$

Accessory recognition function: Included

#### Note

To use this accessory, the IntegratIR mounting kit is required.

The IntegratIR installation kit is required to use this accessory.

- For IRTracer-100 (P/N 206-72715-93)
- For IRPrestige-21 (P/N 206-72715-91)

#### Standard Accessories

Description	P/N	Quantity
IntegratIR A main unit		1
Gold diffusion mirror with protective cap	208-97272-12	1
Test tube (pack of 25)	208-97272-14	2
Test tube holder	208-97271-17	1

#### Options

Description	P/N
Test tube (pack of 25)	208-97272-14
Purge tube for IRTracer-100	208-97272-20



Spectrum of a Tablet (Antipyretic)

# Optional Software

## For LabSolutions IR

### Rapid Scan (P/N 206-30200-91)

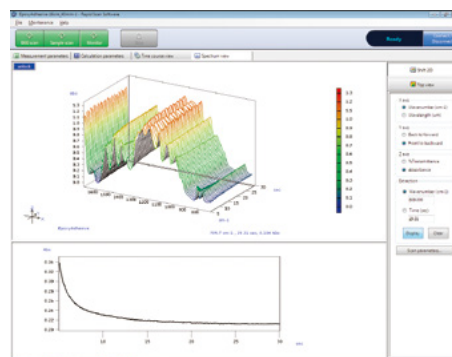
The Rapid Scan option provides the capability of collecting and recording a maximum of 20 spectra/second. This is especially suitable for fast reactions kinetics, where reactions are completed in a few seconds.

Spectra obtained from Rapid Scan measurements can be used to calculate peak heights and areas, which are used to determine kinetic rates.

The Rapid Scan interval is dependent on the resolution, number of scans, and mirror speed. The fastest speed under a  $16\text{ cm}^{-1}$  resolution and a mirror speed of  $40\text{ mm/s}$  is 0.05 seconds for 1 accumulated scan. Maximum measurement time depends on scan parameters.

The 3D Processing Program is required for analysis of Rapid Scan spectra.

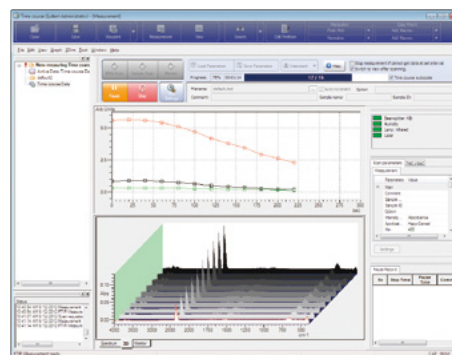
Note: The Rapid Scan is only for IRTracer-100 and IRXcross.



### Time Course Software (P/N 206-74558-91)

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 (bird's eye view) or in a contour plot. Simply modify parameters to recalculate the information.

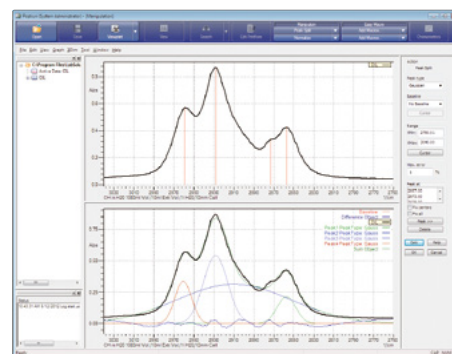
The scan interval is dependent on resolution, number of scans, and mirror speed. The fastest speed under a  $8\text{ cm}^{-1}$  resolution and a mirror speed of  $9\text{ mm/s}$  is 7seconds for 1accumulated scan. The time course software includes a 3D Processing Program.



### Curve-Fitting (Peak-Splitting) Program (P/N 206-74561-91)

Usually, absorption bands in infrared spectra consist of overlapping peaks. The curve-fitting (peak-splitting) program can be used to separate absorption bands into individual peaks, separate peaks that have been influenced by hydrogen bonding, and identify the peaks of functional groups that are hidden by absorption bands. Six types of curves, including Gaussian, Lorentzian, and Gaussian+Lorentzian, are available for separation analysis.

The curve can be selected in accordance with the form of the peaks in the absorption band. The separated component peaks are displayed together with the resultant spectra making it possible to evaluate the separation accurately.



### PLS Quantitation Program (P/N 206-74560-91)

Like multiple linear regression analysis, PLS (partial least squares) is a chemometrics method widely used for the simultaneous quantitation of multiple components. The PLS quantitation program incorporates PLS I and PLS II methods. It is possible to display calculation values based on input values. PLS factors are based on "PRESS" values, loading vectors, and score values. Analysis can be performed on the regression equations obtained with the PLS method.

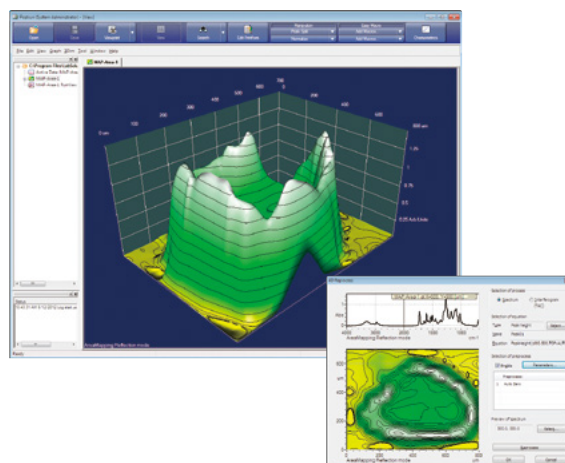
## 3D Processing Program

(P/N 206-74563-91)

The 3D processing program offers the following functionality:

- ▶ **Changes the method of displaying data**
  - Display data in bird's eye view (3D), as an intensity distribution or using contour lines, as a spectral overlay, or rotated.
- ▶ **3D data processing**
  - Isolate changes at specific wavenumbers.
  - Functions include data extraction, data points thinning, smoothing, zero-baseline, background correction, normalization, log conversion, first- or second-order derivative, and ATR correction.
- ▶ **Creation of 3D data from spectra**
  - Create 3D data by consecutively arranging spectra measured at fixed intervals, such as by repeated measurements.

\*1 The 3D processing program cannot control mapping measurements or infrared microscopes.



## For AMsolution

### High-Speed Mapping Program (P/N 206-36299-41)

Using the high-speed mapping program, measurements can be performed with the specified number of accumulations at points determined to contain samples based on the spectra<sup>\*2</sup>. Points determined to contain no samples are measured at a single accumulation, which allows faster performance while maintaining the spectra's quality.

\*2 The high-speed mapping function is only available in the area mapping mode for infrared (transmission/reflection) measurements.

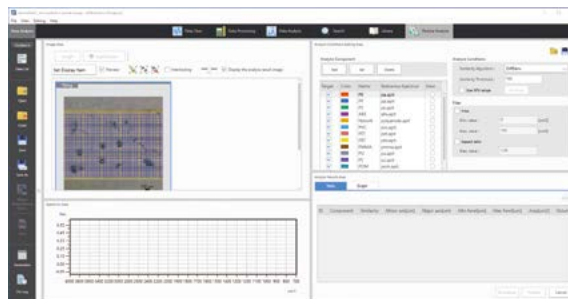
### Particle Analysis Program (P/N 206-36628-41)

By adding a particle analysis program to AMsolution, the chemical images obtained from mapping measurements<sup>\*3</sup> can be used to calculate individual particle qualities, as well as the major axis, minor axis, mass<sup>\*4</sup>, and volume<sup>\*4</sup>. In addition, this statistical information can be easily displayed. The program can be used from the [Particle Analysis] tab page, thereby maintaining the same operational setup as the AMsolution analysis software. The particle analysis program can be used for a variety of analyses, including the analysis of microplastics and contaminant analysis.

\*3 The optional High-Speed Mapping Program is separately required.

\*4 Mass and volume are calculated based on the theoretical formula (Formula (1)  $[\log_{10}(M)=b \cdot \log_{10}(S)+a]$ ) used in the article referenced below. This theoretical formula applies only to microplastics. Shimadzu cannot guarantee the validity of the mass results.

Tomoya Kataoka, Yota Iga, Rifqi Ahmad Baihaqi, et al. Geometric relationship between the projected surface area and mass of a plastic particle. Water Research. 2024;261:122061.



## For AMsolution and AIMsolution

### AIMsolution DB/CS (P/N 206-33541-41)

The software enables the database management of data acquired from the AIMsight and AIM-9000 infrared microscopes, as well as user management for AIMsolution DB/CS. Login to AIMsolution DB/CS is performed through LabSolutions IR, which controls FTIR. Data acquired in AIMsolution DB/CS is automatically transferred to LabSolutions IR and registered in the database.



## KnowItAll Bundle (P/N 206-36793-41)

Activate John Wiley & Sons, Inc. KnowItAll\* from a button in the LabSolutions IR or AMsolution 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.

\* AMsolution does not work with KnowItAll Version 2018 and earlier.

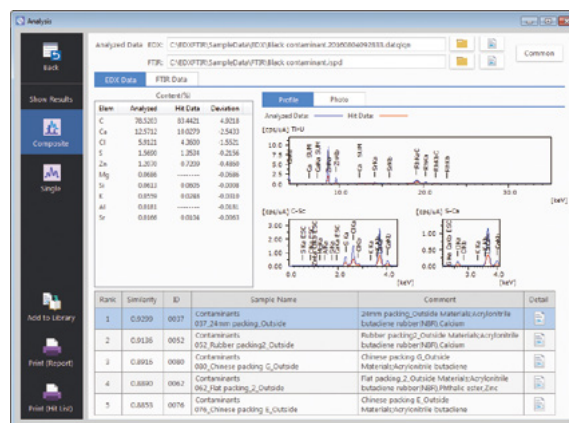
## Macro Platform (P/N 206-74562-91)

Customized macro programs can be prepared by Shimadzu (for a fee). A macro platform is required for running customized macro programs. For procedures that cannot be accomplished using simple macro program functionality, for automatic measurement systems that include an auto sample changer, or for other requirements, contact your Shimadzu sales representative.

## EDX-FTIR Contaminant Finder/Material Inspector EDXIR-Analysis Software

English (P/N 206-33175-92) Chinese (P/N 206-33175-93)

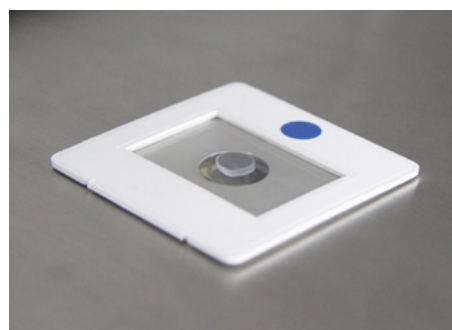
EDXIR-Analysis software is specially designed to perform qualitative analysis using data acquired by an energy dispersive X-ray (EDX) fluorescence spectrometer and a Fourier transform infrared (FTIR) spectrophotometer. This software is used to perform an integrated analysis of data from FTIR, which is 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.



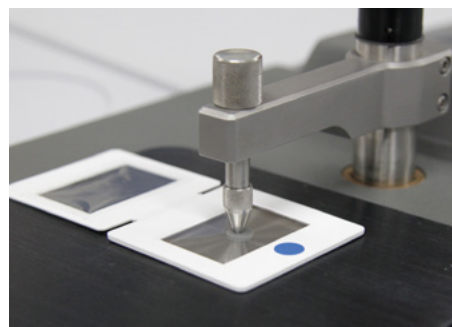
Integrated Data Analysis Results

## EDXIR-Holder Sample Holder/Stocker for Contaminant Measurement (P/N 212-25890-41)

This foldable holder consists of an adhesive layer with samples attached and a polypropylene film designed for fluorescence X-ray. 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. This enables the replacement of samples, at a minimum, saving on labor and making analysis more efficient. Close the holder after the measurement and it can be used as a sample stocker. It is not necessary to transfer the samples to other containers, so there is no danger of losing samples.



Measurement with EDX



Measurement with FTIR

# Materials for Cell Window Plate

Sample cells have a window made of various materials to meet the requirements of your analyses, such as wavenumber range and physical and chemical characteristics of the sample.

The characteristics and features of the materials popularly used for the window of sample cells are described below. Some of the materials are used only rarely due to the difficulty of processing and high costs.

## Materials of Sample Cell Windows

Material	Wavenumber Range cm <sup>-1</sup> (μm)	Refractive Index (1000 cm <sup>-1</sup> )	Water Solubility at 20 °C (g/100 g H <sub>2</sub> O)	% Transmission (thickness)	Max.Temp. (Melting Point)	Knoop Hardness (200 g)
KBr	40,000~340 (0.25~29.4)	1.52	65	90 (5 mm)	300 (730)	7.0<100>
NaCl	50,000~600 (0.2~16.6)	1.49	36	90 (5 mm)	400 (801)	18.2<100>
KCl	40,000~500 (0.25~20.0)	1.46	34	90 (10 mm)	(776)	9.3<100>
CsI	33,000~200 (0.3~50.0)	1.74	44 (0 °C)	90 (5 mm)	200 (621)	—
KRS-5 (TlBr+TlI)	16,600~250 (0.6~40.0)	2.37	0.05	70 (2 mm)	200 (414)	40.2
ZnS	10,000~725 (1.0~13.3)	2.2	Insoluble	70 (1 mm)	300 (1,180 Sublimate)	354
ZnSe	10,000~550 (1.0~18.1)	2.4	Insoluble	65 (1 mm)	350 (1,700)	250
BaF <sub>2</sub>	50,000~770 (0.2~12.9)	1.42	0.004	90 (1 mm)	500 (1,280)	82 (500 g)
CaF <sub>2</sub>	50,000~1,100 (0.2~9.0)	1.39 (2,000 cm <sup>-1</sup> )	Insoluble	95 (3.6 mm)	900 (1,402)	158 (500 g)
Si	8,000~660 (1.25~15.1)	3.4	Insoluble	55 (2.5 mm)	300 (1,420)	1,150
Ge	5,500~660 (1.8~16.6)	4.0	Insoluble	50 (2 mm)	270 (936)	780
Diamond, type II	40,000~12.5 (0.25~800)	2.38	Insoluble	70 (1 mm)	(400)	10 Mohs Scale
SiO <sub>2</sub> (Fused Silica)	50,000~2,500 (0.20~4.0)	1.42 (3,000 cm <sup>-1</sup> )	Insoluble	85 (1 mm)	1,710 Soften	500

%Transmission values given are typical ones, in the wavenumber range applicable to the respective materials, including the loss due to surface reflection.

Max. Temp. values given assume atmospheric conditions.

## Characteristics of Cell Window Materials

- Only the main characteristics of the cell window materials are described below.
- The "Clean-up" lists present only the representative solvents used to wash the cell windows. Even if a solvent is listed as "Clean-up", confirm that the solvent does not react with the samples.
- The "Harm" solvents can destroy the window plate through corrosion or dissolving. Some solvents not listed as "Harm" can be harmful to the material.

### KBr (Potassium Bromide)

- Low cost and wide wavenumber range.
- Easy to process with alcohol anhydride.
- Most popularly used.
- High mechanical strength.
- Store under humidity conditions lower than 50%.

"Clean-up": chloroform, carbon tetrachloride

"Harm":

- Aqueous solution
- Lower alcohol

### NaCl (Sodium Chloride)

- Most inexpensive.
- Wide wavenumber range.
- Store under humidity conditions lower than 50%.

"Clean-up": chloroform, carbon tetrachloride

"Harm":

- Aqueous solution
- Lower alcohol

### KCl (Potassium Chloride)

- Similar characteristics as NaCl and KBr.
- Not popularly used.

### CsI (Cesium Iodide)

- Soft and hence liable to injure.
- Applicable to analysis in far-infrared region.
- Highly deliquescent.
- Store under humidity conditions lower than 40%, and handle with care.

"Clean-up": chloroform, carbon tetrachloride

"Harm":

- Aqueous solution
- Lower alcohol

### KRS-5 (Thallium Bromide-Iodide)

- Wide wavenumber range.
- High refractive index.
- Most widely used for ATR prisms.
- Almost insoluble in water.
- Toxic; must be processed at an authorized manufacturer's site.
- KRS is an abbreviation of "Kristalle aus dem Schmelzfuß" ("crystals that don't melt" in German).

"Clean-up": chloroform, carbon tetrachloride, xylene

"Harm":

- Acetone
- Ammonium salt solution
- Sulfuric acid, ammonia, EDTA
- A solution of a compound that reacts with thallium to form a complex

### ZnS (Zinc Sulfide)

- Non-water soluble.
- Resistant against mechanical and thermal shocks.
- High refractive index.
- Effectively used for evaporation depositing.

"Clean-up": acetone, alcohol

"Harm":

- Acidic solution

### ZnSe (Zinc Selenide)

- Non-water soluble.
- Resistant against weakly acidic or alkaline solution.
- Applicable pH range: 5-9
- High refractive index.
- Used for ATR prisms.
- If used for measuring acidic samples, harmful hydrogen selenide may be generated.

"Clean-up": acetone, H<sub>2</sub>O

"Harm":

- Acidic solution
- Strongly alkaline solution

### BaF<sub>2</sub> (Barium Fluoride)

- Soluble in acidic solution and ammonia.
- Usable up to 500 °C.
- Almost insoluble in water.

"Clean-up": acetone, H<sub>2</sub>O

"Harm":

- Ammonium salt solution
- Acidic solution

### CaF<sub>2</sub> (Calcium Fluoride)

- Soluble in ammonium salt solution.
- Resistant against acidic or alkaline solution.
- Hard, high mechanical strength.
- Suitable for high-pressure cell.
- CaF<sub>2</sub> that occurs in nature is called fluorite.

"Clean-up": acetone, H<sub>2</sub>O

"Harm":

- Ammonium salt solution
- Strongly acidic solution

### Si (Silicon)

- Widely used as the material for semiconductors.
- Rarely used as cell window material.
- Ge can substitute Si as cell window material.

"Clean-up": acetone, H<sub>2</sub>O

"Harm":

- HF-HNO<sub>3</sub> mixture

### Ge (Germanium)

- Widely used as the material for semiconductors.
- Useful as the material for vapor deposition.
- Easily processed to be lenses.
- High refractive index, suitable as the material for ATR prism used in analysis of highly refractive samples.
- Non-watersoluble.

"Clean-up": toluene, H<sub>2</sub>O

"Harm":

- Hot sulfuric acid

### Diamond Type II (Diamond)

- Harder than any other material.
- Applicable to wavelength range from ultraviolet to far infrared, though a gradual absorption is seen in the range from 3,000 to 1,500 cm<sup>-1</sup>.
- Natural diamond is classified as Type I and Type II, and only the Type II is used as the material for cell window.
- Extremely expensive.
- Recommended for the window of high-pressure cell.

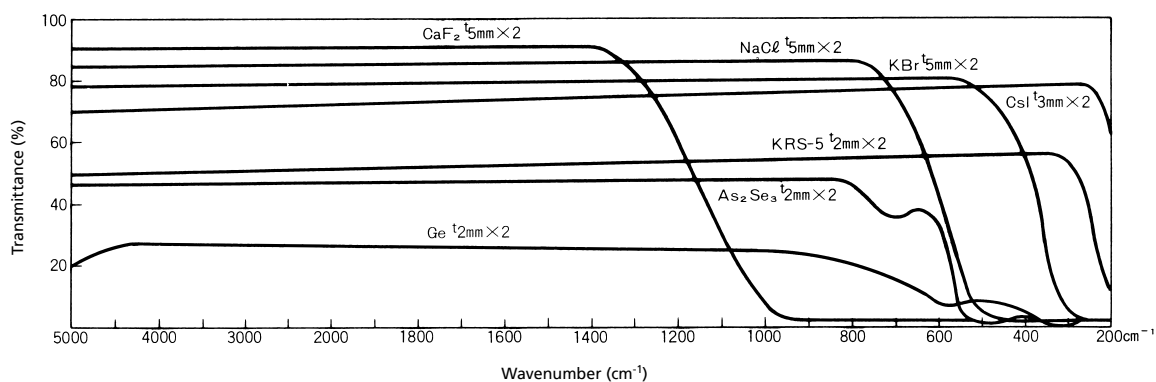
"Clean-up": ethanol, acetone

### SiO<sub>2</sub> (Fused Silica)

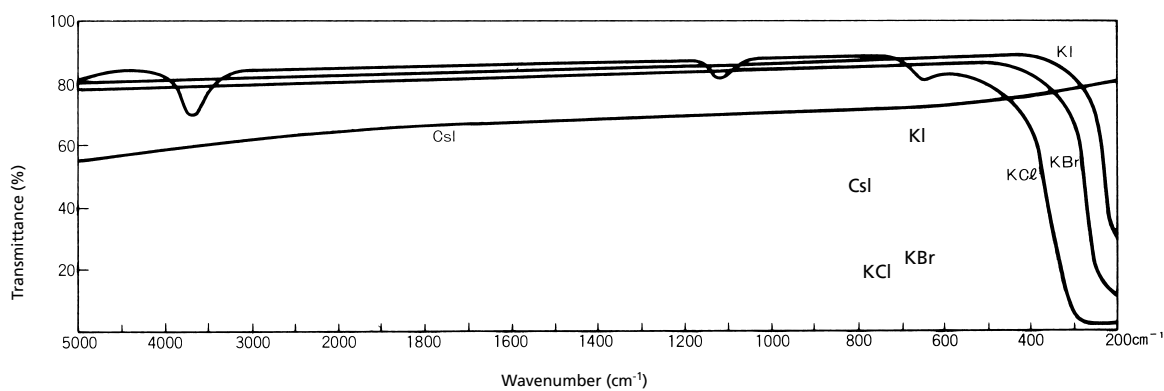
- Effective for analysis in the ultraviolet and visible regions.
- Though useful up to 4 μm in the IR region, this material ensures high stability and is easy to process.

"Clean-up": ethanol, acetone

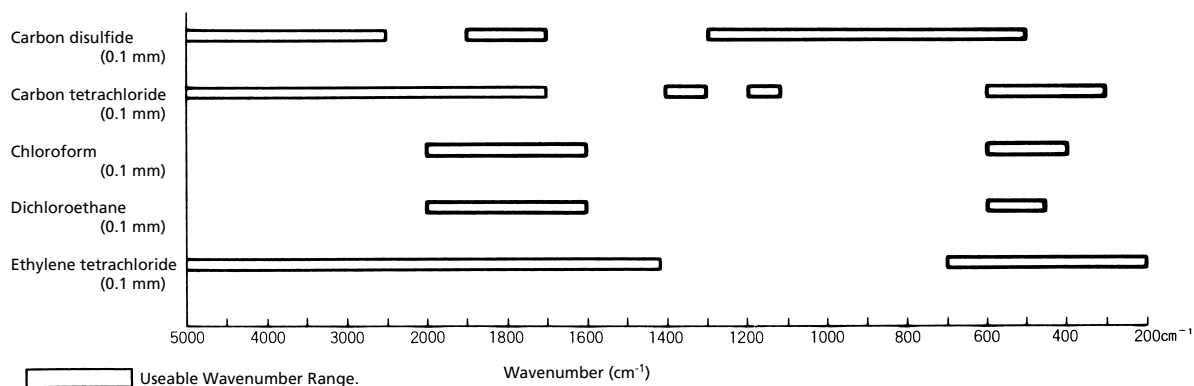
## Transmittance Characteristics of Representative Cell Window Materials



## Transmittance of Alkali Halide Pellet (1 mm thick)



## Wavenumber Range of Solvent.





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