# FRONTIER OPTICA FT-IR



# **User's Guide**



#### **Release History**

| Part Number | Release | Publication Date |
|-------------|---------|------------------|
| L1050103    | В       | July 2013        |

Any comments about the documentation for this product should be addressed to:

User Assistance PerkinElmer Ltd Chalfont Road Seer Green Beaconsfield Bucks HP9 2FX United Kingdom

Or emailed to: info@perkinelmer.com

#### Notices

The information contained in this document is subject to change without notice. Except as specifically set forth in its terms and conditions of sale, PerkinElmer makes no warranty of any kind with regard to this document, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. PerkinElmer shall not be liable for errors contained herein for incidental consequential damages in connection with furnishing, performance or use of this material.

#### **Copyright Information**

This document contains proprietary information that is protected by copyright. All rights are reserved. No part of this publication may be reproduced in any form whatsoever or translated into any language without the prior, written permission of PerkinElmer, Inc.

Copyright © 2013 PerkinElmer, Inc.

Produced in the UK

#### Trademarks

Registered names, trademarks, etc. used in this document, even when not specifically marked as such, are protected by law.

PerkinElmer is a registered trademark of PerkinElmer, Inc. Spectrum and Frontier are trademarks of PerkinElmer, Inc.

# Contents

| Introduction  |     |
|---|-----|
| About This Manual   | . 6 |
| Conventions Used in this Manual                             |     |
| Notes, Cautions and Warnings                                |     |
| Warnings and Safety Information                             | 11  |
| Safety Summary  |     |
| General Safety  |     |
| Location and Ventilation                                    |     |
| To allow for adequate cooling                               |     |
| To allow any nitrogen used to disperse                      |     |
| Use of flammable solvents and samples                       |     |
| Electrical Safety   |     |
| Laser Safety Regulations                                    |     |
| Laser Radiation Hazards and their Classification            |     |
| Labels  |     |
| Warning Signs on the Instrument                             |     |
| EMC Compliance  |     |
| EC Directive  |     |
| FCC rules and regulations                                   |     |
| An Overview of the Frontier Optica FT-IR Spectrometer       | 23  |
| A Guided Tour of the Frontier Optica FT-IR Spectrometer     | 24  |
| Optical system  | 25  |
| Top panel controls  | .26 |
| The sample compartment                                      |     |
| Accessories for the Frontier Optica FT-IR spectrometer      | .27 |
| Storage compartment   | 28  |
| Power switch and communication ports                        | .28 |
| Unpacking and Installation                                  | 29  |
| Requirements  | .30 |
| Electrical requirements                                     | .30 |
| Environment   | .30 |
| Unpacking the Spectrometer                                  | .32 |
| Opening the shipping container                              | .32 |
| The Desiccant Indicator                                     |     |
| Connecting up the Spectrometer                              | 35  |
| Connecting to the PC  | 35  |
| Other connectors  | 36  |
| Connecting the spectrometer to the electrical supply        | 37  |
| Installing the Instrument in the Software                   |     |
| Installing the software                                     | 39  |
| The Instrument Install Wizard                               | 39  |
| Using the Spectrometer                                      | 41  |
| Basics of Software Control                                  |     |
| Starting Spectrum software                                  | 42  |
| Scanning samples  |     |
| Working with the instrument display and Go button           | 44  |
| Using the Spectrum on-screen Help system                    | 44  |
| Atmospheric (CO <sub>2</sub> /H <sub>2</sub> O) Suppression | 45  |
| What is atmospheric suppression?                            | 45  |
| What does atmospheric suppression do?                       | 45  |
| AVI Correction  |     |
| What is AVI correction?                                     |     |
| What does AVI correction do?                                | 47  |
| Look Ahead  |     |
| What is Look Ahead?   |     |
| What does Look Ahead do?                                    | 48  |

| Quality Checks   |    |
|--|----|
| What are Quality Checks?                               | 49 |
| What do Quality Checks do?                             | 49 |
| Measuring Optical Components                           | 51 |
| Optimizing Your Instrument Settings                    | 52 |
| J-stop   |    |
| B-stop   | 53 |
| Resolution   | 53 |
| Phase correction                                       | 54 |
| Apodization  | 54 |
| Sample Properties                                      | 55 |
| Sample wedge   | 55 |
| Sample tilt  | 55 |
| Sample thickness                                       |    |
| Non-planar samples                                     | 56 |
| Small samples  | 56 |
| Samples with near-parallel reflecting surfaces         |    |
| Summary  | 57 |
| Reflection measurements                                | 57 |
| Routine Maintenance                                    |    |
| Cleaning the Spectrometer                              | 60 |
| Cleaning the display                                   |    |
| Moving the Spectrometer                                |    |
| Condensation   |    |
| The Desiccant Indicator in Detail                      |    |
| Changing the Desiccant                                 |    |
| Renewing the instrument desiccant                      | 64 |
| Installing rechargeable desiccant in the instrument    | 65 |
| Purging the Spectrometer                               | 66 |
| Changing the External Fuse                             |    |
| Advanced Maintenance                                   | 71 |
| Opening the Main Cover                                 | 72 |
| Replacing the Source                                   | 75 |
| Installing/Replacing Windows                           |    |
| Installing Filters in the Filter Wheel                 | 79 |
| Replacing the Laser and Power Supply                   |    |
| Appendices   | 85 |
| Appendix 1: Changing the Sampling Accessory            | 86 |
| Appendix 2: Instrument Self-Checks                     | 88 |
| Appendix 3: Instrument Performance Validation Kit      |    |
| Appendix 4: Decontamination and Cleaning               | 91 |
| Appendix 5: WEEE Instructions for PerkinElmer Products | 92 |
| Index  |    |

# **Introduction**

## About This Manual

This manual contains the following sections:

- Introduction
- Warnings and Safety Information
- An Overview of the Frontier Optica FT-IR Spectrometer
- Unpacking and Installation
- Using the Spectrometer
- Measuring Optical Components
- Routine Maintenance
- Advanced Maintenance
- Appendices.

For further information on collecting, viewing and processing spectra using Spectrum software, refer to the Help file that you can access from the Help menu.

## **Conventions Used in this Manual**

Normal text is used to provide information and instructions.

Bold text refers to text that is displayed on the screen.

UPPERCASE text, for example ENTER or ALT, refers to keys on the PC keyboard. '+' is used to show that you have to press two keys at the same time, for example, ALT+F.

All eight digit numbers are PerkinElmer part numbers unless stated otherwise.

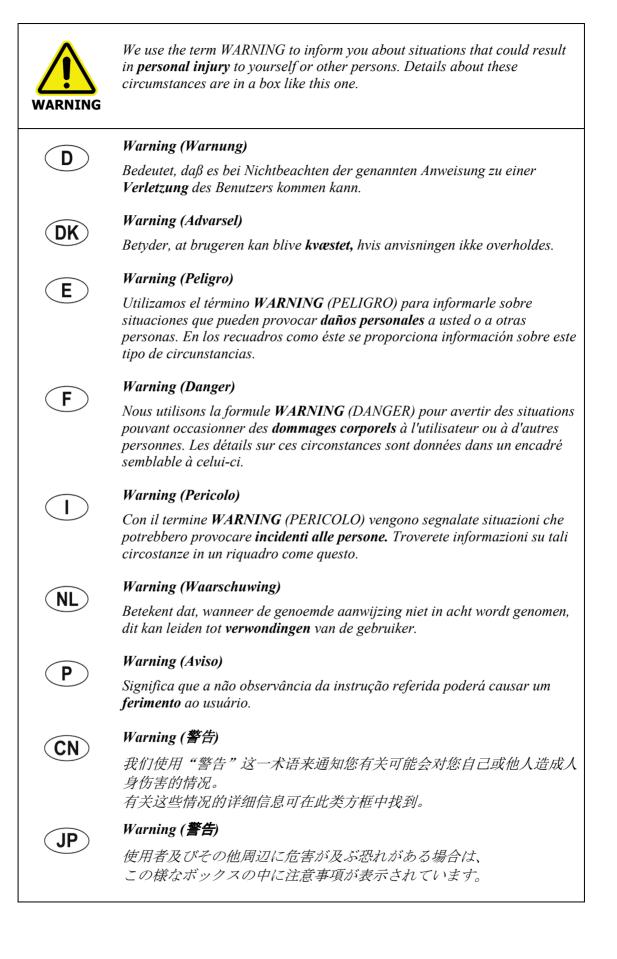
The term "instrument" refers to the Frontier Optica FT-IR spectrometer, and any sampling accessory fitted.

#### Notes, Cautions and Warnings

Three terms, in the following standard formats, are also used to highlight special circumstances and warnings.

**NOTE:** A note indicates additional, significant information that is provided with some procedures.

| CAUTION | We use the term CAUTION to inform you about situations that could result in <b>serious damage to the instrument</b> or other equipment. Details about these circumstances are in a box like this one.   |
|---------|---|
| D       | <b>Caution (Achtung)</b><br>Bedeutet, daß die genannte Anleitung genau befolgt werden muß, um<br>einen <b>Geräteschaden</b> zu vermeiden.   |
| DK      | <b>Caution (Bemærk)</b><br>Dette betyder, at den nævnte vejledning skal overholdes nøje for at undgå<br>en <b>beskadigelse af apparatet</b> .   |
| E       | <b>Caution (Advertencia)</b><br>Utilizamos el término <b>CAUTION</b> (ADVERTENCIA) para advertir sobre<br>situaciones que pueden provocar <b>averías graves en este equipo</b> o en otros.<br>En los recuadros como éste se proporciona información sobre este tipo de<br>circunstancias.                     |
| F       | <b>Caution (Attention)</b><br>Nous utilisons le terme <b>CAUTION</b> (ATTENTION) pour signaler les<br>situations susceptibles de provoquer de <b>graves détériorations de</b><br><b>l'instrument</b> ou d'autre matériel. Les détails sur ces circonstances figurent<br>dans un encadré semblable à celui-ci. |
|         | <b>Caution (Attenzione)</b><br>Con il termine <b>CAUTION</b> (ATTENZIONE) vengono segnalate situazioni<br>che potrebbero arrecare <b>gravi danni allo strumento</b> o ad altra<br>apparecchiatura. Troverete informazioni su tali circostanze in un<br>riquadro come questo.                                  |
| NL      | <i>Caution (Opgelet)</i><br>Betekent dat de genoemde handleiding nauwkeurig moet worden<br>opgevolgd, om <b>beschadiging van het instrument</b> te voorkomen.   |
| P       | <b>Caution (Atenção)</b><br>Significa que a instrução referida tem de ser respeitada para evitar a<br><b>danificação do aparelho</b> .  |
| CN      | Caution (小心)<br>我们使用"小心"这一术语来通知您有关可能会对<br><b>本仪器或其它设备造成严重损害</b> 的情况。<br>有关这些情况的详细信息可在此类方框中找到。   |
| JP      | <b>Caution (注意)</b><br>分光器や他の機材等に深刻なダメージを与える恐れがある場合は、<br>この様なボックスの中に表示しています。  |



10 . Frontier Optica FT-IR User's Guide

# <u>Warnings and Safety</u> <u>Information</u>

## Safety Summary

The Frontier Optica FT-IR spectrometer has been designed to comply with a wide variety of international standards governing the safety of laboratory equipment. In routine use, the instruments pose virtually no risk to you. If you take some simple, common-sense precautions, you can make sure that you maintain the continued safe operation of your instrument:

DO make sure that the instrument is properly connected to the electrical supply; in particular, make sure that the ground (earth) is securely connected.

DO disconnect the electrical power cable before opening the main cover of the instrument.

DO keep the instrument dry. Avoid spilling liquid into the instrument. Clean all external spills immediately. If anything that is spilled enters the main body of the instrument, switch off the power and contact a PerkinElmer Service Engineer.

DO NOT stare into the internal laser beam under the instrument cover. The instrument contains a low power, visible (red) laser; momentary exposure to the beam is not dangerous, but deliberate, direct viewing of the beam along its axis could damage your eye.

DO NOT use a flammable gas to purge the instrument. The instrument contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.

DO read the more detailed information on warnings and safety in the following pages to ensure the safe operation of the instrument.

## **General Safety**

The Frontier Optica FT-IR spectrometer has been designed and tested in accordance with PerkinElmer specifications and in accordance with the safety requirements of the International Electrotechnical Commission (IEC). The instruments conform to IEC publication 61010-1 ("Safety requirements for electrical equipment for measurement, control, and laboratory use") as it applies to IEC Class 1 (earthed) appliances and therefore meets the requirements of EC low voltage directive 2006/95/EC.

If the instrument is used in a manner not specified by the manufacturer, the protection provided by the instrument may be impaired. Only use the instrument indoors and under the following conditions:

Temperature15 °C to 35 °CRelative Humidity80% maximum (non-condensing)

If possible, avoid any adjustment, maintenance and repair of the opened, operating instrument. If any adjustment, maintenance and repair of the opened, operating instrument is necessary, this must only be done by a skilled person who is aware of the hazard involved.

Whenever it is likely that the instrument is unsafe, make it inoperative. The instrument may be unsafe if it:

- Shows visible damage
- Fails to perform the intended measurement
- Has been subjected to prolonged storage in unfavorable conditions
- Has been subjected to severe transport stresses.

The instrument has been designed to be safe under the following environmental conditions:

- Indoor use
- Altitude up to 2000 m (above mean sea level)
- Ambient temperatures of 5 °C to 40 °C
- A maximum ambient relative humidity of 80% for temperatures up to 31 °C, decreasing linearly to 50% relative humidity at 40 °C
- Mains supply fluctuations not exceeding  $\pm 10\%$  of the nominal voltage.

# Location and Ventilation



Make sure that the switch at the electrical supply inlet on the rear of the instrument is not obstructed.

## To allow for adequate cooling

Do not site the instrument near to room heating equipment, for example, central heating radiators.

During operation, there should be a minimum gap of:

- 15 cm (6 inches) between any surface and the cooling louvers at the rear of the instrument.
- 7 cm (3 inches) between the instrument and adjacent equipment.
- 45 cm (18 inches) between any surface and the top surface of the closed sample area lid (to allow for the lid to be opened fully).

## To allow any nitrogen used to disperse



Do not site the instrument in a poorly ventilated area if nitrogen will be used as a purge gas.

Oxygen depletion in an enclosed space does not trigger a gasping reflex, and errors of judgment, confusion, or unconsciousness can occur in seconds and without warning.

The spectrometer includes a coupling that enables the instrument body, and another that enables the sample compartment, to be purged using clean, dry, oil-free air or nitrogen. The recommended flow rate to each connector is 10 l/min, and both the instrument and the sample compartment vent to their surroundings.

### Use of flammable solvents and samples



The instrument contains a hot source and contact with flammable vapors may cause an explosion. When working with flammable solvents or samples, particularly during unattended operation with flow-cells, it is recommended that the instrument optics area should be continuously purged with dry air or nitrogen to maintain a positive pressure and prevent flammable vapor entering the instrument.



If flammable solvents or samples are spilled on the instrument and there is any possibility that they have entered the interior (by coming into contact with cover gaskets for example) then the instrument must be switched off immediately and disconnected from the power supply. The optics area should then be thoroughly purged with dry air or nitrogen, or the main cover should be opened to thoroughly ventilate the optics area before proceeding.



Flammable solvents or samples should not be stored on or near the instrument. Handling of such materials during preparation should be performed in a safe area away from the instrument such as a fume cabinet.

# **Electrical Safety**

- Connect the instrument to a power supply line that includes a switch or other means of disconnection from the electricity supply.
- Only plug the instrument into an electricity-supply socket that is provided with a protective earth connection.
- When fuses need replacing, use only those with the required current rating and of the specified type. Do not use makeshift fuses and do not short-circuit fuse holders.
- When the instrument is connected to its electricity supply, terminals may be live and the removal of covers other than those which can be removed by hand is likely to expose live parts.
- Capacitors inside the instrument may still be charged even if the instrument has been disconnected from all voltage sources.
- The instrument must be disconnected from all voltage sources before it is opened for any adjustment, replacement, maintenance or repair.



Any interruption of the protective earth conductor inside or outside the instrument or disconnection of the protective earth terminal can make the instrument dangerous.

The instrument has an IEC Insulation class I rating for external circuits – only connect equipment that meets the requirements of IEC 61010-1, IEC 60950 or equivalent standards.

# Laser Safety Regulations

The Frontier Optica FT-IR spectrometer is a Class 1 laser product as defined by IEC 60825-1. The optical module contains a Class 2 Helium Neon (HeNe) laser, which emits visible, continuous wave radiation at a wavelength of 633 nm and has a maximum output power of 1 mW. Some diffuse HeNe laser radiation, within Class 1 limits, emerges from:

- The window in the left side of the sample compartment when an internal beampath is selected.
- An external beam port when the beam port cover is removed, no accessory is fitted at the port, and the beampath to the port is selected.



Do not stare into any laser beam. Staring into a laser beam (intrabeam viewing) can cause permanent damage to your eyes.

The laser is automatically shut down when the main cover of the instrument is raised.



Do not attempt to override or modify the interlock system.

Use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous radiation exposure.

The instrument complies with the following laser safety regulations:

- 1. 21 CFR Part 1040.10 and 1040.11 except for deviations pursuant to Laser Notice No. 50 dated 24 June 2007. Administered by the Center for Devices and Radiological Health, U.S. Department of Health and Human Services.
- 2. European Standard EN 60825-1:2007 "Safety of laser products Part 1: Equipment classification and requirements".

# *Laser Radiation Hazards and their Classification*

Indirect observation of the laser beam radiation in the optical path is not hazardous. Directly viewing the laser beam along its axis (allowing the laser beam radiation to pass into the eye) can be hazardous, depending upon the power of the beam, the length of time that the eye is exposed to the beam and the optical efficiency of the exposed eye. Direct viewing of a laser beam along its axis is termed intrabeam viewing.

Protection of the eye during accidental, momentary intrabeam viewing of a Class 2 laser beam is normally given by the eye's aversion response, including the blink reflex, which limits exposure of the eye to less than 0.25 seconds.

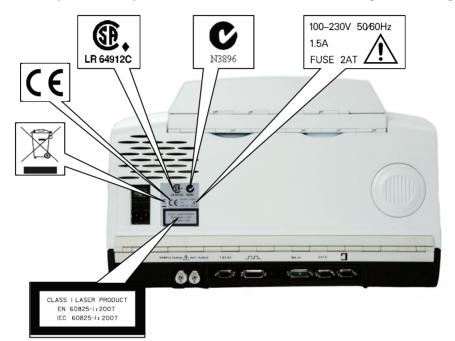
Class 1 levels of laser radiation are not considered to be hazardous.

# Labels



When this label is attached to an instrument it means "Caution, risk of danger". Refer to the manual to find out the nature of the potential hazard and any actions that have to be taken.

The product identification label is on the front of the instrument. Other labels are fixed to the Frontier Optica FT-IR spectrometer in the locations shown in Figure 1 and Figure 2:



#### Figure 1 Labels (rear of instrument)

**NOTE:** The label with a crossed-out wheeled bin symbol and a rectangular bar indicates that the product is covered by the Waste Electrical and Electronic Equipment (WEEE) Directive. Refer to *Appendix 5: WEEE Instructions for PerkinElmer Products* on page 92.

#### 20 . Frontier Optica FT-IR User's Guide

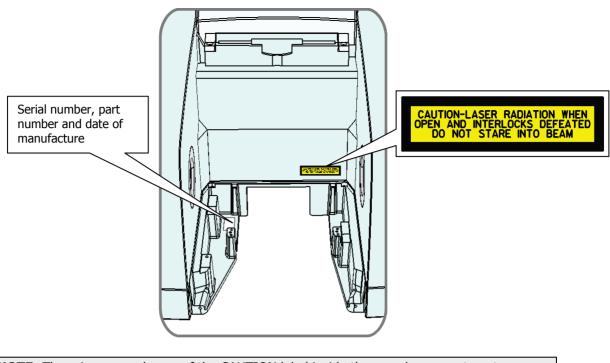
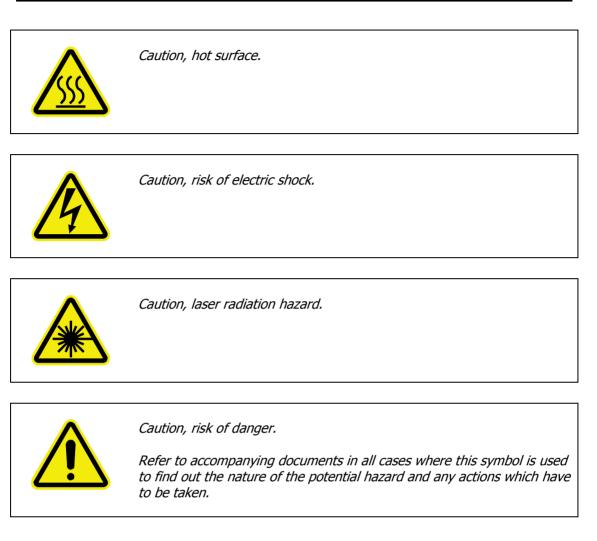




Figure 2 Labels (sample compartment)

# Warning Signs on the Instrument



# **EMC Compliance**

## EC Directive

The Frontier Optica FT-IR spectrometer has been designed and tested to meet the requirements of the EC Directive 2004/108/EC. The instrument complies with the EMC standard EN 61326-1 (EMC standard for electrical equipment for measurement, control and laboratory use).

## FCC rules and regulations

These products are classified as digital devices used exclusively as industrial, commercial, or medical test equipment. They are exempt from the technical standards specified in Part 15 of the FCC Rules and Regulations, based on Section 15.103(c).

# An Overview of the Frontier Optica FT-IR Spectrometer

# A Guided Tour of the Frontier Optica FT-IR Spectrometer

The PerkinElmer Frontier Optica FT-IR spectrometer (Figure 3) is a bench-top instrument that has been designed to provide high ordinate accuracy for measurements on optical components.



#### Figure 3 Frontier Optica FT-IR spectrometer

The following are all provided in one, self-contained unit:

- The instrument can operate in ratio, single-beam, or interferogram mode.
- The optical system enables you to collect data over a total range of 7800 to 350  $\rm cm^{-1}$  (1.28 to 28  $\mu m$ ) with a best resolution of 0.4  $\rm cm^{-1}.$
- The optical system has two variable, software controlled apertures: a beamsplitter stop (B-stop) and a Jaquinot stop (J-stop).
- A LiTaO<sub>3</sub> (lithium tantalate) mid-infrared detector as standard.

The instrument is connected to a PC, either point-to-point or over a network. The Spectrum software package supplied enables you to control the instrument and to manipulate the spectra that you collect.

## **Optical system**

The optical system is under the main cover of the instrument. Usually the main cover of the instrument is closed, but to perform most maintenance tasks the cover has to be open. When you do this, a safety interlock automatically switches off the power. Nevertheless, the instrument should be disconnected from the mains before opening the main cover for maintenance.

Consistent, reliable performance is achieved by having few moving or adjustable parts, and by extensive insulation of the optical system from the effects of humidity and vibration.

#### Stability of the optical system

The entire optical system is purged and sealed at the factory. A supply of desiccant placed within the system removes any water vapor and carbon dioxide that may enter. A desiccant indicator is fitted in the top cover, which warns you when the desiccant needs changing (an internal humidity sensor is available as an option).

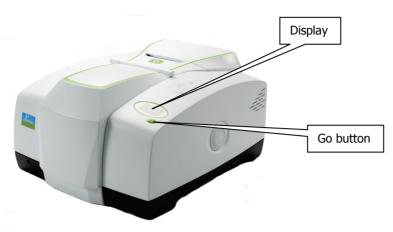
In the Frontier Optica FT-IR spectrometer, KBr windows separate the sample compartment from the purged optical system. You can purge the sample compartment with clean, dry, oil-free air or nitrogen. Either one removes water vapor; however, nitrogen is preferable because it also removes atmospheric carbon dioxide.



Do not use a flammable gas to purge Frontier Optica FT-IR instruments. The instrument contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.

The optics are kinematically mounted to ensure accurate positioning and to make them rugged. The interferometer is enclosed and mounted on anti-vibration mounts to guard against air and bench borne disruptions. The interferometer uses very low-friction point bearings and a frictionless electromagnetic drive to ensure long life.

### Top panel controls



#### Figure 4 Top panel controls

The display on the front right of the top of your instrument has two purposes:

- To display messages generated by the instrument's firmware, such as those that monitor initialization and diagnostics when the instrument is switched on.
- To display prompts and other messages generated by Spectrum software.

The instrument's Go button is used in concert with the displayed prompts and other messages generated by Spectrum software. It allows you to Start and Halt data collection while you are away from your computer.

### The sample compartment

The instrument has a large, purgeable sample compartment (Figure 5) located at the front of the instrument.

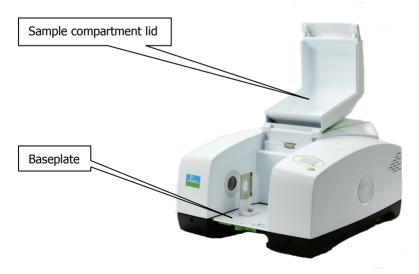


Figure 5 Sample compartment

**CAUTION** The Frontier Optica FT-IR spectrometer is fitted with sample compartment windows that are composed of KBr that, although coated, can be damaged by high levels of humidity.

If you spill a liquid in the sample compartment, wipe it up quickly. When working with water-based samples open to the air, either purge the sample compartment or leave the cover open.

| CAUTION | A relative humidity higher than 80% can damage the windows of the sample compartment. If you expect the humidity to exceed 80%, continually purge or desiccate the sample compartment. |
|---------|--|
|---------|--|

Open the sample compartment by lifting the cover using the recess at the front.

The infrared beam enters the sample compartment through an aperture on the left. After passing through the sample, it enters the detector area through an aperture on the right side of the sample compartment.

Standard accessories are mounted on a baseplate. The standard baseplate has a sample holder located by a knurled screw.

# Accessories for the Frontier Optica FT-IR spectrometer

There is a range of specialized sampling accessories available for the Frontier Optica, including Universal Attenuated Total Reflectance (UATR), Horizontal Attenuated Total Reflectance (HATR) and sample shuttle accessories. These accessories are easily installed (see *Appendix 1: Changing the Sampling Accessory* on page 86) and will be automatically recognized and controlled by the software. Further information about the use of these accessories can be found on the *IR & Raman Manuals CD* (L1050002).



Figure 6 Frontier Optica FT-IR with Universal ATR accessory

#### Storage compartment

You can store your polystyrene reference film, sample slides and other small accessories in the storage compartment on the top of the spectrometer (Figure 7).



Figure 7 Storage compartment on top of the spectrometer

### Power switch and communication ports

The power switch, AC power cable connector, and communication ports are on the rear of the instrument. The power switch is marked **I/O** (on/off).

**NOTE:** It can take the instrument about 2 hours to equilibrate when switched on after being switched off overnight. To save time, we suggest that you leave the instrument switched on at all times.

<u>Unpacking and</u> <u>Installation</u>

## Requirements

**NOTE:** Read the warnings and safety information at the start of this manual before you install the instrument. They contain important information.

#### **Electrical requirements**

The Frontier Optica FT-IR spectrometer can operate on electricity supplies of 50 or 60 Hz and in the 100 V to 230 V range without any adjustment.

The nominal power consumption of the instrument is 120 VA.

The line supply must be within 10% of the nominal voltage.

If possible, do not connect the instrument to circuits that have heavy duty equipment connected, such as large motors.

If possible, do not use photocopiers, discharge lamps, radio transmitters, and other equipment with large or frequent transient loads on the same supply circuit.

The primary fuse (2 AT, 250 V) is in the drawer on the rear of the instrument next to the mains inlet: the spare fuse is in the same drawer. The primary fuse is connected in the live line.

#### Environment

To obtain the best performance from your instrument:

- Place the instrument in an environment that is relatively dust-free.
- Make sure that the bench top is free from vibration or mechanical shocks.
- Do not place the instrument or the PC near to room-heating equipment, such as central-heating radiators.
- Do not position the instrument in direct sunlight, as this may cause overheating.
- Leave at least 15 cm (6 inches) from any surface and the cooling louvers at the rear of the instrument.
- Leave at least 7 cm (3 inches) from any vertical obstacle to the sides of the instrument, to permit an adequate flow of cooling air.
- Make sure that there are no overhanging shelves, and no water pipes or faucets that could leak onto the instrument.
- The area near the PC must be free of strong magnetic fields, direct sunlight, and heating or cooling units or ducts.

The instrument has been designed for indoor use and operates correctly under the following conditions:

Ambient temperature 15 °C to 35 °C

Ambient relative humidity 80% maximum (non-condensing).

# Unpacking the Spectrometer



The spectrometer is a heavy precision instrument, so two people are required for safe handling.

The instrument weighs approximately 34 kg unpacked (40 kg packed) and has a lifting recess on either side. Consult the local codes of practice issued by safety advisors before attempting to lift it.

Take care not to injure yourself or others, or to drop the instrument.

#### CAUTION

Take great care when installing your Frontier Optica FT-IR spectrometer, and follow the procedures described in this manual. If you require assistance, contact your local PerkinElmer Service Engineer.

### Opening the shipping container

Your spectrometer is packed inside the box in a silver bag that protects it from condensation.

1. First remove the manuals/software box, leads, and so on from the box, and check that all the following parts are present:

| Part Number | Description                    |   |
|-------------|--------------------------------|---|
| L1202057    | Polystyrene calibration film   | 1 |
| 04974265    | Quick-release purge coupling   | 2 |
| L1200466    | Ethernet crossover cable       | 1 |
| 04790839    | 2 A, 250 V time lag fuse       | 2 |
| L9003693    | 8.0 mm hexagonal wrench        | 1 |
| L1050002    | IR & Raman Manuals CD          | 1 |
| L1250450    | Germanium test sample kit      | 1 |
| LX108873    | Spectrum Standard Software Kit | 1 |
| L1250230    | Spectrum Configuration Disk    | 1 |

If any items are missing or damaged, contact your local PerkinElmer office.

2. Carefully remove the instrument from the shipping container, but not from the bag in which it was shipped.

**CAUTION** The spectrometer must be allowed to reach the temperature of its surroundings before it is removed from the bag. This means leaving it overnight if it has been moved from a cold area, and at least 4 hours after removal from the shipping container.

3. When the spectrometer has been allowed to warm to the temperature of its surroundings, remove it from the bag and place it on the bench where it is to be used. Ensure that you can reach the rear of the spectrometer to connect the cables.

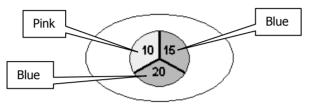
**NOTE:** Any accessories will be shipped in separate boxes.

# The Desiccant Indicator

The optical system of the spectrometer is purged at the factory. This protects the beamsplitter and the sample compartment windows from being damaged by humidity. Replaceable packs of desiccant keep the optics dry and free of  $CO_2$ .

The top panel of the instrument includes a desiccant indicator, whose sectors change sequentially from blue to pink as the desiccant packs are exhausted (Figure 8). Change the desiccant in the instrument when the sector marked 10 becomes pink, but while the sectors marked 15 and 20 are still blue.

Refer to *The Desiccant Indicator in Detail* on page 62 for more information about the appropriate action to take if the sectors marked 15 and 20 are pink.



#### Figure 8 The desiccant indicator

CAUTIONIf all three sectors of the desiccant indicator are pink, then you must<br/>change the desiccant.The instrument optics may be fogged. Do not switch the instrument<br/>either ON or OFF until all sectors are blue.

# Connecting up the Spectrometer

### Connecting to the PC

**NOTE:** To control your instrument from a PC, use the crossover cable supplied. To control your instrument over your network, use a standard Ethernet cable (not supplied).

1. Plug one end of the cable into the connector port on the right-hand side of the instrument (Figure 9).



#### Figure 9 PC connection port

2. Plug the other end of the cable into the network connection on your PC (if you are using the crossover cable) or network hub (if you are using a standard Ethernet cable).

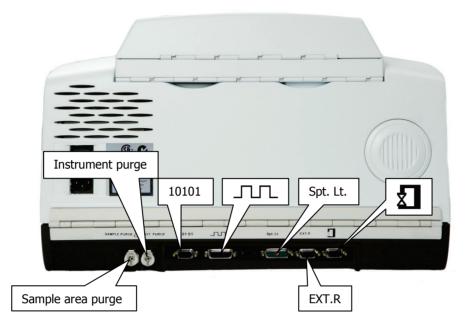
| <b>CAUTION</b> Do not attempt to connect a monitor to either the EXT.R port or the MICROSCOPE port, or you will cause serious damage to the instrument when it is switched on. |
|--|
|--|

#### **Connector details**

| Description   | Connector<br>Type | Voltage | Maximum<br>Current |
|---|-------------------|---------|--------------------|
| 10/100 Base-T Ethernet connector. This is the<br>standard interface between the PC and the<br>instrument, or between a Local Area Network<br>(LAN) and the instrument. If connecting directly<br>from the PC to the instrument use the Category 5<br>UTP Cross-Over cable supplied. If you are<br>connecting to your network, use a standard<br>Ethernet cable.<br>DO NOT USE THE CROSS-OVER CABLE TO<br>CONNECT TO YOUR NETWORK. | Ethernet          | <5 V    | <100 mA            |

### Other connectors

The communication ports for peripheral devices are shown in Figure 10.



#### Figure 10 Communication ports

Icons that identify the function of each of the Communication ports are printed on the hinge molding directly above the port.

| Connector | details |
|-----------|---------|
|-----------|---------|

| Icon   | Description   | Connector<br>Type                | Voltages | Maximum<br>Currents |
|--|---|----------------------------------|----------|---------------------|
| <b>10101</b> Serial port. Connects a PC to the<br>instrument using an RS232<br>interface cable. This connector is<br>only used for service diagnostics.9-way<br>D-type |   | ,                                | +12 V    | <100 mA             |
|  | D-type  | -12 V                            | <100 mA  |                     |
| <u></u>  | General Purpose Optical Bench<br>(GPOB). Allows synchronization<br>between the instrument and an<br>external accessory. | 26-way<br>high density<br>D-type | +5 V     | <50 mA              |
| Spt. Lt  | Spotlight. Used to connect the instrument to a Spotlight Imaging System.  | 11-way<br>mixed<br>D-type        | +5 V     | <100 mA             |
|  |   |                                  | ±12 V    | 50 mA               |

| Icon   | Description   | Connector<br>Type      | Voltages | Maximum<br>Currents |
|--------|---|------------------------|----------|---------------------|
| EXT. R | Right external detector module.<br>Connects to an external detector   | 15-way<br>high density | +12 V    | 0.65 A              |
|        | Microscope external detector<br>module. Usually the detector is<br>placed in an accessory placed on<br>the right of the instrument.<br>Microscope external detector<br>module. Connects to a<br>PerkinElmer infrared microscope,<br>placed on the left of the | D-type                 | -12 V    | 0.65 A              |
|        |   |                        | +5 V     | 4 A                 |
| x      |   | 15-way<br>high density | +12 V    | 0.65 A              |
|        |   | D-type                 | -12 V    | 0.65 A              |
|        | instrument.   |                        | +5 V     | 4 A                 |

## Connecting the spectrometer to the electrical supply

The power cable for the electrical supply plugs into the rear of the instrument. It has a molded socket at one end. If it is necessary to fit a plug on the power cable, use the wire color code below:

| Plug Pin Wire Color (100–120 V) |                       | Wire Color (220–240 V) |  |  |
|---------------------------------|-----------------------|------------------------|--|--|
| Ground (Earth)                  | Green or Green/Yellow | Green/Yellow           |  |  |
| Live                            | Black                 | Brown                  |  |  |
| Neutral                         | White                 | Blue                   |  |  |



To ensure safe and satisfactory operation of the instrument, it is essential that the green or green/yellow ground (earth) wire of the power cord is connected to a ground that complies with the regulations of the local electricity supply authority (or equivalent body); ground circuit continuity is essential for safe operation of the equipment. The Frontier Optica FT-IR spectrometer can operate on electricity supplies of 50 Hz or 60 Hz and in the 100 V to 230 V range without any adjustment.

1. Fit the molded socket of the power cable into the electrical supply inlet (Figure 11) of the instrument.



#### Figure 11 Electrical supply inlet

- 2. Switch on the power at the supply.
- Switch on the instrument at the switch above the supply inlet.
   I is on and O is off.

After a short diagnostic check, which takes about two minutes and is described in *Appendix 2: Instrument Self-Checks* on page 88, your instrument will be ready to communicate with the PC.

## Installing the Instrument in the Software

Before you can use the instrument it must be set up in the software.

#### Installing the software

# **NOTE:** If you are supplying your own computer, make sure that it meets the minimum requirements for hardware and software set out in the "PC Requirements" section of the *Administrator's Guide* for your software, which can be found on the *IR & Raman Manuals CD* (part number L1050002) supplied with your instrument.

> To install Spectrum software, insert the supplied DVD and follow the instructions on the screen. Details of the installation program are given in the *Administrator's Guide*.

## The Instrument Install Wizard

After installing your software you will need to install your instrument.

Select Add Instrument from the Administration group on the Setup menu in Spectrum software.

The Instrument Install Wizard starts.

Details of the instrument install wizard are given in the Administrator's Guide.

40 . Frontier Optica FT-IR User's Guide

# **Using the Spectrometer**

## Basics of Software Control

#### Starting Spectrum software

1. Switch on the power to the instrument using the switch on the rear of the instrument. The instrument will initialize, which will take approximately 2 minutes.

**NOTE:** It can take the instrument about two hours to equilibrate when switched on after being switched off overnight. To save time, we suggest that you leave the instrument switched on at all times.

2. From the Start menu select **Programs**; the **PerkinElmer Applications** group; the **Spectrum** sub-group and then the **Spectrum** application.

OR

Double-click the shortcut icon  $\bigcirc$  on the desktop.

The Spectrum start-up splash-screen is displayed, followed by a dialog that may require your login details:

| PerkinElmer Login                  |
|------------------------------------|
| Enter your user name and password. |
| User name                          |
|                                    |
| Password                           |
|                                    |
| Change Password                    |
| OK Cancel                          |

3. If required, enter your User name and Password, and then click OK.

If you already have an instrument set up in Spectrum for this user on this PC, the Instrument Connection dialog may be displayed, unless Auto Connect is set up for the instrument. If Auto Connect is enabled Spectrum will automatically connect to the instrument.

4. Select the **Instrument** you want to use.

OR

If you want to work with data that has been collected previously, without connecting to an instrument, select **work offline**.

**NOTE:** Working offline can free a networked instrument for use by another user.

Spectrum starts.

## Scanning samples

When you connect to your spectrometer the instrument settings will default to appropriate values for your instrument type and accessory.

The configurable Scan toolbars at the top of the workspace include the tools you need to collect a sample spectrum. The default Instrument Settings toolbar contains settings that are appropriate for the Frontier Optical FT-IR (Figure 12).

| Start (µm) | End (µm) | Accumulations | Sample ID                   | Description | Resolution (cm-1) | J-Stop (mm) | B-Stop (mm) |
|------------|----------|---------------|-----------------------------|-------------|-------------------|-------------|-------------|
| 2.5        | 25       | 1 Minutes     | <ul> <li>User 01</li> </ul> | Sample 0 😆  | 8 🔻               | 6           | 6           |

#### Figure 12 Instrument Settings toolbar

**NOTE:** The Scan toolbars are not displayed if you have chosen to work offline.

To scan a sample:

1. Check and set the instrument parameters.

Here you set the **Start** and **End** points of the scan range (by default in microns, but the abscissa units can also be set to nanometers or wavenumbers on the Setup Instrument Basic tab) and the **Accumulations** required, either as a number of scans, or as a length of time. You can enter a unique **Sample ID** and **Description** for the sample. You can also set the **Resolution** (in cm<sup>-1</sup>). This will set the **J-Stop** size (in mm) to the default for that resolution, which you can then edit.

By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar. The values applied depend on your instrument and accessory. To amend any value, select the parameter and then enter your new value, or select a value from the drop-down list.

2. If a background scan is required, the **Scan** button includes a small background flag. Clear the instrument beampath, or insert a suitable background material, and then click

lo collect a background spectrum.

The background spectrum is displayed briefly, and then the Viewing Area is prepared for data collection from your sample.

By default, the Measurement bar includes **Scan**, **Halt**, **Background** and **Monitor** buttons. You can also select these commands from the Measurement menu.

We recommended that you run a background scan before every sample.

**NOTE:** You can use the Sample Shuttle Accessory (L1200302) to set up an interleaved cycle scan so that you do not have to open the sample compartment between the background and sample scans. This helps to reduce changes in the concentration of carbon dioxide and water vapor in the sample compartment. Set the **Scan Type** to **Interleaved** on the Setup Instrument Basic tab. See the Spectrum on-screen Help for more information.

**NOTE:** If you wish to run a background scan with a filter in place, you must set the **Scan Type** to **Background** on the Setup Instrument Basic tab, rather than using the toolbar button. See the Spectrum on-screen Help for more information. 3. Place your sample in the instrument and then click for begin scanning your sample.

By default, during scanning the sample data is displayed on the Live tab in the Viewing Area.

The completed spectrum is displayed on the Graph tab, and added to the current Samples View in the Data Explorer.

4. If, for any reason, you want to stop scanning your sample, click

## Working with the instrument display and Go button



#### Figure 13 Top panel controls

The display on the front right of the top of your instrument is used to display prompts and other messages generated by Spectrum software.

Simply follow the prompts in the instrument display and use the Go button located on the instrument to complete a series of sample scans.

#### Using the Spectrum on-screen Help system

Use the Spectrum Help system to find further information about using Spectrum software to control, set up and adjust your instrument.

To open the Help file, select **Contents** from the **Help** menu. This menu also includes links to on-screen tutorials (**Tutorials**), and information about the software (**About**).

## Atmospheric (CO<sub>2</sub>/H<sub>2</sub>O) Suppression

Atmospheric suppression can be selected in the Setup Instrument Advanced tab (Figure 14).

| Setup Instrument Auto-Name | Setup Instrument Data Collection | Setup Instrume | nt BeamPath              | Setup Instrument Adv | anced | Setup Instrument Basic |
|----------------------------|----------------------------------|----------------|--------------------------|----------------------|-------|------------------------|
|                            | ed Settings Quali                | ty Checks      |                          |                      |       |                        |
| ToolBox 🔽 CO               | 02/H20                           | Name Ir        | nclude                   | Range                |       | All Checks Off         |
| AV                         | a Base                           | eline High     | <ul> <li>80 -</li> </ul> | 95                   |       |                        |
|                            | Base                             | eline Low      | ✓ 50 -                   |                      |       |                        |
| Lo                         | ok Ahead Bas                     | eline Sloping  | ✓ 50 -                   | 65                   | =     | Restore Defaults       |
| _                          |                                  | n Noise        | ✓ 10 -                   | 60                   |       |                        |
|                            |                                  | ng Band        | ✓ 30 -                   | 50                   |       |                        |
| 0.2                        | 💌 Wea                            | ak Band        | 25 -                     |                      | _     |                        |
| Phase                      | Correction Stra                  | y Light        | ✓ 30 -                   |                      |       |                        |
| Magnit                     | tude 🔽 Wat                       | er Vapor       | <ul> <li>30 -</li> </ul> |                      |       |                        |
| Apodiz                     | Carb                             | oon Dioxide    | <ul> <li>80 -</li> </ul> | 95                   |       |                        |
| Strong                     | Vian                             | etting         | ✓ 50 -                   | - 85                 |       |                        |
| Stiong                     | Fring                            | jes            | V 0                      | 70                   |       |                        |
| Scan S                     | Start Delay (s) Bloc             | ked Beam       | 40 -                     | 70                   |       |                        |
| 0                          | Neg                              | ative Bands    | 99 -                     | 99                   |       |                        |
|                            |                                  | ÷ · ·          | -                        |                      |       |                        |

Figure 14 Setup Instrument Advanced tab in Spectrum

## What is atmospheric suppression?

This is an atmospheric correction routine. This routine is more powerful than simple subtraction, overcoming the following issues:

- Non-linearity due to resolution
- The measured spectrum is temperature dependent
- Lineshape and calibration are affected by J-stop and sample or accessory.

#### What does atmospheric suppression do?

When **CO2/H2O** is switched on, the software uses a single reference spectrum derived from high resolution data and our understanding of the instrument to model the lineshape, then finds the current real instrument parameters by least squares fitting to the measured spectrum.

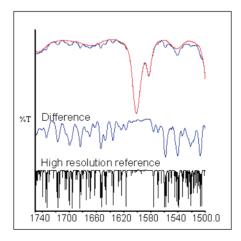
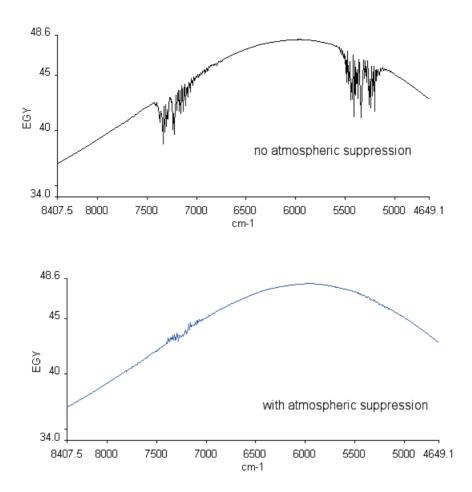


Figure 15 Correction of an MIR spectrum at 4 cm<sup>-1</sup> resolution



#### Figure 16 Atmospheric suppression

**NOTE:** Atmospheric suppression should be used with caution when measuring optical components. For example, when measuring a 1600 cm<sup>-1</sup> CO<sub>2</sub> passband filter suppressing the CO<sub>2</sub> absorption may produce errors in that region of the spectrum.

## **AVI** Correction

AVI correction can be selected in the Setup Instrument Advanced tab in Spectrum (Figure 14).

AVI correction can only be performed if an AVI Calibration has been set up for the current configuration and resolution. Select **AVI** from the **Adjustments Toolbox**, available from the Setup Instrument Advanced Tab. Follow the instructions on-screen. For further information, refer to the Spectrum on-screen Help file.

## What is AVI correction?

The objectives of Absolute Virtual Instrument (AVI) correction are:

- Consistent performance over time and between instruments
- Traceability for all measurements.

Although FT-IR spectrometers use a reference laser, the wavenumber calibration and lineshape are affected by differences in beam divergence and uniformity. This is true for all FT-IR spectrometers. Differences can occur between instruments, when using different sampling accessories and when components are changed. AVI allows calibration and lineshape to be maintained.

The Absolute Virtual Instrument is an instrument with theoretical performance, such that the result of measuring a known sample on such an instrument can be predicted. So, if we measure with a real instrument and calculate the software transform to match the theoretical result, we can apply this transform to future measurements.

The Absolute Virtual Instrument is defined by wavenumber calibration, instrument lineshape and ordinate accuracy.

## What does AVI correction do?

When **AVI** is switched on, the software measures the current instrument profile relative to an absolute standard (a methane cell) and an ideal lineshape function, and applies a correction. If you have an automated, internal filter wheel, this can provide correction for any sampling configuration.

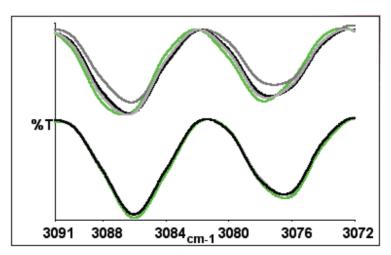


Figure 17 Spectra of methane at 4 cm<sup>-1</sup> resolution as measured (top) and with AVI (bottom)

## Look Ahead

Look Ahead can be selected in the Setup Instrument Advanced tab (Figure 14).

## What is Look Ahead?

Look Ahead is a novel system where the spectrometer scans continuously and uses the properties of the measured spectrum to identify changes corresponding to sample removal, sample insertion, or sample change, automatically.

This information is used to identify the scans that are being collected, and to accumulate sample scans. This can decrease the overall scanning time required for those samples that require scan accumulation.

## What does Look Ahead do?

If **Look Ahead** has been enabled, the spectrometer scans continuously. When you request a sample scan, the scan collected is compared to the scans that have already been collected. If identical scans are found, the number of scans requested is decreased by the number of scans found, so decreasing the overall scanning time.

## **Quality Checks**

Quality Checks can be selected in the Setup Instrument Advanced tab (Figure 14).

#### What are Quality Checks?

Quality checking is a tool for less experienced IR users that identifies possible problems in the spectrum being collected and suggests ways of improving the measurement.

### What do Quality Checks do?

Simply select the **Quality Checks** that you want to perform from the list in the Setup Instrument Advanced tab and, if required, adjust the threshold range using the slider bars. To display more information about an individual test, double-click on its name in the list.

When you collect your spectrum, the selected tests are performed as the data is collected and a signal light (green <sup>o</sup>, amber <sup>o</sup>, or red <sup>o</sup>) indicates the result.

The results from the Quality Checks imply:

**Okay** (**•**) – the quality of the spectra is satisfactory.

**Caution** (•) – the software identified a problem that you may want to investigate in order to improve the quality of the spectra you are collecting.

**Warning** (•) – the software has identified a serious problem that you should attempt to cure before collecting further spectra.

**NOTE:** Some quality checks may not be appropriate when measuring optical components. Before applying a quality check, ensure that you fully understand the implications of doing so. 50 . Frontier Optica FT-IR User's Guide

# <u>Measuring Optical</u> <u>Components</u>

## **Optimizing Your Instrument Settings**

The Frontier Optica FT-IR instrument has been designed to have high ordinate accuracy for use in applications such as optical component measurements. This section contains some guidelines to help you to get the best performance out of your instrument.

## J-stop

The J-stop is a variable aperture that has been partially blanked off to prevent back reflections propagating through the interferometer. It defines the size of the beam at the sample and on the detector. If the beam is deviated by the sample, there is a chance that the beam, or part of the beam, could miss the detector. If the diameter of the beam is small in relation to the detector there is more tolerance for this deviation. The diameter of the beam at the beam at the sample position will be about 1.2 times the diameter of the J-stop.

For high ordinate accuracy we recommend that you use a 6 mm or smaller J-Stop when making transmittance measurements. However, the smaller the diameter of the J-stop, the lower the level of signal reaching the detector and, therefore, the lower the signal-to-noise ratio.

For a given **J-stop Image Size**, the selected resolution is only achievable in the spectrum up to a wavenumber value known as the **J-Stop Wavenumber** (Figure 18). Increasing the J-stop size beyond the default value will decrease the J-stop wavenumber, and thus the wavelength range over which a particular spectral resolution can be achieved.

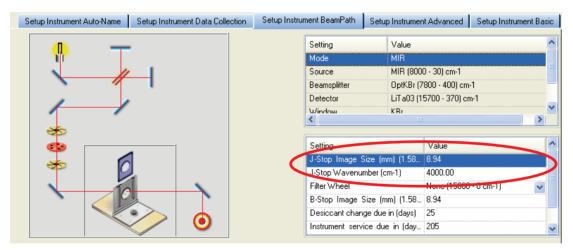


Figure 18 Setup Instrument BeamPath tab in Spectrum software

**NOTE:** If you change the resolution in Spectrum software, the **J-Stop Image Size** will be set to the default size for that resolution. However, for resolutions ≥2 cm<sup>-1</sup> we recommended that you reset the **J-Stop Image Size** to 6 mm.

#### **B-stop**

The B-stop is a circular, variable aperture that defines the area of the beam passing through the interferometer. It also controls the divergence of the beam at the sample position (by restricting the angle of the cone of radiation).

The beam angle is proportional to the B-stop diameter. For high ordinate accuracy when measuring transmittance we recommend that you use a 6 mm or smaller **B-Stop Image Size**. A 6 mm B-stop image size produces a beam in the sample area with a cone half-angle of 4° (70 milliradians).

Reducing the B-stop size decreases the optical beam distortions at the detector, increasing the ordinate accuracy. Reducing the B-stop size may also improve the wavelength accuracy of multi-layer optical filter measurements by decreasing the divergence of the beam.

However, the smaller the diameter of the B-stop, the smaller the amount of signal reaching the detector and, therefore, the lower the signal-to-noise ratio.

## Resolution

FT-IR measurements in wavenumbers (cm<sup>-1</sup>) have constant resolution over the entire range. If wavenumbers are converted to wavelength (for the Frontier Optica FT-IR, measured in microns or nanometers) the resolution varies as a function of wavelength.

The relationship between wavenumber resolution, wavenumber, wavelength resolution and wavelength is given by:

$$\frac{\Delta \upsilon}{\upsilon} = \frac{\Delta \lambda}{\lambda}$$

This relationship is demonstrated in the following table.

| Wavelength                                | Resolution (nm)<br>corresponding to 16 cm <sup>-1</sup> | Resolution (nm)<br>corresponding to 4 cm <sup>-1</sup> |  |  |
|---|---|--|--|--|
| 2500 nm (2.5 μm, 4000 cm <sup>-1</sup> )  | 10  | 2.5  |  |  |
| 5000 nm (5.0 μm, 2000 cm <sup>-1</sup> )  | 40  | 10   |  |  |
| 10 000 nm (10 µm, 1000 cm <sup>-1</sup> ) | 160   | 40   |  |  |
| 20 000 nm (20 μm, 500 cm <sup>-1</sup> )  | 640   | 160  |  |  |

**NOTE:** If the resolution is changed in Spectrum, the software automatically resets the **J-stop Image Size** to the default for that resolution.

#### **Phase correction**

Phase correction is a necessary part of the process of converting the measured interferogram into a spectrum. There are three options available:

#### Background

**Background** uses the information in the interferogram of the background scan to correct both the background and sample spectra.

This is the recommended option for optical measurements.

If there is a long time delay between background and sample measurements this could introduce errors. In this case, it is advisable to collect a new background before your sample spectrum.

#### Magnitude

**Magnitude** is not suitable when transmittance values very close to zero have to be measured. Any transmittance values that are negative due to noise will be rectified to appear positive. This will result in average values that are offset to be slightly above zero, with the size of the offset depending on the noise level. This problem can be avoided by using Background phase correction.

#### Self

**Self** uses the background and sample interferograms separately to correct the respective spectra. As with Magnitude, there can be problems when transmittance values are close to zero. There is no phase information from regions where transmittance is zero, leading to inaccurate transmittance values in those regions and in sharp band edges adjoining these regions. This problem can be avoided by using Background phase correction.

**NOTE:** Phase correction is set on the Setup Instrument Advanced tab in Spectrum software (Figure 14). See the on-screen Help for more information.

#### Apodization

The true interferogram of a light source is infinite in length. A spectrometer can only measure a finite part of the interferogram. This means that unwanted oscillations or sidelobes are produced on either side of narrow bands in the spectrum. Apodization is a mathematical function applied to the interferogram to remove the sidelobes. The influence of apodization on lineshape may become important when, for example, measuring narrow passband filters.

The Spectrum software has a number of types of Apodization available.

For optical measurements we recommend **Filler**. The Apodization function is defined on the Setup Instrument Advanced Tab (Figure 14).

Please refer to the Spectrum on-screen Help for more information.

## Sample Properties

When you measure the transmittance of your sample, you are effectively measuring the change in energy of the beam as it passes through the sample. The properties of your sample – for example, the shape, position and material – will affect the path taken by the beam. Deflections and multiple reflections may decrease the accuracy of your %T value.

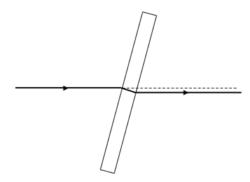
## Sample wedge

The beam will be deflected by samples with non-parallel faces. The greater the wedge angle (the angle by which one face deviates from parallel to the other face) the greater the deflection of the beam. This increases the probability that part, or all, of the beam will miss the detector.

The angular deviation of the beam is the wedge angle multiplied by (n-1), where *n* is the refractive index of the sample material. You may find reduced accuracy when, for example, measuring zinc selenide ( $n \approx 2.4$ ) samples with wedge angles of more than 0.2° or when measuring germanium ( $n \approx 4$ ) samples with wedge angles of more than 0.1°.

## Sample tilt

If a sample is tilted, then the beam will be displaced from its axis. Any multiple reflections will also be displaced. The detector optics in the Frontier Optica FT-IR are more susceptible to error when the beam is displaced horizontally (when, for example, the sample is tilted about a vertical axis) than when displaced vertically. Therefore, we recommend that if a sample is tilted it should be about the horizontal axis. Figure 19 shows the displacement of the beam as a sample is tilted.



## Figure 19 Sample tilt about a horizontal axis showing the vertical displacement of the beam

When the sample is tilted the deflection of the beam (and any multiple reflections) will increase with the thickness of the sample.

You may find reduced accuracy when measuring, for example, a germanium sample ( $n \approx 4$ ) with a thickness of 1 mm that is tilted by more than 5° about a horizontal axis.

## Sample thickness

The sample thickness impacts on the image focus at the detector, and therefore may affect the accuracy of the measurement. You may find reduced accuracy when, for example, measuring germanium ( $n \approx 4$ ) samples with sample thicknesses greater than 6 mm. Sample thickness effects can also be significant when tilting samples (see *Sample tilt* on page 55).

#### Non-planar samples

You should be aware that taking measurements from non-planar samples will introduce errors. You may be able to improve the accuracy of such measurements by, for example, comparing a coated component with a similar uncoated component.

## Small samples

We advise that you mount small samples over an aperture in an opaque mask to prevent the beam from passing round the edge of the sample. However, the mask *must* be in the same position for both background and sample measurements.

## Samples with near-parallel reflecting surfaces

An optical substrate with parallel reflecting surfaces can act as an etalon. If the free spectral range of the etalon (the fringe spacing) is finer than the resolution selected on the Frontier Optica FT-IR, the fringes will not be seen directly.

However, in spectral regions with atmospheric absorption, the spectral filtering due to the etalon fringes can interfere with the atmospheric absorption lines, resulting in apparent excess noise in the atmospheric absorption region. This is shown in Figure 20, in the region  $2000-1300 \text{ cm}^{-1}$  (water vapor) for a 2 mm thick sample of uncoated germanium with near-parallel surfaces.

This can be reduced by purging the sample area with dry nitrogen (see *Purging the Spectrometer* on page 66), and by ensuring that the instrument desiccant is changed regularly (see *Changing the Desiccant* on page 63).

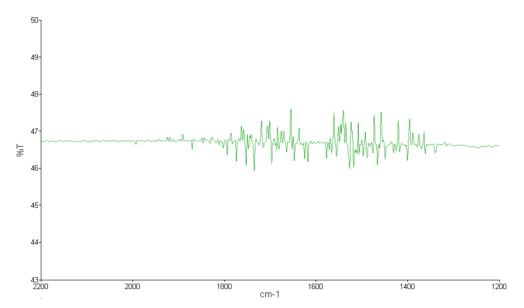


Figure 20 Water vapor interference in an FT-IR spectrum of a 2 mm thick sample of uncoated germanium

## Summary

In this chapter, we have described a number of parameters that affect the accuracy of your optical measurements when measuring transmittance.

It is important to ensure that the resolution is good enough to measure the features of interest, with the limitation that using higher resolution will increase the noise or the measurement time.

To achieve high ordinate accuracy at non-zero %T values the J-stop and B-stop image sizes should be set to 6.00 mm or lower. However, when measuring regions that are close to 0%T, for example to determine blocking efficiency, it may be advisable to use the maximum J-stop and B-stop image sizes to reduce noise.

#### **Reflection measurements**

Reflection measurements can be made using the appropriate accessories. They do not require the reduced J-stop and B-stop image sizes that are needed to minimize beam distortions caused by transmission samples.

58 . Frontier Optica FT-IR User's Guide

## **Routine Maintenance**

## Cleaning the Spectrometer

Clean the outside of the instrument using a damp cloth. If necessary, a mild detergent may be used. Before you clean the entire instrument, always perform a patch test on an inconspicuous area.

Avoid spilling liquid into the instrument. Clean all external spills immediately. If anything that is spilled enters the main body of the spectrometer, switch off the power and contact a PerkinElmer Service Engineer.

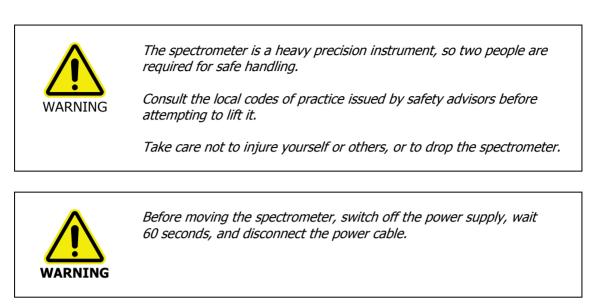
#### CAUTION

Do not touch or attempt to clean any optical surface in the instrument, because this will impair its performance and may easily damage the component.

## Cleaning the display

Clean grease and dirt off the display using a soft damp cloth and a mild detergent.

## Moving the Spectrometer



The spectrometer can be lifted using the shaped handholds on its sides, as shown in Figure 21. Two people are needed to lift it because its basic weight is approximately 34 kg.



Figure 21 Frontier Optica FT-IR lifting points

## Condensation

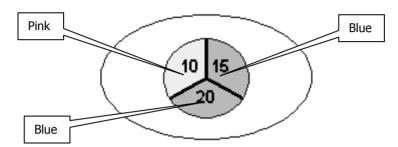
Be aware that condensation caused by moving your spectrometer from a cooler environment to a warmer one can damage the windows of the sample compartment. To prevent this damage from occurring:

- Make sure that the windows are protected by placing fresh bags of desiccant in the sample compartment.
- Leave the spectrometer to reach the temperature of the surroundings before removing the desiccant.

## The Desiccant Indicator in Detail

The optical system of the spectrometer is purged at the factory. This protects the KBr beamsplitter and the sample compartment windows from being damaged by humidity. Replaceable packs of desiccant maintain the purge.

The top panel of the instrument includes a desiccant indicator whose sectors change sequentially from blue to pink as the desiccant becomes exhausted. Change the desiccant packs in the instrument when the sector marked 10 becomes pink, but while the sectors marked 15 and 20 are still blue. These numbers correspond to the approximate % Relative Humidity in the instrument.





CAUTION

If all three sectors of the desiccant indicator are pink, then you **must** change the desiccant.

The instrument optics may be fogged. Do not switch the instrument either ON or OFF until all sectors are blue.

| Sector              | Action Required   |
|---------------------|---|
| All sectors blue    | None.   |
|                     | The humidity levels in the instrument are below approximately 10% Relative Humidity.  |
| Sector 10 pink      | Desiccant change is recommended.  |
|                     | If the instrument has been switched OFF for an extended period, do<br>not switch ON until you have changed the desiccant and all sectors<br>are blue. |
| Sector 10 & 15 pink | Replace desiccant the immediately to avoid instrument damage.   |
|                     | Do not switch the instrument ON or OFF until you have changed the desiccant and all sectors are blue.   |

## Changing the Desiccant

| CAUTION | Expect to change the desiccant in the spectrometer every six months.<br>Old, used desiccant releases moisture. |
|---------|--|
|         | In regions experiencing high humidity levels we recommend you change<br>the desiccant more often.              |

The desiccant change interval is set in the **Desiccant change due in (days)** option on the Setup Instrument BeamPath tab in Spectrum software (Figure 23).

| Setup Instrument Auto-Name Setup Instrument Data Collection | n Setup Instrum | ent BeamPath     | Setup Instrumer  | it Advanced 📗 S  | etup Instrument Basic |
|---|-----------------|------------------|------------------|------------------|-----------------------|
| <b>—</b>  | [               | Setting          | Value            |                  | <u>^</u>              |
|   |                 | Mode             | MIR              |                  |                       |
|   |                 | Source           | MIR (800         | 0 - 30) cm-1     | =                     |
|   |                 | Beamsplitter     | OptKBr (7        | 800 - 400) cm-1  |                       |
| 1 1   |                 | Detector         | LiTa03 (1        | 5700 - 370) cm-1 |                       |
|   |                 | Window<br><      | KBr              |                  | ×                     |
| *   | 6               |                  |                  | 1                | (=)                   |
|   |                 | Setting          |                  | Value            | <u>^</u>              |
|   |                 | J-Stop Image S   | ize (mm) (1.58   | 8.94             |                       |
|   |                 | J-Stop Wavenun   | nber (cm-1)      | 4000.00          | E                     |
|   |                 | Filter Wheel     |                  | None (15000 - 0  | cm-1) 🗸               |
|   |                 | B-Stop Image 3   | ize (mm) (1.58   | 0.34             |                       |
|   |                 | Desiccant chang  | ge due in (days) | 25               |                       |
|   |                 | Instrument servi | ce due in (day   | 205              | ~                     |

Figure 23 Setup Instrument BeamPath tab in Spectrum

If an instrument desiccant change is overdue, a warning will be displayed in the Status Bar and in the Setup Instrument BeamPath table.

The warning is displayed until you tell the software that the desiccant has been changed. To reset the desiccant change interval, select the current value, click **Changed** to clear any warning messages, and then enter the number of days before the next desiccant change is due.

#### Renewing the instrument desiccant

# CAUTIONOld, used desiccant releases moisture and can cause catastrophic failure<br/>of KBr optics.Do not use damaged packs of desiccant. Make sure that the packs you<br/>use have not been left in contact with the air.

You can purchase disposable desiccant kits from PerkinElmer (part number N0171159). A kit contains two packs of desiccant, and three kits are required.

- 1. Inspect the humidity indicator card in the plastic bags in which the spare desiccant packs are packed. If the card indicates humidity in the bag, discard the desiccant pack.
- 2. Remove the sample area cover, if fitted, by opening the cover, pressing the clip and pulling the cover vertically to remove.



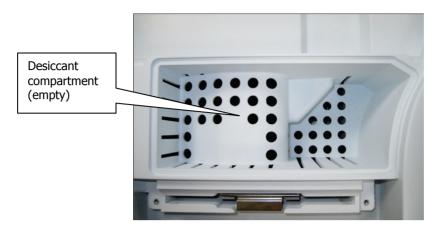
#### Figure 24 Removing the sample compartment cover

3. Undo the two captive screws securing the desiccant cover (Figure 25).



Figure 25 Captive screws securing the desiccant cover

4. Open the cover and remove all the exhausted desiccant packs (Figure 26), noting how they are installed.



#### Figure 26 Desiccant removed

5. Place the first three packs of desiccant upright in the recess on the right of the desiccant holder then, one at a time, lay the three remaining packs flat in the upper part of the holder.

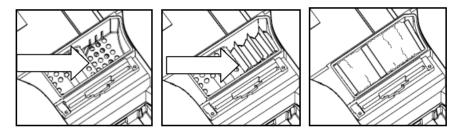


Figure 27 Stowing the desiccant packs

Ensure that when the packs have been installed they do not rise above the level of the black rubber purge seal.

- 6. Close the cover and tighten the screws.
- 7. Refit the sample area cover.

#### Installing rechargeable desiccant in the instrument

There is also a rechargeable desiccant kit available (part number L1250311).

To install rechargeable desiccant packs follow the *Renewing the instrument desiccant* procedure starting on page 64.

The instrument requires two rechargeable desiccant packs; the packs are sized to fit into the left (70 mm  $\times$  78 mm  $\times$  33 mm) or right (102 mm  $\times$  78 mm  $\times$  84 mm) of the desiccant container.

The standard kit contains two pairs of rechargeable desiccant packs. This is so you can immediately replace the desiccant in the instrument with re-activated packs.

The desiccant packs can be re-activated by baking them in an oven at 250 °C for approximately 8 hours. They should be cooled in a dry atmosphere. For optimum results, re-activate the packs immediately before re-use.

## Purging the Spectrometer

Under most circumstances, you do not need to purge the optical system. However, after performing any maintenance tasks that involved opening the main cover, you may purge the optical system to remove water vapor and  $CO_2$  that entered while the system was open.

Purge the sample compartment if you need to make sure that no residual water vapor or  $\mbox{\rm CO}_2$  peaks are visible in the spectrum.

There are two separate sets of connectors for purge gas lines, one for the sample compartment and one for the optical system. You can purge with either dry air or nitrogen. Both remove water vapor; however, nitrogen is preferable because it also removes atmospheric carbon dioxide.

A typical cylinder of dry nitrogen (or dry air) stores 6.26 m<sup>3</sup> at 1.4  $\times$  104 kPa (220 ft<sup>3</sup> at 2200 lbf/in<sup>2</sup>). Make sure that the gas is free of oil, water, or dirt particles larger than 25  $\mu m$  (0.001 inch).



Do not site the instrument in a poorly ventilated area if nitrogen will be used as a purge gas.

Oxygen depletion in an enclosed space does not trigger a gasping reflex, and errors of judgment, confusion, or unconsciousness can occur in seconds and without warning.



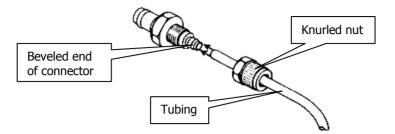
Do not use a flammable gas to purge the instrument. The spectrometer contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.



Never connect the purge tubing directly to a gas cylinder or other high pressure supply; always use a pressure regulator and set the pressure to a maximum of 1  $lbf/in^2$  (6.9 kPa) before you start the flow.

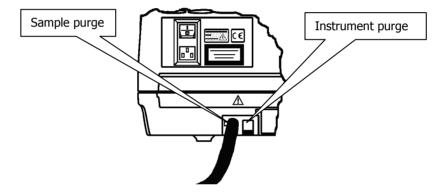
A length of clear plastic tubing (4 mm internal diameter) will be required to transfer the gas from the gas bottle to the instrument purge connectors.

1. The tubing is connected to the instrument by a universal pipe fitting which is secured to the tubing with a nut. Two sets of fittings are supplied with the instrument. Assemble the fittings to the tubing as illustrated in Figure 28.



#### **Figure 28 Purge fittings**

- 2. Tighten the nut, ensuring it is not over tightened.
- 3. Push the connector on the end of the tubing into the purge connector of the compartment to be purged (Figure 29).



#### Figure 29 Connector fitted to purge port

4. Connect the free end of the tubing to the gas regulator.

**NOTE:** Ensure the regulator is set to a pressure not greater than 6.9 kPa (1 lbf/in<sup>2</sup>).

5. Open the gas flow valve on the regulator until a flow rate of 28 l/minute (1 ft<sup>3</sup>/minute) is achieved.

The instrument compartment is purged in 10 minutes. The sample compartment is purged in 2 minutes.

6. Once purging is complete turn off the gas supply.

7. Disconnect the fitting from the instrument by pushing the locking clip located on the side of the purging port (Figure 30).

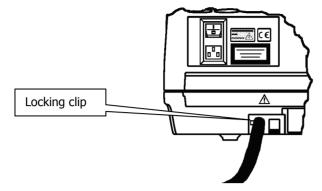


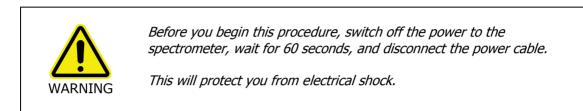
Figure 30 Disconnect the locking clip

## Changing the External Fuse

Very occasionally, a fuse may fail with age and will need to be changed.

**NOTE:** If fuses fail repeatedly, there is an electrical fault: disconnect the power supply and contact your PerkinElmer Service Engineer.

There is one spare fuse in the fuse drawer. If you need more, order 2 A, 250 V Time Lag fuses (part number 04970839) from PerkinElmer. You must only replace the fuse with one of this type and rating. Do not use makeshift fuses and do not short-circuit fuse holders.



The external fuse drawer is located at the rear of the instrument between the power switch and the power socket (Figure 31).

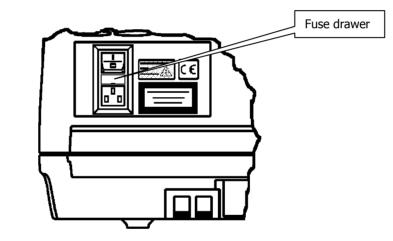
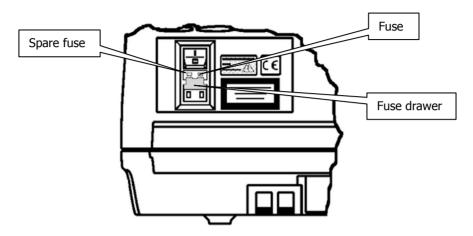


Figure 31 Fuse drawer closed

- 1. Lever out the fuse drawer so that it swings down over the power socket. The fuse is in the right hand slot.
- 2. Remove the old fuse and discard it.
- 3. Fit the new fuse into the slot (Figure 32).



#### Figure 32 Fuse fitted; drawer open

- 4. Close the drawer. The new fuse is now installed.
- 5. Reconnect the power cable and switch on the instrument.

## **Advanced Maintenance**

## **Opening the Main Cover**

To perform most maintenance tasks, you have to open the main cover of the spectrometer.

**NOTE:** If you have any samples or reference materials in the storage compartment, you are advised to remove these before opening the main cover.



Switch off the mains power supply to the spectrometer, wait 60 seconds and disconnect the power cable before you open the cover of the spectrometer. This makes sure that you are safe from electrical shock and laser radiation.

# CAUTIONDo not open the main cover if the humidity is >80% relative humidity for<br/>an instrument fitted with KBr optics.The humidity sensitive optics will be damaged if subjected to a relative<br/>humidity in excess of the specified levels.

The main cover is hinged at the back of the instrument and opens from the front. Figure 33 identifies the locking bolts, which are on the front of the instrument.



#### Figure 33 Main cover locking bolts

- 1. Switch off the power supply to the spectrometer.
- 2. Wait for 60 seconds.
- 3. Disconnect the power cable.
- 4. Remove the sample compartment cover, if fitted; open the cover, press on the cover retaining clip and then pull the cover vertically to remove it.



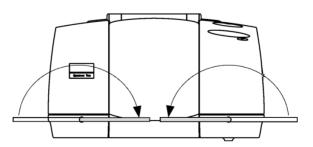
#### Figure 34 Removing the sample compartment cover

5. Remove the fitted sampling accessory, by pulling the release handle towards you and sliding the accessory towards you.



#### Figure 35 Removing the sampling accessory

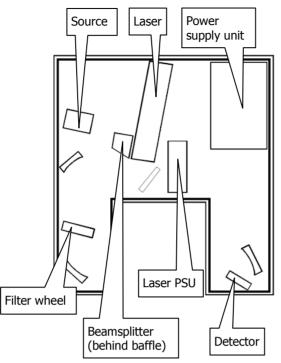
6. Undo the two locking bolts on the front of the instrument using the hexagonal wrench supplied; insert the wrench, so that the free end is pointing horizontally away from the instrument and then rotate the wrench 180° in the direction indicated by the arrows in the figure.



#### Figure 36 Undoing the locking bolts

- 7. Lift the main cover from the front.
- 8. Ensure the cover is fully open and retained by the stay.

Perform the necessary maintenance inside the instrument.
 Figure 37 illustrates the primary component parts of a Frontier Optica FT-IR spectrometer.



#### Figure 37 Frontier Optica FT-IR component parts

- 10. Close the cover.
- 11. Lock the two locking bolts by inserting the wrench into each bolt in turn and rotating it opposite to the direction indicated by the arrows in Figure 36.
- 12. If required, reinstall the sampling accessory by sliding it on the ledge and pushing it into the sample compartment until it engages with the connector.
- 13. If required, refit the sample cover by inserting the hinge into the grooves and pushing the cover downwards until the clip engages.
- 14. Reconnect the power cable and switch the power back on.
- 15. If required change the desiccant (see page 62), and/or purge the instrument (see page 66).If the cover is left open for more than 1 hour, the desiccant should be replaced.

# Replacing the Source

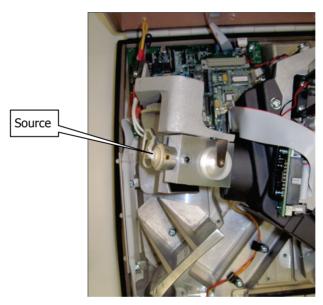


Switch off the mains power supply to the spectrometer, wait 60 seconds and disconnect the power cable before you open the cover of the spectrometer. This makes sure that you are safe from electrical shock and laser radiation.



Due to its high operating temperature allow sufficient time for the source to cool before attempting to remove it.

1. Open the main cover of the instrument as detailed on page 72 and identify the source (Figure 38).



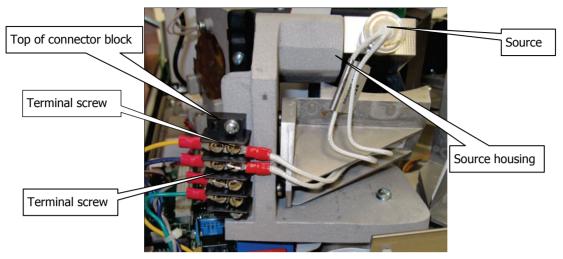
#### Figure 38 Source location



Caution, hot surface.

The source housing and source itself will be hot if recently switched on. Allow to cool before performing the following procedure.

2. Slacken the two terminal screws (Figure 39) securing the wires leading to the source. Disconnect the white MIR source wires from the connectors.



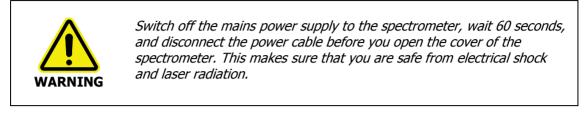
#### Figure 39 Terminal screws

- 3. By grasping the round metal source body, NOT the wires, remove the source from its housing by pulling, noting its installed position.
- 4. Install the new source in its housing, by pushing in until it clicks into place.
- 5. Reconnect the two wires to the terminals and secure by tightening the two terminal screws.
- 6. Close and secure the main cover. Refer to page 74, steps 10 to 15.

Allow the source temperature to stabilize for approximately 2 hours before using the instrument.

# Installing/Replacing Windows

The following procedure describes how to install a window in one of the external beam ports. The details apply equally to windows in the sample compartment.



- 1. Open the main cover of the instrument, as detailed on page 72.
  - Using the hexagonal wrench supplied with the new window kit, slacken and remove the screws and washers securing the beam port cover or current window to the main cover.

Remove the screws carefully, and ensure that the washers do not fall into the instrument.

- Remove the beam port cover or current window and seal. Retain for further use.

CAUTION

Be careful not to get moisture on the optical surface of the window. Do not touch or breathe on the optical surface of the window.

2. Ensure the seal is fitted to the window and is correctly seated (Figure 40).

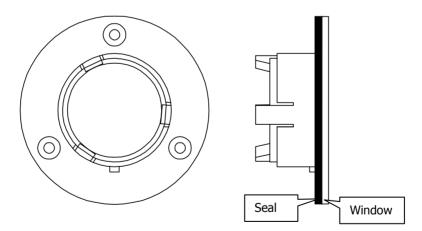
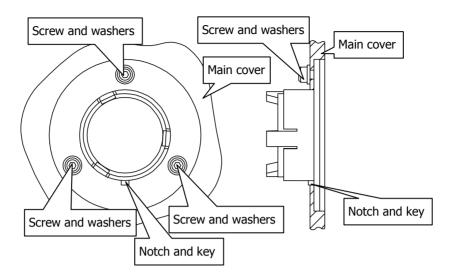


Figure 40 Seal fitted to window

3. Fit the window to the main cover from the outside in.

Ensure the seal is fully seated and the key on the window lines up with the notch in the main cover.



#### Figure 41 Window installed in main cover

- 4. Secure the window to the main cover by fitting the screws and washers and tightening the screws using the hexagonal wrench (Figure 41).
- 5. Close and secure the main cover. Refer to page 74, Steps 10 to 15.

# Installing Filters in the Filter Wheel

The following procedure describes how to install a filter in the filter wheel. The same procedure should be followed when replacing a filter or the methane cell.

The filter wheel assembly is removed from its mounting and placed on the standard sample slide baseplate.

1. Set the **Filter Wheel** to the Position 1 on the Setup Instrument BeamPath tab in the Spectrum software.

Position 1 will be labelled as **None 15000 – 0 cm**<sup>-1</sup> and be the first option in the dropdown list.



Switch off the mains power supply to the spectrometer, wait 60 seconds, and disconnect the power cable before you open the cover of the spectrometer. This makes sure that you are safe from electrical shock and laser radiation.

2. Open the main cover of the instrument as detailed on page 72 and identify the filter wheel.

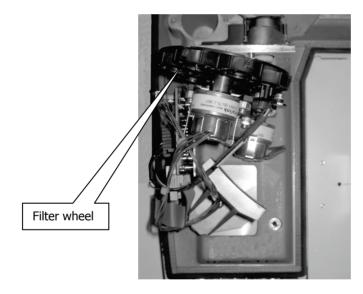


Figure 42 Filter wheel location

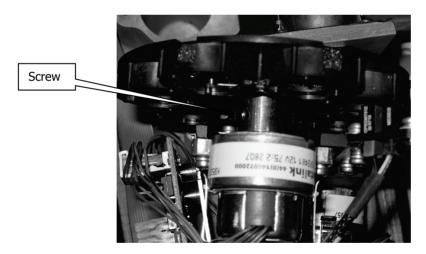
3. Install the standard sample holder baseplate, but remove the sample holder itself by unscrewing the knurled screw.



#### Figure 43 Knurled screw

4. To remove the filter wheel, loosen the set screw that secures it to its shaft using a 1.5 mm Allen key, and then gently ease the filter wheel off the shaft, rotating the filter wheel as required to clear the filter wheel from the other instrument components. Take care not to remove the spacer ring from the spindle, as this may be lost.

**NOTE:** If the set screw is not accessible, you may not have moved the filter wheel to **Position 1** as described in Step 1.



#### Figure 44 Filter wheel securing screw

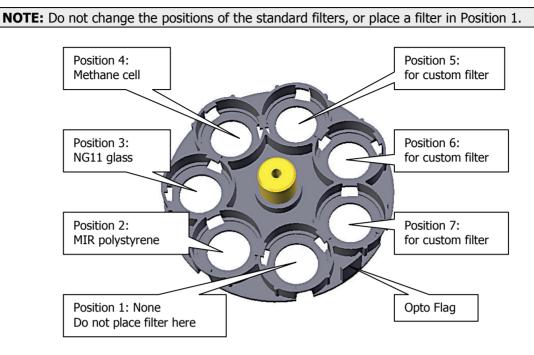
CAUTION

Avoid touching the filters.

Some of the filters are quite difficult to see.

5. Place the assembly face down on the sample holder baseplate.

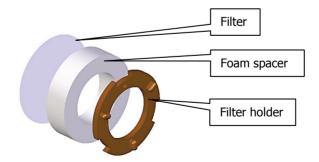
By default, three of the seven filter wheel positions are filled, leaving Positions 5, 6 and 7 are available for your custom filters.



#### Figure 45 Filter wheel positions

- 6. Working clockwise around the filter wheel, identify the next available filter position.
- 7. Release the filter holder by turning it about 30 degrees counter-clockwise, and then remove the filter holder and foam spacer.
- 8. Place the filter in the hole, place the foam spacer on top of it, and then fit the filter holder. Figure 46 illustrates the assembly sequence.

Align the notches of the holder with the indents in the filter wheel. You must twist the holder clockwise to lock it to the filter wheel.



#### Figure 46 Filter, foam spacer and filter holder

When fitted correctly, the small hole in the filter holder is close to the outer edge of the filter wheel.

9. Refit the filter wheel to its spindle, gently pressing it against the spacer ring, and secure it with the set screw.

CAUTIONMake sure that you tighten the set screw onto the flat of the shaft.If the set screw is tightened onto a round portion of the shaft the filter<br/>wheel may loosen.

- 10. Refit the sample holder onto the baseplate with the knurled screw.
- 11. Close the main cover (refer to Steps 10 to 15 on page 74).
- 12. Select the filter you would like to use in the beampath from the Filter Wheel drop-down list in the Setup Instrument BeamPath tab in Spectrum software.

**NOTE:** If you wish to run a background scan with a filter in place, you must set the **Scan Type** to **Background** on the Setup Instrument Basic tab, rather than using the

**Background** toolbar button **I**. See the Spectrum on-screen Help for more information.

# Replacing the Laser and Power Supply

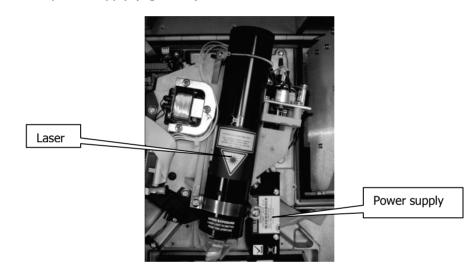


Switch off the main power supply to the spectrometer, wait 60 seconds and disconnect the power cable before you open the cover of the spectrometer. This makes sure that you are safe from electrical shock and laser radiation.



Do not attempt to separate the Laser from the power supply. The Laser retains an electrical charge even when the main power is switched off.

1. Open the main cover of the instrument as detailed on page 72 and identify the laser and laser power supply (Figure 47).



#### Figure 47 Laser and power supply

- 2. Slacken the two screws securing the laser power supply.
- 3. Disconnect the thin black and red cables from the board connector which is located under the rear of the laser assembly (Figure 48).



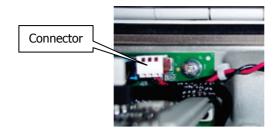
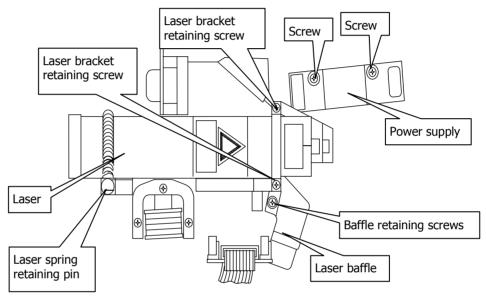


Figure 48 Laser Board connector

4. Unhook the spring and remove the two screws on the retaining bracket, as shown in Figure 49.



#### Figure 49 Laser and power supply installation

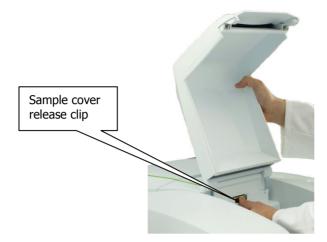
- 5. Remove the laser and power supply; noting the way the cabling is routed.
- 6. Install the new laser and power supply.
- Ensure the laser is pushed fully home to the stop at the front of the housing. The laser must be installed so that the yellow laser warning label is facing directly upwards.
- 8. Refit the laser retaining bracket and secure with the two securing screws.
- 9. Secure the spring on the retaining pin.
- 10. Reconnect the PSU Laser cable to the board connector.
- Secure the laser power supply with the two securing screws.
   Make sure that the laser cabling is secured so that it does not get trapped in the cover.
- 12. Close and secure the main cover. Refer to page 74, steps 10 to 15.

**NOTE:** Allow the Frontier Optica FT-IR spectrometer to equilibrate for approximately 2 hours before using the instrument.



# Appendix 1: Changing the Sampling Accessory

1. Remove the sample area cover if fitted by opening the cover, pressing the clip and pulling the cover vertically to remove (Figure 50).



#### Figure 50 Removing the sample area cover

2. Remove the current sampling accessory by pulling the release handle (under the baseplate of the accessory) towards you and then sliding the accessory towards you (Figure 51).



Figure 51 Removing a sampling accessory

3. Install the new accessory (Figure 52) by sliding it onto the ledge and pushing it into the sample compartment until it engages with the connector.



#### Figure 52 Installing the sampling accessory

Spectrum automatically recognizes which accessory is installed, and displays the accessory information on the Setup Instrument tabs.

| Setup Instrument Auto-Name            | Setup Inst | trument Data Collection  | Setup Instrument BeamPath | Setup Instrument Advanced | B Setup Instrument B                           | lasic    |
|---------------------------------------|------------|--|---------------------------|---------------------------|--|----------|
| Actions<br>Restore Def<br>Load and Sa |            | Settings<br>Abscissa Units<br>Wavenumber V<br>Ordinate Units<br>&T V | Start (cm-1) 4000         | 4 💌 S.                    | can Type<br>ample v<br>ccumulations<br>Scans v |          |
|                                       |            | Accessory  | Shu                       | ttle                      |  |          |
|                                       |            | Item   |                           | Value                     |  |          |
|                                       |            | Move Shuttle   |                           | OUT                       | ×  |          |
|                                       |            | Sampling   |                           | Not Specified             | ~  | <u>.</u> |
|                                       |            |  |                           |                           |  |          |

Figure 53 Setup Instrument Basic tab

# Appendix 2: Instrument Self-Checks

**NOTE:** It can take the instrument up to 2 hours to equilibrate when switched on after being switched off overnight. To save time, we suggest that you leave the instrument switched on at all times.

 When you switch on the instrument, the instrument display provides this sequence of messages:

> Initializing Initializing Checking Program Integrity Checking Instrument Configuration Checking Source Checking Laser Checking Scan Checking Calibration Initialization Complete.

 When initialization is complete the last message fades, leaving the instrument identity message:

*PerkinElmer Frontier FT-IR* When connected to a PC, the instrument display adds *Ready*.

• When collecting data, the instrument display provides prompts generated by the PerkinElmer application software.

#### Initialization errors

If your instrument generates one of the following error messages, switch off the instrument, then switch the instrument on again. Consult your PerkinElmer Service Engineer if the problem persists.

| Error message                      | Action   |
|------------------------------------|--|
| Program Integrity Failed           | The instrument's firmware may be corrupt, so must be reinstalled.  |
| Instrument Configuration<br>Failed | Suggests that one or more internal devices is failing. If<br>the problem persists, note any associated error<br>messages and consult your PerkinElmer service<br>representative. |
| Scan Failed                        | If the problem persists, note any associated error messages and consult your PerkinElmer service representative.   |
| Laser Failed<br>Replace Laser      | Refer to <i>Replacing the Laser and Power Supply</i> on page 83.   |
| Source Failed<br>Replace Source    | Refer to <i>Replacing the Source</i> on page 75.   |
| Calibration Failed                 | Too little energy may be reaching the detector. Make sure the sample compartment is clear.   |

# *Appendix 3: Instrument Performance Validation Kit*

The MIR Performance Validation Kit (L1250404) available for the Frontier Optica FT-IR contains a polystyrene reference sample.

Macros are supplied with Spectrum software (version 10.3 or later) that can be used with the Performance Validation kits to produce a report certifying your instrument.

# Appendix 4: Decontamination and Cleaning

Before using any cleaning or decontamination methods except those specified by PerkinElmer, users should check with PerkinElmer that the proposed method will not damage the equipment.

#### Decontamination

#### Customers wishing to return instrumentation and/or associated materials to PerkinElmer for repair, maintenance, warranty or trade-in purposes are advised that all returned goods must be certified as clean and free from contamination.

The customer's responsible body is required to follow the "Equipment Decontamination Procedure" and complete the "Certificate of Decontamination". These documents are available on the PerkinElmer public website:

http://las.perkinelmer.com/OneSource/decontamination.htm

Alternatively, if you do not have access to the internet contact Customer Care:

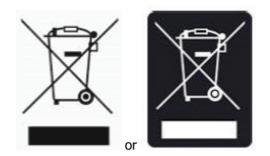
| Customer Care USA:        | 1-800-762-4000    | (inside the USA)  |
|---------------------------|-------------------|-------------------|
| (8:30 a.m. – 7 p.m. EST ) | (+1) 203-925-4602 | (outside the USA) |
| Customer Care Canada:     | 800-561-4646      |                   |
| Customer Care EU:         | 0800 40 858       | (Brussels)        |
|                           | 0800 90 66 42     | (Monza)           |

If you are located outside of these regions, please call your local PerkinElmer sales office for more information.

#### Cleaning the Instrument

Exterior surfaces may be cleaned with a soft cloth, dampened with a mild detergent and water solution. Do **not** use abrasive cleaners or solvents.

# Appendix 5: WEEE Instructions for PerkinElmer Products



A label with a crossed-out wheeled bin symbol and a rectangular bar indicates that the product is covered by the Waste Electrical and Electronic Equipment (WEEE) Directive and is not to be disposed of as unsorted municipal waste. Any products marked with this symbol must be collected separately, and in accordance with the regulatory guidelines in your area.

The objectives of this program are to preserve, protect and improve the quality of the environment, protect human health, and utilize natural resources prudently and rationally. Specific treatment of WEEE is indispensable in order to avoid the dispersion of pollutants into the recycled material or waste stream. Such treatment is the most effective means of protecting the customer's environment.

The requirements for waste collection, reuse, recycling, and recovery programs are set by the regulatory authority at your location. Contact your local responsible person (such as your laboratory manager) or authorized representative for information regarding applicable disposal regulations.

See the PerkinElmer web address below for information specific to PerkinElmer products, and contact details for the Customer care department in your region.

http://las.perkinelmer.com/OneSource/Environmental-directives.htm

Products from other manufacturers may also form a part of your PerkinElmer system. These other manufacturers are directly responsible for the collection and processing of their own waste products under the terms of the WEEE Directive. Please contact these manufacturers directly before discarding any of their products.

Consult the PerkinElmer web site (above) for manufacturer's names and web addresses.

# Index

# A

| About this manual      | 6  |
|------------------------|----|
| Accessory              |    |
| Changing               | 86 |
| Release handle         | 86 |
| Apodization            |    |
| Theory                 | 54 |
| Atmospheric suppresion | 45 |
| AVI correction         | 47 |
|                        |    |

# В

| B-stop |    |
|--------|----|
| Theory | 53 |

# С

| Capacitors 16                      |
|------------------------------------|
| Cleaning 60                        |
| Display 60                         |
| External 60                        |
| Cleaning the instrument            |
| Communication ports 28             |
| Communications ports               |
| Component parts 74                 |
| Condensation 61                    |
| Connecting to electrical supply 37 |
| Connecting to the PC 35            |
| Conventions                        |
| Notes, Cautions and Warnings 7     |
| Text                               |
| Cooling 14                         |
|                                    |

# D

| Decontamination     | 91     |
|---------------------|--------|
| Desiccant           |        |
| Changing            | 63     |
| Disposable          | 64     |
| Indicator           | 34, 62 |
| Rechargeable        |        |
| Removed             |        |
| Stowed              | 65     |
| Desiccant cover     |        |
| Captive screws      | 64     |
| Desiccant indicator |        |
| Display             | •      |
|                     |        |

| E                          |  |
|----------------------------|--|
| Electrical supply inlet 38 |  |
| EMC                        |  |
| Compliance 22              |  |
| EC Directive 22            |  |

| FCC rules           | 22 |
|---------------------|----|
| Standard EN 61326-1 | 22 |

# F

| FCC rules and regulations 22      |
|-----------------------------------|
| Filter wheel                      |
| Filter 81                         |
| Filter holder 81                  |
| Foam spacer 81                    |
| Installing filters 79             |
| Location79                        |
| Retaining screws                  |
| Flammable solvents and samples 15 |
| Fuse                              |
| Changing69                        |
| Drawer 69                         |

# G

| Go button      | 26 |
|----------------|----|
| Guided tour of | 24 |

### Н

| HTML help | 6 |
|-----------|---|
| Humidity1 | 3 |

# Ι

| Initialization errors               | 9 |
|-------------------------------------|---|
| Installing software                 | 9 |
| Installing the instrument           | 9 |
| Instrument controls                 |   |
| Description26, 4                    | 4 |
| Display 20                          | 6 |
| Go button20                         | 6 |
| Instrument display and Go button 44 | 4 |
| IPV                                 | 0 |
|                                     |   |

### J

| J-stop            |   |
|-------------------|---|
| In sample area 52 | 2 |

### L

| 20 |
|----|
| 21 |
|    |
| 17 |
| 33 |
| 34 |
| 34 |
| 34 |
|    |
| 34 |
|    |

| Installation             | 84 |
|--------------------------|----|
| Replacing                | 83 |
| Laser safety regulations |    |
| Lifting points           | 61 |
| Locking bolts            |    |
| Undoing                  | 73 |
| Look Ahead               | 48 |

### Μ

| Main cover    |    |
|---------------|----|
| Locking bolts | 72 |
| Opening       | 72 |
| Mains supply  |    |
| Fluctuations  | 13 |
| Moving        | 61 |

### Ν

| Nitrogen | 14 |
|----------|----|
|          |    |

#### 0

| Optical system | . 25 |
|----------------|------|
| Stability      | . 25 |

#### Ρ

| PC connection port<br>Phase correction | 35 |
|--|----|
| Theory                                 | 54 |
| Power switch                           | 28 |
| Purge fittings                         | 67 |
| Purge ports                            | 67 |
| Purging                                | 66 |
| Connectors                             | 66 |
| Gas regulator pressure                 | 67 |
| Purge gas lines                        | 66 |

# Q

| Quality Checks49 |
|------------------|
|------------------|

### R

| Requirements | 30 |
|--------------|----|
| Electrical   |    |
| Environment  | 30 |

### S

| Safety     |    |
|------------|----|
| Electrical | 16 |
| General    | 13 |

| Laser                                 |
|---------------------------------------|
| Laser radiation hazard                |
| Location and ventilation14            |
| Summary12                             |
| Use of flammable solvents and samples |
|                                       |
| Use of nitrogen14                     |
| Safety interlock25                    |
| Sample area cover                     |
| Release clip                          |
| Sample compartment                    |
| Sample properties                     |
| Near-parallel surfaces                |
| Non-planar samples                    |
| Small samples                         |
| Thickness                             |
| Tilt                                  |
| Wedge55                               |
| Sampling accessory                    |
| Changing                              |
| Removing                              |
| Shipping container                    |
| Opening                               |
| Software                              |
| Installation                          |
| Software control                      |
| Basics                                |
| Source                                |
| High operating temperature75          |
| Location                              |
| Replacing                             |
| Terminal screws                       |
| Switching on42                        |
|                                       |

### Т

| Temperature1         | 3 |
|----------------------|---|
| Top panel controls20 |   |

### U

```
Unpacking ......32
```

#### W

| WEEE Directive       | .92 |
|----------------------|-----|
| Windows              |     |
| in main cover        | .78 |
| Installing/Replacing | .77 |
| Seal                 | .77 |
| Windows Start menu   | .42 |