Spectrum GX
User's Guide

Release History

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CLASS 1 LASER PRODUCT
BS EN 60825-1 : 1994
IEC 825-1 :1993

C.D.R.H. Class IIa Laser Product
Avoid Long-Term Viewing
of Direct Laser Radiation.

WARNING

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

Contents

Warnings and Safety Information 1

Summary

The Spectrum GX has been designed to comply with a wide variety of international standards governing the safety of laboratory equipment. In routine use, the Spectrum GX poses 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 the instrument:

DO make sure that the Spectrum GX 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 lid of the optical module.

DO keep the Spectrum GX dry. Avoid spilling liquid into the instrument, especially into the top rear cover of the optical module, which contains a high-voltage supply. Clean all external spills immediately. If anything that is spilled enters the main body of the Spectrum GX, switch off the power and call a PerkinElmer Service Engineer.

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

DO NOT use a flammable gas to purge the Spectrum GX. The Spectrum GX 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 safety, starting on page 12.

General Safety

WARNING

If the equipment is used in a manner not specified herein, the protection provided by the equipment may be impaired.

The Spectrum GX has been designed and tested in accordance with PerkinElmer specifications and in accordance with the safety requirements of the International Electrotechnical Commission (IEC). The spectrometer conforms 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.

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

Whenever it is likely that the instrument is unsafe, it must be made 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.

WARNING

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

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

- Indoor use.
- Altitude up to 2000 m.
- 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.
- Electrical supply fluctuations not exceeding ± 10% of the nominal voltage.

Location and Ventilation

The Spectrum GX is installed by a Service Engineer, who will be able to advise on the siting of the system. To allow for adequate cooling, the system should not be sited near to room heating equipment, for example, central heating radiators. There should be a minimum gap of:

- 7 cm (3 inches) between any surface and the heat sink at the rear of the Spectrum GX optical module.
- 15 cm (6 inches) between any surface and the ventilation louvers on the instrument.

WARNING

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

Electrical Safety

Connect the Spectrum GX to a power supply line that includes a switch or other adequate means of disconnection from the electricity supply.

Only plug the Spectrum GX into an electrical 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 that 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 they are opened for any adjustment, replacement, maintenance or repair.

WARNING

Any interruption of the protective ground (earth) conductor inside or outside the instrument, or disconnection of the protective ground (earth) terminal, is likely to make the instrument dangerous.

The Spectrum GX has been designed and tested in accordance with PerkinElmer specifications and in accordance with the safety requirements of the International Electrotechnical Commission (IEC). The spectrometer conforms to IEC publication 61010-1 (*Safety Requirements for Electrical Equipment for Measurement, Control and Laboratory Use: General Requirements*) as it applies to IEC Class 1 (earthed) appliances and therefore meets the requirements of EC Directive 73/23/EEC, amended by 93/68/EEC.

The Spectrum GX has:

- An IEC Installation Category (Overvoltage Category) II classification – suitable for connection to local level power supplies.

- An IEC Pollution Degree 2 classification – usually only non-conductive atmospheric pollution of the equipment occurs; occasionally, however, a temporary conductivity caused by condensation must be expected.

EMC Compliance

EC directive

The Spectrum GX has been designed and tested to meet the requirements of the EC Directive 89/336/EEC. The Spectrum GX complies with the EMC standards EN 55 011 Class A (rf emissions) and EN 61326 (*Electrical Equipment for Measurement, Control and Laboratory Use – EMC requirements*).

FCC rules and regulations

This product is classified as a digital device used exclusively as industrial, commercial, or medical test equipment. It is exempt from the technical standards specified in Part 15 of the *FCC Rules and Regulations*, based on Section 15.103 (c).

Laser Safety Regulations

The Spectrum GX is a CDRH Class IIa, BS EN 60825-1/IEC 825-1 Class 1 laser product. The optical module contains a ClassII/2 Helium Neon (HeNe) laser, which emits visible, continuous wave radiation at a wavelength of 633 nm and has a maximum output power of less than 1 mW.

Some of the HeNe laser radiation, with a maximum power level of less than 3.9 μW, may be accessed in an infrared sample compartment. The laser is automatically shut down when the outer lid of the optical module is raised.

The Spectrum GX complies with the following laser safety regulations:

1. 21 CFR Chapter 1, Subchapter J, *Radiological Health*, Part 1040.10 - administered by the Center for Devices and Radiological Health, U.S. Department of Health and Human Services.

2. British Standard BS EN 60825-1 (1994) - *Safety of laser products; Part1. Equipment classification, requirements and user's guide.*

3. IEC Publication 825-1 (1993) - *Safety of laser products; Part1. Equipment classification, requirements and user's guide.*

Explanation of the Laser Radiation Hazard and Laser Radiation Classifications

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 the laser beam along its axis is termed intrabeam viewing.

Protection of the eye during accidental, momentary intrabeam viewing of a Class II/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 0.025 seconds.

CDRH regulations state that Class IIa levels of laser radiation are not considered to be hazardous if directly viewed for any period of time less than or equal to 1000 seconds.

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

The CDRH, BS EN 60825-1 and IEC 825-1 laser radiation classification limits are described below:

CDRH Class Limits

Classification	**For 633 nm Laser Radiation**
Class II	> 3.9 µW to 1000 µW
Class IIa	> 0.39 µW to 3.9 µW
Class I	0.39 µW

BS EN 60825-1 and IEC 825-1 Class Limits

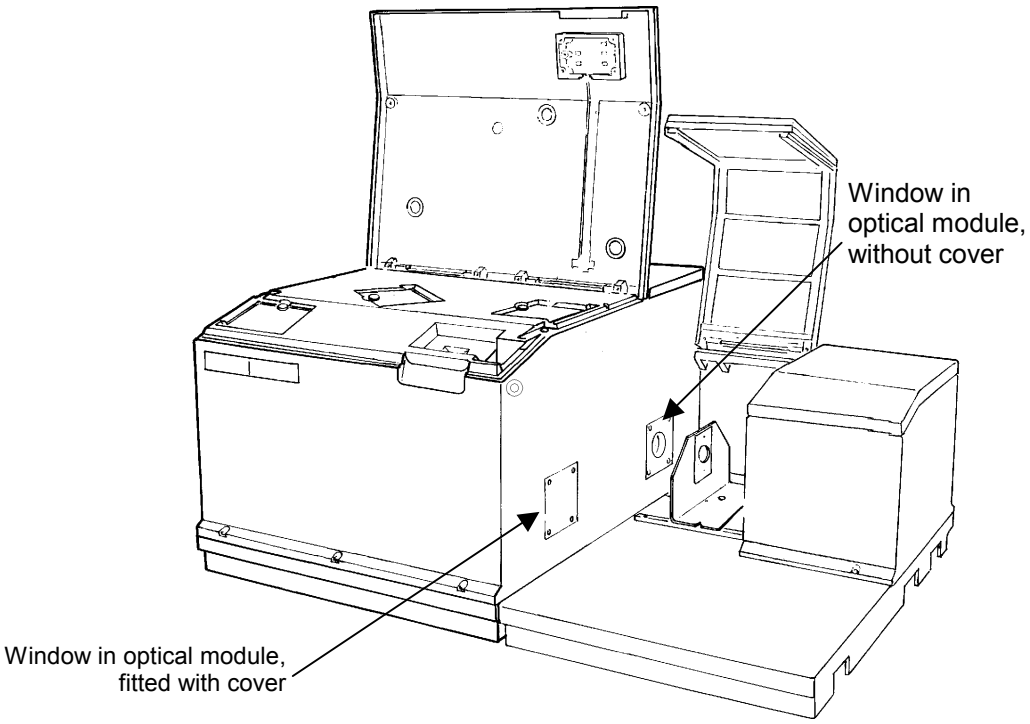
Classification	**For 633 nm Laser Radiation**
Class 2	> 6.8 µW to 1000 µW
Class 1	6.8 µW

WARNING

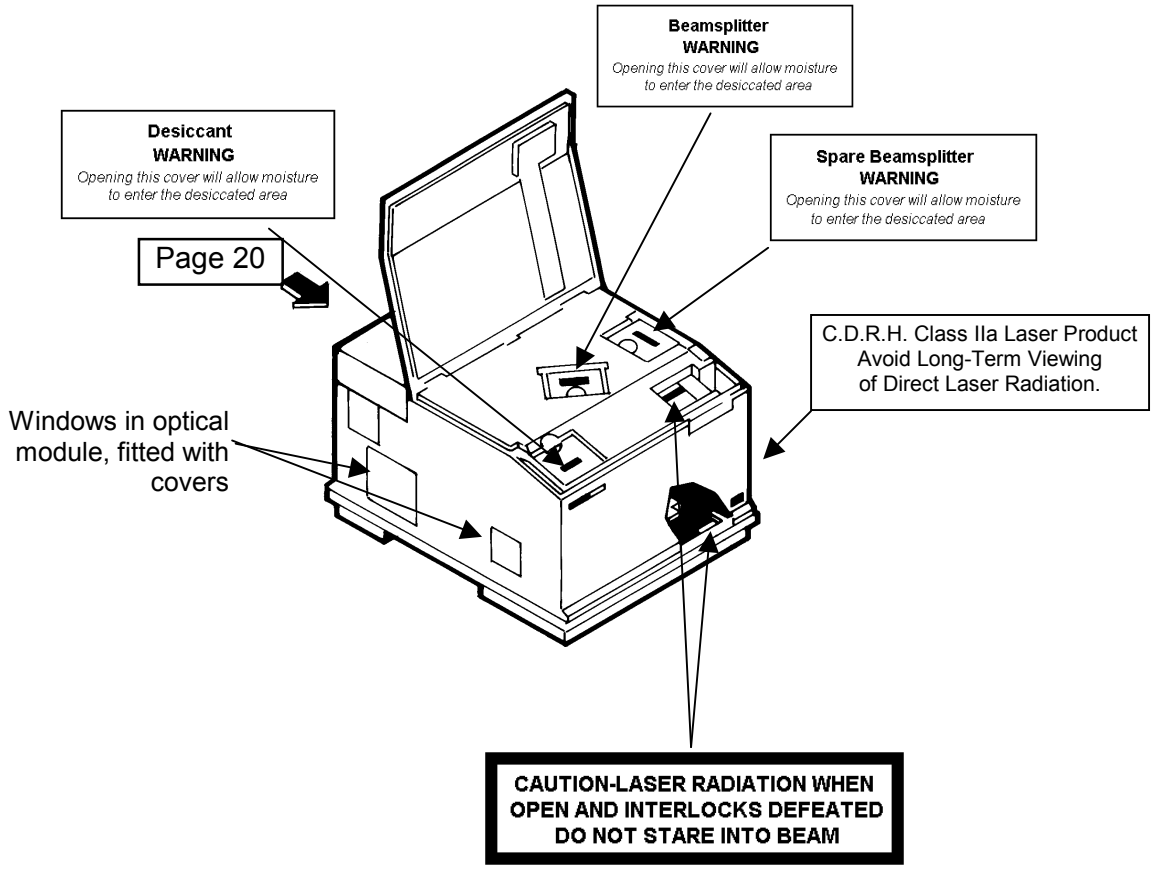
Do not stare into any laser beam. Staring into a laser beam (intrabeam viewing) can cause permanent damage to your eyes.

Laser Labels and Laser Apertures

The Spectrum GX is a modular instrument, which has up to four sample compartments. Sample area windows are located on both sides of the optical module (see illustrations below and on the next page). You can change the beam path using the Spectrum GX Beam Setup dialog – when the beam enters a sample compartment, laser radiation is emitted from the window in the optical module, into the sample compartment. If a sample compartment is not fitted, the sample area window is fitted with a cover.

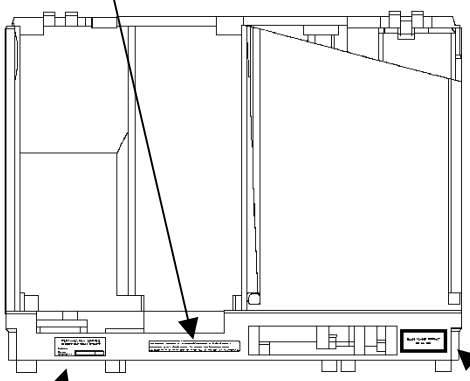


This manual contains information and warnings that must be heeded by the user to ensure safe operation of the instrument. Warning labels are fixed to the Spectrum GX in the locations shown in the diagrams below and on the following pages.



NOTE: *This label is for Service use only – the interlocks can only be defeated by a Service Engineer.*

This product conforms to all applicable standards of 21CFR Chapter 1. Subchapter J, Part 1040.10, Center for Devices and Radiological Health, U.S. Department of Health and Human Services, at the date of manufacture.



PerkinElmer™
instruments.
Serial Number
Date of Manufacture

CLASS 1 LASER PRODUCT
BS EN 60825-1 : 1994
IEC 825-1 :1993

View on Arrow on Page 19

Conventions 2

About This Manual

NOTE: *This manual equally applies to the Spectrum 2000 FT-IR. The term Spectrum GX has been used throughout to denote either instrument.*

This manual contains the following sections:

- Warnings and Safety Information.
- Conventions.
- An Overview of the Spectrum GX.
- Using the Spectrum GX.
- Maintenance of the Spectrum GX.
- Theory.
- Glossary.

This is a reference manual, and we assume that you are familiar with Spectrum and your Spectrum GX. If you have not used Spectrum before, we recommend that you work through the on-screen tutorials, which you can access by choosing **Learning Spectrum** from the Help menu. In particular tutorial 3 *Collecting Spectra* describes how to set scan parameters and collect spectra.

Spectrum has on-screen help, which you can access by choosing a command from the Help menu, or by clicking on the **Help** button on a dialog, as discussed in *HTML Help* on page 67.

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.

Notes, warnings and cautions

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

Caution
*We use the term CAUTION to inform you about situations that could result in **serious damage to the instrument** or other equipment. Details about these circumstances are in a box like this one.*

D

Caution (Achtung)
*Bedeutet, daß die genannte Anleitung genau befolgt werden muß, um einen **Geräteschaden** zu vermeiden.*

DK

Caution (Bemærk)
*Dette betyder, at den nævnte vejledning skal overholdes nøje for at undgå en **beskadigelse af apparatet**.*

E

Caution (Advertencia)
*Utilizamos el término **CAUTION** (ADVERTENCIA) para advertir sobre situaciones que pueden provocar **averías graves en este equipo** o en otros. En recuadros éste se proporciona información sobre este tipo de circunstancias.*

F

Caution (Attention)
*Nous utilisons le terme **CAUTION** (ATTENTION) pour signaler les situations susceptibles de provoquer de **graves détériorations de l'instrument** ou d'autre materiel. Les détails sur ces circonstances figurent dans un encadré semblable à celui-ci.*

I

Caution (Attenzione)
*Con il termine **CAUTION** (ATTENZIONE) vengono segnalate situazioni che potrebbero arrecare **gravi danni allo strumento** o ad altra apparecchiatura. Troverete informazioni su tali circostanze in un riquadro come questo.*

NL

Caution (Opgelet)
*Betekent dat de genoemde handleiding nauwkeurig moet worden opgevolgd, om **beschadiging van het instrument** te voorkomen.*

P

Caution (Atenção)
*Significa que a instrução referida tem de ser respeitada para evitar a **danificação do aparelho**.*

WARNING

Warning
*We use the term WARNING to inform you about situations that could result in **personal injury** to yourself or other persons. Details about these circumstances are in a box like this one.*

D

Warning (Warnung)
*Bedeutet, daß es bei Nichtbeachten der genannten Anweisung zu einer **Verletzung** des Benutzers kommen kann*

DK

Warning (Advarsel)
*Betyder, at brugeren kan blive **kvæstet**, hvis anvisningen ikke overholdes.*

E

Warning (Peligro)
*Utilizamos el término **WARNING** (PELIGRO) para informarle sobre situaciones que pueden provocar **daños personales** a usted o a otras personas. En los recuadros como éste se proporciona información sobre este tipo de circunstancias.*

F

Warning (Danger)
*Nous utilisons la formule **WARNING** (DANGER) pour avertir des situations pouvant occasionner des **dommages corporels** à l'utilisateur ou à d'autres personnes. Les détails sur ces circonstances sont données dans un encadré semblable à celui-ci.*

I

Warning (Pericolo)
*Con il termine **WARNING** (PERICOLO) vengono segnalate situazioni che potrebbero provocare **incidenti alle persone**. Troverete informazioni su tali circostanze in un riquadro come questo.*

NL

Warning (Waarschuwing)
*Betekent dat, wanneer de genoemde aanwijzing niet in acht wordt genomen, dit kan leiden tot **verwondingen** van de gebruiker.*

P

Warning (Aviso)
*Significa que a não observância da instrução referida poderá causar um **ferimento** ao usuário.*

An Overview of the Spectrum GX 3

Introduction to FT-IR

The Advantages of FT-IR Spectroscopy

In principle, an interferometer has several basic advantages over a classical dispersive instrument. These advantages are:

Multiplex advantage (Fellgett advantage)

All source wavelengths are measured simultaneously in an interferometer, whereas in a dispersive spectrometer they are measured successively. A complete spectrum can be collected very rapidly and many scans can be averaged in the time taken for a single scan of a dispersive spectrometer.

Throughput advantage (Jacquinot advantage)

For the same resolution, the energy throughput in an interferometer can be higher than in a dispersive spectrometer, where it is restricted by the slits. In combination with the Multiplex Advantage, this leads to one of the most important features of an FT-IR spectrometer: the ability to achieve the same signal-to-noise ratio as a dispersive instrument in a much shorter time.

Connes advantage

The wavenumber scale of an interferometer is derived from a HeNe (helium neon) laser that acts as an internal reference for each scan. The wavenumber of this laser is known very accurately and is very stable. As a result, the wavenumber calibration of interferometers is much more accurate and has much better long-term stability than the calibration of dispersive instruments.

Negligible stray light

Because of the way in which the interferometer modulates each source wavelength, there is no direct equivalent of the stray light found in dispersive spectrometers.

Constant resolution

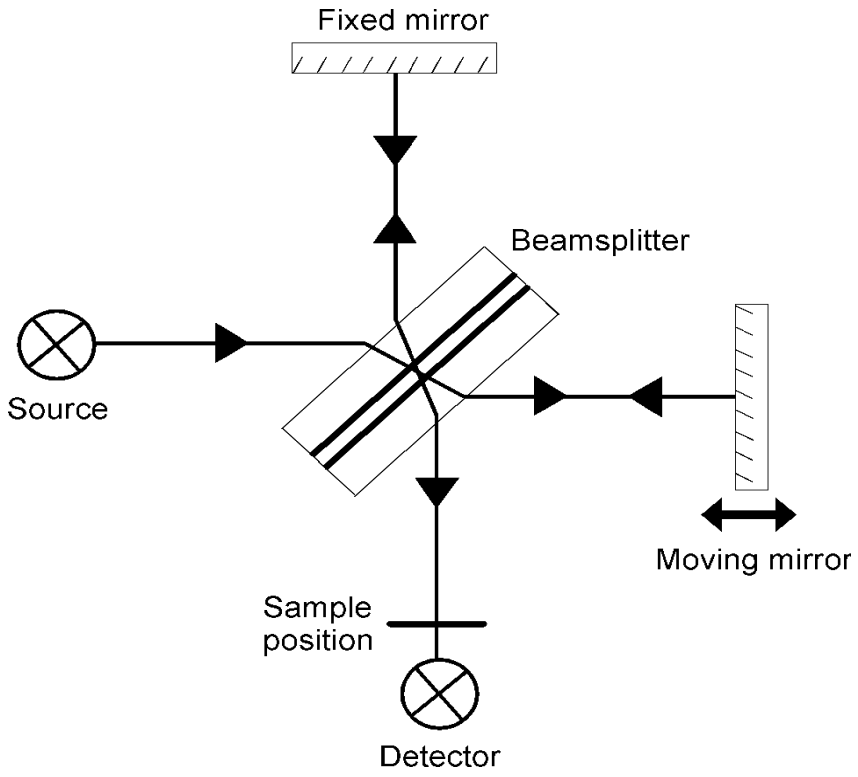
Resolution is constant at all wavenumbers in the defined spectral range but the signal-to-noise ratio varies across the spectrum. FT-IR instruments have a much higher optical throughput than dispersive instruments and do not use slits to define the resolution. Instead, the resolution is defined by the J-stop (Jacquinot stop) aperture size, which does not change during data collection. In dispersive instruments, throughput is typically optimized by adjusting the slit width during the scan. Thus, signal-to-noise is constant but resolution varies.

No discontinuities

Because there are no grating or filter changes, there are no discontinuities in the spectrum.

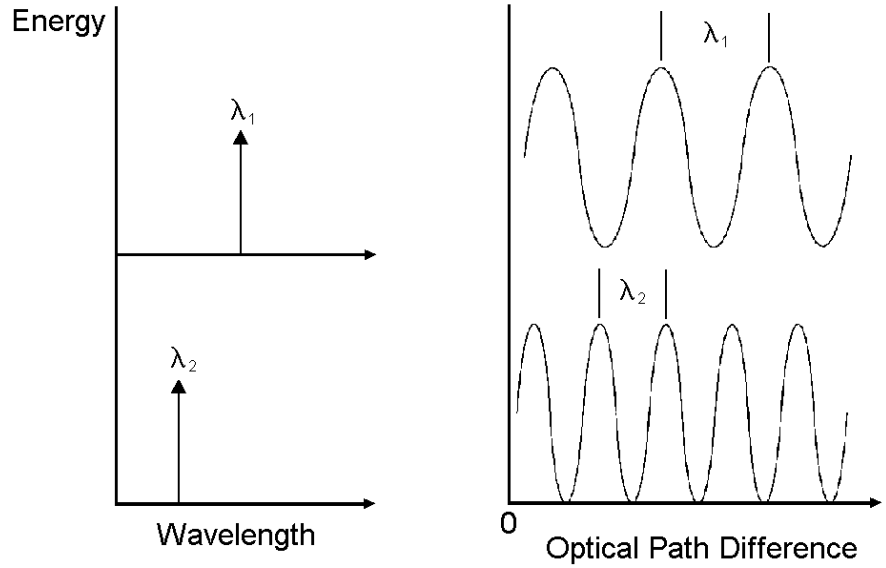
The Principle of the Michelson Interferometer

The essential component of an interferometer is a system for splitting a beam of radiation into two and then recombining the two beams after introducing a path difference. This combined beam passes through the sample to the detector. Division of the beam is achieved with a beamsplitter that transmits about 50% and reflects about 50% of the radiation. One part of the beam goes to a fixed mirror and the other to a mirror that can be moved to introduce a varying path difference.

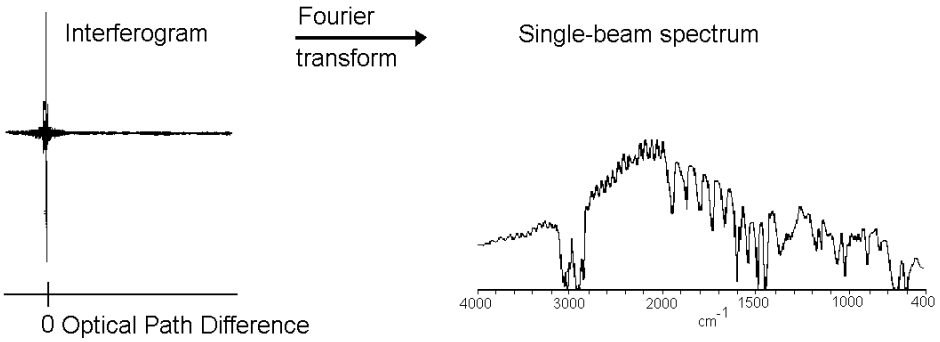


When the beams are recombined, an interference pattern is obtained as the path difference is varied. On recombination, interference between the two beams causes the energy reaching the detector to be modulated as the path difference changes. For a source with a single optical wavelength, this interference (or interferogram) is sinusoidal, with maxima when the two beams are exactly in phase and zero when the two are 180 degrees out of phase. The spacing between the maxima corresponds to a change in path difference proportional to the wavelength of the source (see *OPD Velocity* on page 121). The modulation frequency (f) is proportional to the wavelength and the mirror velocity (v):

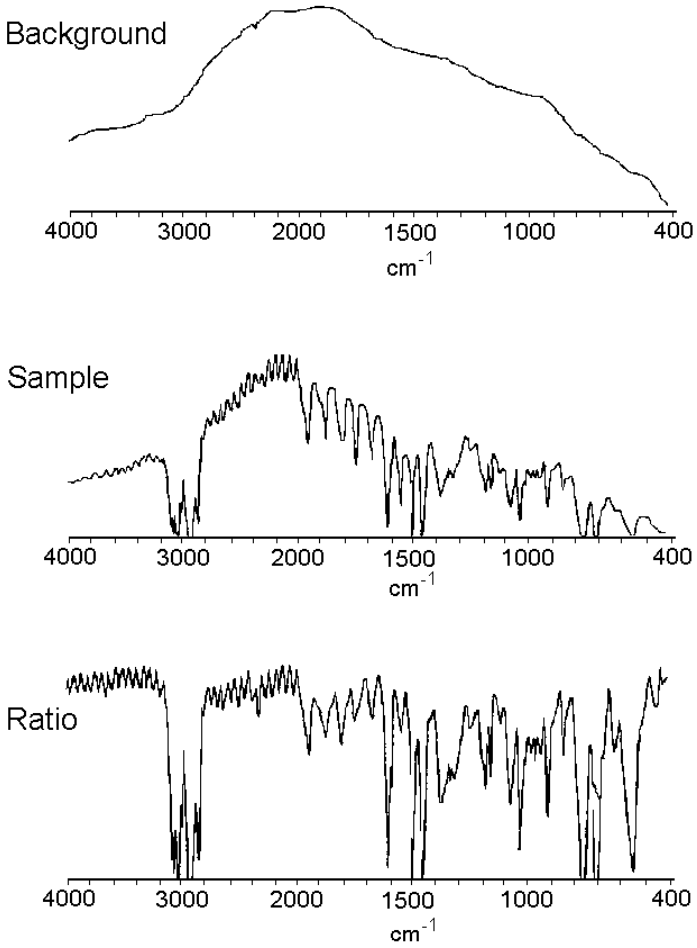
$$f(\mathrm{Hz}) = \frac{2v(\mathrm{cm/s})}{\lambda\ (\mathrm{cm})}$$



For a broad band source, the interference pattern is the sum of the cosine waves for all the wavelengths emitted. This interferogram consists of a strong signal at the point where the path difference is zero, falling away rapidly on either side. The customary spectrum, showing energy as a function of wavenumber, can be obtained from the interferogram by the mathematical process of Fourier Transformation.



When no sample is present this gives a single beam spectrum, the overall shape of which is largely determined by the characteristics of the beamsplitter and source. Normally, interferometers operate by first recording this background and then ratioing the sample spectrum against it.



Generating the Interferogram

Because interferometers operate in a single-beam mode, greater stability is required than in classical double-beam spectrophotometers. While adequate stability can be achieved by appropriate design, the presence of atmospheric absorption is a major inconvenience. Any change in water or carbon dioxide concentration results in extraneous bands in the final ratioed spectrum. When spectrometers are purged, great care has to be taken to ensure that the degree of purge is the same for sample and background measurements.

Optical components

The most commonly used beamsplitter is a plate of KBr (Potassium Bromide) with a Ge (germanium) coating. This covers a range of about 7800 to 400 cm^{-1}. To avoid refractive index effects, both beams in the interferometer must pass through the same thickness of KBr, so a matching compensator plate is needed. The path difference must be the same for all parts of the beam, which means that any divergence of the beam must be limited. The degree of divergence that can be tolerated depends on the resolution required. Higher resolution requires lower divergence to avoid variations in path difference for different parts of the beam. This is achieved by restricting the size of the beam with a variable aperture called a J-stop. One effect of the J-stop is similar to that of the slits in a classical spectrometer: at higher resolution the energy throughput is reduced. When the resolution is doubled, the energy reaching the detector is halved.

The two beams returning to the beamsplitter must be superimposed exactly in order to generate the interferogram. The optical elements of the interferometer have to be carefully aligned to achieve this and to ensure that the path difference is uniform across the beam. This alignment has to be maintained as the interferometer scans. One of the most critical aspects of interferometer design is to avoid any tilt or shear (wobble) of the moving mirror during the scan, because this affects alignment and distorts the final spectrum.

Measuring the Interferogram

The interferogram is measured by recording the detector signal as a function of the path difference between the two beams. The signal has to be sampled at precise intervals corresponding to equal steps in path difference. For signal averaging, successive interferograms have to be measured at exactly the same points. This is achieved by using a HeNe laser as a reference. Monochromatic radiation from the laser at 632.99 nm traverses the same optical path as the infrared beam. A separate detector measures the interferogram produced by the laser, giving a cosinusoidal signal with maxima separated by the laser wavelength. This signal is used to trigger the sampling of the infrared signal very reproducibly.

Path difference

Measurement of the interferogram has to start on one side of the point of zero path difference and continue out on the other side to a maximum path difference that depends upon the required resolution. The laser signal cannot be used to identify the point of zero path difference, so this is found by locating the maximum signal in the infrared interferogram. Although the laser signal precisely monitors changes in path difference, it does not sense the direction in which the mirror is moving and so loses count at the end of each scan. The absolute path difference has to be re-established for each scan so that successive scans start at the same point. One means of doing this has been to use a white light source and detector to produce a sharp spike interferogram for the infrared radiation. This signal is used as a reference point from which to start counting the laser signal.

Recently, an improved system has been introduced, using two laser detectors from which the path difference can be monitored continuously, even when the scan changes direction. This eliminates the need for the white light interferometer, or for any other means of re-establishing the absolute position for each scan. It also opens up the possibility of scanning the interferometer continuously in both directions. The normal procedure has previously been to scan in one direction only and then return rapidly to the starting point to begin the next scan.

Processing the Interferogram

Fourier transformation

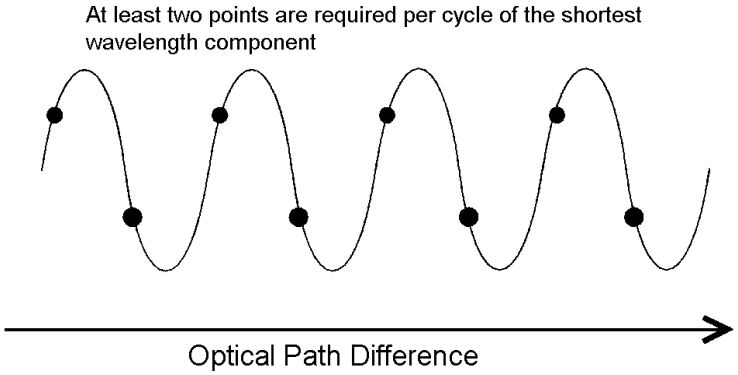
The spectrum is obtained from the interferogram by Fourier Transformation. This process analyzes the interferogram as the sum of a series of sine and cosine waves with discrete frequencies.

Spectral frequency range

The range of frequencies used in the Fourier analysis is limited by the way in which the interferogram is stored as a series of discrete points. There must be at least two data points for each cycle if a wavelength is to be recognized correctly (the Nyquist criterion).

This means that the interferogram must be measured at intervals equal to half of the shortest wavelength from the source to be measured. Radiation at shorter wavelengths may contribute to the interferogram, but will appear at the wrong place in the final spectrum. This effect is known as aliasing.

The problem is avoided by filtering out shorter wavelengths optically or electronically.



The sampling points for measuring the interferogram are derived from the laser signal. If one data point is recorded for each cycle of the laser signal, the data point separation is equal to the laser wavelength (in a vacuum) of 632.99 nm. The shortest wavelength that could be recognized in the spectrum would then be twice this laser wavelength, that is 1266.0 nm, corresponding to a wavenumber of 7899 cm^{-1}.

Resolution

In addition to the J-stop effects described earlier (page 34), the resolution in the final spectrum also depends on the maximum optical path difference in the interferogram. Each wavelength emitted by the source contributes to the interferogram as a cosine wave with a separation between successive maxima equal to the wavelength.

The Fourier transformation analyzes the interferogram as the sum of the contributions from individual wavelengths. However, the Fourier transformation is not able to distinguish properly between wavelengths that differ by less than half a cycle. So two wavenumbers $\tilde{\nu}_1$ and $\tilde{\nu}_2$ cannot be independently determined if they are closer together than:

$$\tilde{\nu}_1 - \tilde{\nu}_2 = \frac{1}{2d_{\max}}$$

Where $d_{\max}$ is the maximum optical path difference.

A useful approximation is that two spectral features must be at least two such spacings apart to be resolved. This means that the resolution is approximately the reciprocal of the maximum optical path difference scanned. So, the longer the scan, the better the resolution: for example a scan to 1 cm OPD gives a resolution of 1 cm^{-1}, but a scan to 2 cm optical path difference gives a resolution of 0.5 cm^{-1}.

The exact relationship for resolution also depends on the instrument line shape.

Data interval

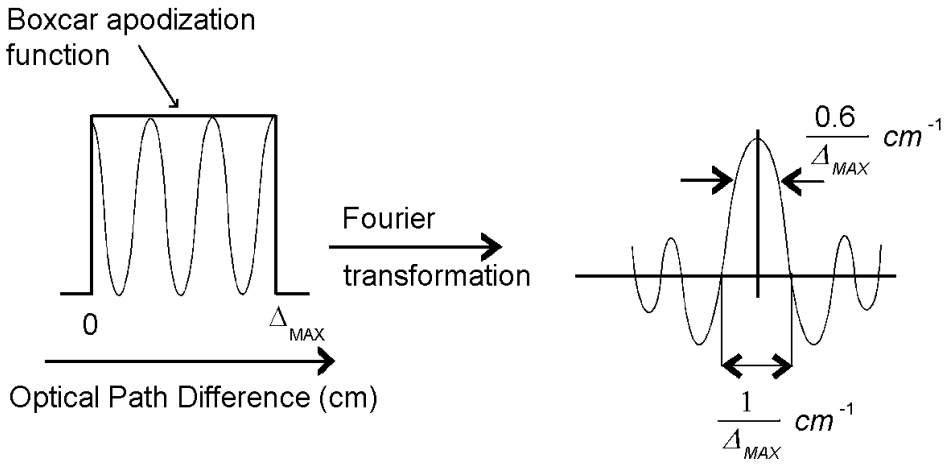
Spectra collected with an FT-IR are stored digitally. The data-points are stored at equal wavenumber intervals: the data interval. The approximate relationship between the data interval and resolution is the same as it is for resolution and wavenumber.

If too large a data interval is chosen, information that may exist between data points is lost, and resolution is reduced. There should be at least two data points per resolution width. For example, if the resolution is 2 cm^{-1}, the data points should be spaced at 1 cm^{-1} or less. In practice, a smaller data interval makes the data easier to visualize.

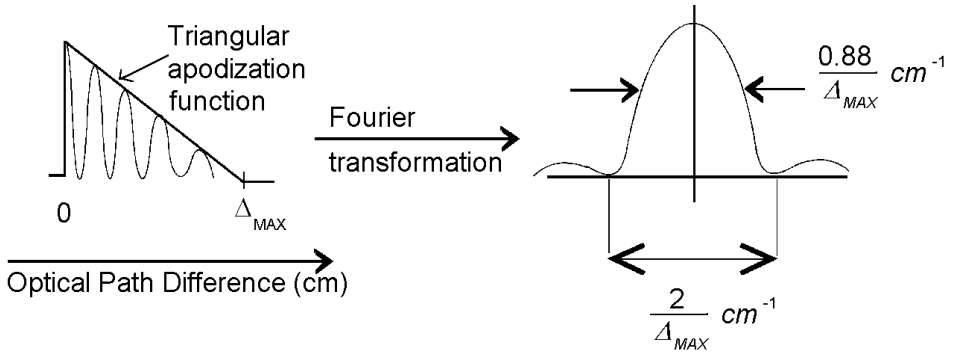
However, the resolution of a spectrum cannot be improved by using a smaller data interval.

Apodization

The contribution to an interferogram from an infinitely narrow line would be a cosine wave that continued indefinitely as the path difference increased. The contribution to an interferogram from any real line with a finite width decreases in amplitude as the path difference increases. To avoid any distortion in measuring the spectrum, the interferogram should be measured out to a path difference where the contribution from the narrowest line has decayed to a negligible value. This is the same criterion as in a classical spectrometer - that the resolution should be much smaller than the line width. If this condition is not met the line is broadened and, in addition, oscillations called sidelobes appear in the baseline on either side. These sidelobes occur because the interferogram has been cut off instead of decaying naturally to zero.



They can be reduced by multiplying the interferogram by a function which itself goes steadily to zero at the maximum path difference. This process is called apodization. The simplest function has a linear slope. Use of such triangular apodization reduces the sidelobes, which no longer become negative, but causes additional broadening.



Various apodizing functions have been used, giving slightly different compromises between line broadening and reduction of sidelobes. Among these, the Norton-Beer functions ensure the smallest sidelobes for a given degree of broadening. The narrowest lines are obtained when no apodizing function is used, a situation sometimes called boxcar truncation.

Apodization also generally reduces noise in the spectrum. The noise in the interferogram comes largely from the detector and affects all points in the single-beam spectrum approximately equally. The proportion of spectral information in the interferogram is decreasing as the path difference increases, so that apodization reduces the contribution from those points in the interferogram where the signal-to-noise ratio is lowest. In this respect, apodizing the interferogram is similar to smoothing the spectrum, because noise is reduced at the expense of some line broadening.

Phase correction

An idealized interferometer would produce an interferogram that was exactly symmetrical about the center. In any real instrument the interferogram is not symmetrical as various effects cause phase differences between the contributions at different wavelengths. To obtain an accurate representation of the spectrum these phase errors must be corrected. The necessary information for doing this is obtained from the central region of the interferogram. The most accurate method of applying the correction involves using a double-sided interferogram, that is, one that is measured for an equal distance on either side of zero path difference. Some instruments use less accurate procedures with single-sided interferograms that are measured for only a short distance on one side of zero path difference and to the maximum path difference on the other. Although measuring a double-sided interferogram requires almost twice as long as a single-sided interferogram it contains effectively as much information as two single-sided scans and so is equally efficient in time.

Trading rules relating resolution, noise level and measurement time

Exactly as in a classical spectrometer, it is possible to obtain lower noise levels or reduce measurement time by sacrificing resolution. Nearly always, spectra are obtained by averaging a number of scans, because the time taken for a single scan is so short. The time taken for a single scan depends upon the mirror velocity and the maximum path difference, which depends on the required resolution.

The mirror velocity depends principally on the type of detector being used. With room temperature DTGS (Deuterated TriGlycine Sulfate) detectors the scan should be relatively slow, because the detector works more efficiently at lower modulation frequencies and this more than offsets the lower number of scans that can be averaged in a given time (see *OPD Velocity* on page 121). Liquid nitrogen cooled MCT (Mercury Cadmium Telluride) detectors have a much faster response, and in general the scan should be much faster in order to optimize the results obtained in a fixed measurement time. Each detector has a default OPD velocity that will give good results under most circumstances.

The time for a single scan is halved if the resolution is decreased by a factor of two, so that twice as many scans can be averaged in the same time. In theory, a larger J-stop can also be used, corresponding to using wider slits in a dispersive spectrometer. However, this possibility is ultimately limited by the diameter of the detector. With a fixed J-stop, changing the resolution by a factor of two halves the noise level in a fixed measurement time, or allows the same noise level to be reached in one quarter of the time. If the ideal J-stop can be used in each case, the energy reaching the detector is doubled when the resolution is halved. The noise is therefore reduced by an overall factor of four, or the measurement time for the same noise level can be reduced by a factor of sixteen.

Signal-to-noise ratio (S/N), measurement time and resolution are related as follows:

For signal averaging:

$S/N \propto \sqrt{}$Measurement time (or $\sqrt{}$Number of scans)

For a fixed measurement time:

$S/N \propto (\text{Resolution in } cm^{-1})^2$ with optimized throughput

$S/N \propto (\text{Resolution in } cm^{-1})$ with constant throughput

In a ratioed spectrum, the signal-to-noise ratio is a function of the individual signal-to-noise ratios of both the average sample and average background spectra. With weakly absorbing samples, approximately the same number of background scans and sample scans must be averaged in order to see the full signal-to-noise ratio improvement, whereas with strongly absorbing samples relatively few background scans are needed.

Optimum measurement times are achieved by selecting a ratio of background scans to sample scans equal to the transmittance of the sample in the region of interest, for example, if the sample has 10% transmittance, averaging ten times as many sample scans as background scans gives approximately the optimum measurement time.

Choice of detector

The most commonly used detector is the DTGS detector. This has a wide wavenumber range and is suitable for most routine applications. When higher speed or sensitivity is needed, liquid nitrogen cooled MCT detectors are available. These have faster response, allowing faster scanning and considerably lower noise levels.

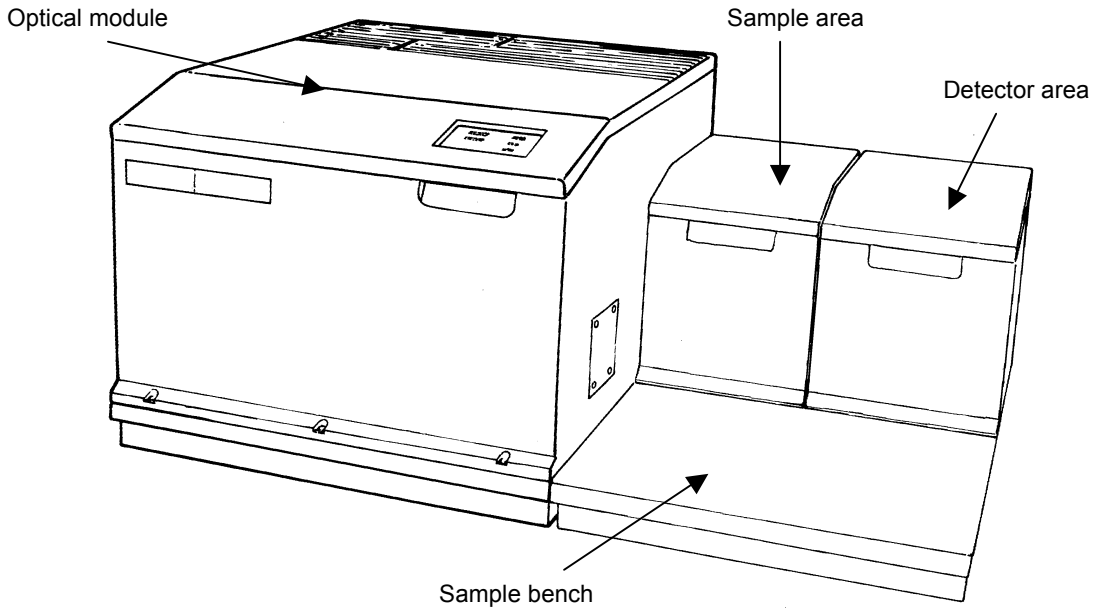
Wide Band MCT	10000 - 400 cm^{-1}
Medium Band MCT	10000 - 700 cm^{-1}
Narrow Band MCT	10000 - 750 cm^{-1}

The narrow range detector is about three times more sensitive than the wide range, and approximately ten times more sensitive than the TGS. MCT detectors work most efficiently with low-transmittance samples and energy-restricting accessories. They are typically partly saturated by the full instrument energy, leading to non-linearity and serious spectral distortion. Other more sensitive detectors, for example, Indium Antimonide (InSb), are available for studies in the near infrared region of the spectrum.

Introduction to the Spectrum GX

The Spectrum GX FT-IR spectrometer is a modular instrument featuring:

- A dual-level optical module that is sealed and desiccated.
- Up to four independent sample beams that are equivalent in their performance and optical characteristics.
- Up to four sampling stations that can accommodate sample and detector areas: the GC-IR Interface, the TG-IR Interface, an infrared microscope and the Raman sample bench.
- Up to two independent, software-controlled, internal sources and an external source position.
- A choice of user-changeable beamsplitters and up to eight detectors covering an infrared wavenumber range from 15 000 cm^{-1} in the near infrared to 30 cm^{-1} in the far infrared. Note that you cannot change the beamsplitter if you have a fixed-range instrument.
- PC control using Spectrum software.
- Transputers (parallel processors) in the PC that enhance computational speed and efficiency.



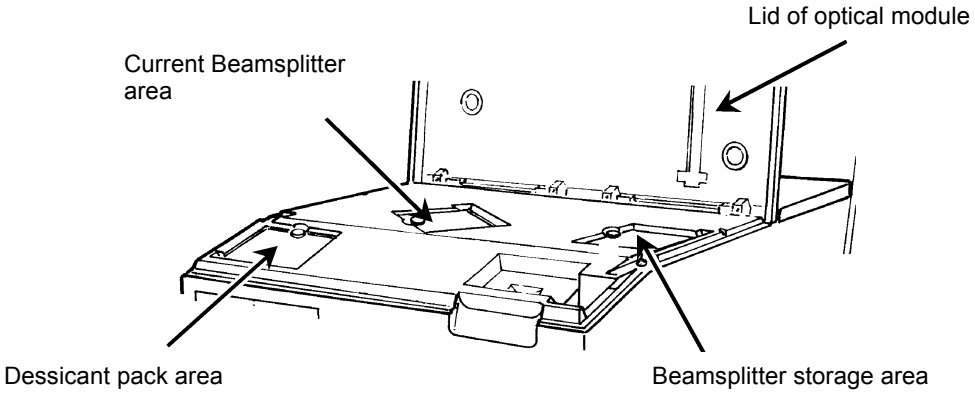
The Optical Module

The optical module contains components on two levels:
on the upper level are the source, Jacquinot- and Beamsplitter-stops, filterwheel and beamsplitter; on the lower level, where the polarizers are located, the optical system directs the beam to the selected sample area.

The optical module is a sealed, desiccated area for the interferometer and optical components. This area may be purged. The indicator panel on the lid of the optical module contains five LEDs that are illuminated to show the status of the instrument.

The lid of the optical module can be opened to access the three hatches in the cover below. These three hatches provide access to the current beamsplitter, a spare beamsplitter and the desiccant pack.

NOTE: *If you have a fixed-range instrument you never need to open the hatches to the beamsplitter areas, except to change the desiccant. The beamsplitter area is desiccated. If the hatch is opened the area below the cover must be purged with dry nitrogen.*



Laser interlock

The interlock system protects you from exposure to hazardous laser radiation. When the lid of the optical module is raised, for example, if you are changing the beamsplitter, the HeNe reference laser shuts down.

Source

The source, or sources, of radiant energy can be located inside the instrument or on an external bench.

Internal source

The internal source is in the back left corner of the upper level. It may be either a single source or a carousel that accommodates two independent sources.

Two types of source are available: both are voltage-stabilized and air-cooled:

- Near infrared radiation is produced by a tungsten-halogen lamp with a quartz envelope.

- Mid and far infrared radiation is produced by a temperature stabilized, wire coil that operates at 1350 K.

Source carousel

The software-controlled carousel enables you to select one of two sources and switch it on without removing the instrument covers or re-adjusting and re-aligning the optics.

External source position

A window located above the rear, left output port enables the use of external sources for Raman, emission or remote sensing applications. After passing through the window the beam follows the standard path through the instrument.

The beam from the source is focused by a paraboloidal mirror and passes through the B-stop (beamsplitter stop), filterwheel and J-stop.

Stops and Filter Wheel

B-stop

The B-stop defines the area of the beam passing through the interferometer. It also controls the convergence of the beam at the sample position. The B-stop is available as a fixed aperture or, alternatively, a software-controlled iris. It can act as a variable attenuator if it is an iris aperture.

Filter wheel

The filter wheel enables various filters and attenuators to be positioned in the beam under software control. The introduction of a filter enables you to scan a small, defined region of the spectrum and to study weakly transmitting samples. The reference materials used in internal IPV (Instrument Performance Validation) are installed in the filter wheel.

The standard filter size is 25.4 mm in diameter and 2 - 3 mm thick (5 mm maximum thickness).

J-stop

The circular J-stop limits the divergence angle of rays passing through the interferometer and thus affects the resolution of the instrument. By adjusting the J-stop, throughput is optimized for any combination of resolution and scan range. The J-stop is available as a fixed-size aperture or a software-controlled iris. The fixed J-stop restricts the resolution to a maximum of 4 cm^{-1} up to 4000 cm^{-1}. If one of the sample area J-stops supplied in the shipping kit is installed in the sample carrier, resolutions of 0.3 cm^{-1}, 1 cm^{-1} or 2 cm^{-1} can be achieved.

The sample area J-stops have the following part numbers:

J-stop Resolution (at 4000 cm^{-1}) / cm^{-1}	**Part Number**
0.3	L1362340
1.0	L1361238
2.0	L1361289

The J-stop resolution can be defined independently from the interferometer resolution and both the J-stop wavenumber and image size can be changed from their default values.

After the J-stop the infrared beam is made parallel and directed onto the beamsplitter by a paraboloidal mirror.

Interferometer

An interferometer consists of a moving mirror, a fixed mirror and a beamsplitter. The interferometer modulates the infrared beam. The beamsplitter divides the beam in two and the moving mirror creates an optical path difference (OPD) between them. The PerkinElmer Dynascan™ interferometer gives 0.15 cm^{-1} resolution unapodized and 0.2 cm^{-1} resolution with the default apodization.

Beamsplitter

A variety of beamsplitters is available to cover the instrument operating range from 15000 to 30 cm^{-1} and enable the use of near, mid and far infrared options.

NOTE: *You cannot change the beamsplitter if you have a fixed-range instrument.*

Beamsplitter	Range/cm^{-1}	Hygroscopic
Quartz	15000 - 2700	
CaF_2	14000 - 1200	
Raman	12000 - 5000	
Wide Range KBr	10000 - 370	Yes
Optimized KBr	7800 - 370	Yes
Mid-IR CsI	6500 - 220	Yes
Far IR grid	710 - 30	
6 µm Mylar film	500 - 50	
12 µm Mylar film	250 - 30	
25 µm Mylar film	120 - 30	

The laser beam path through the interferometer is offset from the infrared beam path.

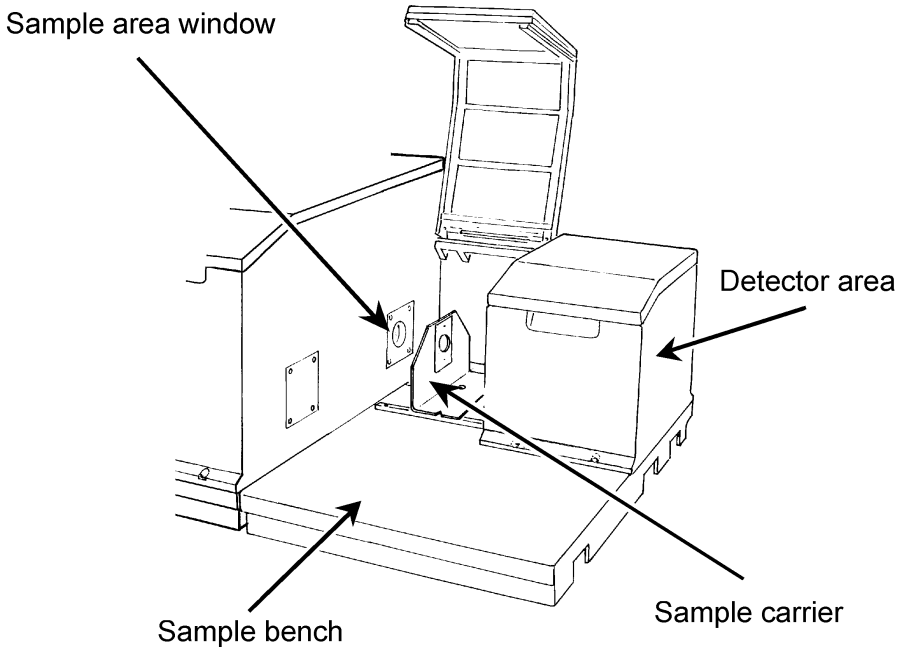
Polarizer

When the infrared beam leaves the interferometer, it is directed to the lower level of the optical module by two flat periscope mirrors. A paraboloidal central mirror directs the beam either to the right or left hand side of the instrument and a flat side mirror directs the beam to the front or rear sampling area on the selected side.

A polarizer can be mounted between the central mirror and the side mirror on both the left and right hand sides of the optical module. The introduction of a polarizer enables orientational and structural studies to be performed on, for example, stressed polymers. The polarizing element is moved in and out of the beam under software control and can be rotated from 0 to 180° in one-degree increments. The polarizers that are available are:

Position	Far or Mid Infrared	Material	Part Number
Right	Far	Wire grid on KRS-5 (thallous bromide/iodide)	L1302810
Left	Far	Wire grid on KRS-5 (thallous bromide/iodide)	L1302820
Right	Mid	Polyethylene	L1302830
Left	Mid	Polyethylene	L1302840

Sample Area



Sampling stations can be fitted to, and interchanged between, output beams as required.

Sample area window

The optical module is supplied with the appropriate windows for the detectors that are fitted in each of the detector areas. Film windows, for use in the far infrared, KBr for mid infrared and quartz windows are available. Generally, a sample area should be dedicated to a particular beamsplitter so that window changes are not required. The window seals the optical module, which is purged and desiccated, from the sample area. The optical module must be purged after changing one of the sample area windows.

Sample carrier

The sample carrier can hold sample slides, sampling accessories, cells, and other small items. It is reversible and can be moved to enable focusing of the sample.

White dots on the base of the sample area indicate the optimum position of the sample holder (that is the nominal position of the J-stop image for a KBr beamsplitter and windows). In either orientation this is achieved by aligning the notches in the base of the sample carrier with the white dots (see *Aligning the Sample Carrier* on page 115).

Sample shuttle

The sample shuttle accessory can be installed in any of the four sample ports. It is interchangeable with the basic sample port baseplate and sample holder assembly.

The sample shuttle enables either of two sample slides to be positioned in the optical beam of the spectrometer. Its primary function is to enable interleaved operation, where the sample is moved smoothly in and out of the beam as the instrument accumulates sample and background scans respectively. This use of an interleaved scanning mode enables you to ratio the sample against an effectively simultaneously recorded background, and thus eliminates residual atmospheric absorptions from the final spectrum. This is of particular benefit for far-infrared spectroscopy. An alternative use of the shuttle is to enable an accessory to be switched in and out of the beam without disturbing the alignment of the accessory.

Detector Area

Each detector module can accommodate up to two internal detectors. The cover of the detector module provides access for liquid nitrogen cooling and a purge seal. Both cooled and room temperature detectors can be fitted.

Detector filters

Near infrared filters are available for use with near infrared detectors. They enable the throughput to be matched to detector response. They can be removed very easily if the same sample compartment is to be used for mid infrared measurement.

Detector types

The detector types available are Deuterated TriGlycine Sulfate (DTGS), Mercury Cadmium Telluride (MCT), Indium Antimonide (InSb) and Photo-acoustic (PAS). A near infrared integrating sphere uses a dedicated Lead Sulfide (PbS) detector. The detectors are automatically recognized and their gain is set by the software.

Cooled detectors

Cooled detectors are housed in a standard 8 or 12 hour dewar. The dewar can be refilled without breaking the purge seal in the detector area or in the GC-IR interface, and spillage of liquid nitrogen into the instrument is inhibited. Cooled detectors have a coolant level sensor that detects when the coolant level is low and a message is then displayed on the screen (see *Cooling the Detector* on page 107).

Instrument Specification

NOTE: *The figures quoted in the following specification correspond to the maximum tolerance limits permitted in the manufacture of the instrument. The performance of each instrument will be equal to or better than that specified. Measurements and calibration are made at an ambient temperature of approximately 20 °C, having allowed the temperature of the instrument to stabilize for 20 minutes with power switched on. This stabilization takes longer for a near infrared instrument.*

Principle

Single beam Michelson interferometer with rotary bi-directional scan and stationary beamsplitter. Interferometer auto alignment. Magnetic drive.

Optics

Choice of user-installed, interchangeable beamsplitters covering the wavenumber range 15 000 to 30 cm^{-1}.

Sealed, desiccated optics. Purging possible but not an instrumental requirement.

Source

Near infrared:
Voltage-stabilized, air-cooled, tungsten halogen source with a quartz envelope.

Mid and far infrared:
Voltage-stabilized, air-cooled wire coil operated at 1350 K.

Detector

Near infrared:
A liquid nitrogen cooled InSb (Indium Antimonide) detector is available. Near infrared FR-DTGS (Fast Recovery Deuterated TriGlycine Sulfate) detectors have a calcium fluoride window.

Mid infrared:
Wide, medium or narrow band, liquid nitrogen cooled MCT (Mercury Cadmium Telluride) detector available. Mid infrared FR-DTGS detectors have a KBr window; a CsI window is also available.

Far infrared:
Far infrared FR-DTGS detectors have a polyethylene window.

J-stop

Fixed: 2 to 16 cm^{-1} up to 15000 cm^{-1}
Variable: 0.2 to 16 cm^{-1} up to 15000 cm^{-1}

Abscissa range

15000 to 30 cm^{-1} with appropriate combination of beamsplitters, sources and detectors.

Signal-to-noise

Measured under the following conditions:

DTGS detector with KBr window
Wide-range KBr beamsplitter
Resolution at 4000 cm^{-1} = 4 cm^{-1}
Scan speed = 0.2 cm/s
Apodization = Strong
Bi-directional double-sided scanning
Measured over 50 cm^{-1} intervals around 2000 cm^{-1}
Scan time = 5 seconds

r.m.s. S:N = 45 000:1 (Spectrum GXI = 30 000:1)

Peak-to-Peak = 9000:1 (Spectrum GXI = 6000:1)

Resolution

0.2 to 64 cm^{-1} (Spectrum GXI = 0.5 to 64 cm^{-1})

Scan speeds

Variable between 0.05 and 5.0 cm/s optical path difference (OPD) velocity.

Apodization

Choice of weak, medium or strong Beer-Norton, triangular, raised cosine, filler, Kaiser-Bessel or boxcar.

Sample/accessory alignment

Energy throughput indicator (on the Monitor dialog) for optimum alignment.

External requirements

200 to 250 V; 50 or 60 Hz
100 to 127 V; 50 or 60 Hz
Power requirements: 320 VA

Purging

Near and mid infrared: Purging possible but not essential.

Far infrared: Recommended in detector and sample areas.

Size and weight

Module	Length cm	Height cm	Depth cm	Weight Kg
Optical	50.0	42.0	63.0	62.5-71.5
Sample Compartment	41.0	32.0	63.0	34.0

4 Using the Spectrum GX

Switching on the Instrument

1. Connect the mains cable to the electrical supply.

2. Switch on the instrument and the PC. The ON/OFF switch for the Spectrum GX spectrometer is located on the back of the optical module, high on the right-hand side.

   The **POWER ON** and **LASER ON** lights on the indicator panel are illuminated.

NOTE: *To obtain the best results, we recommend that the instrument is kept switched on at all times.*

NOTE: *If the instrument is switched off and on without exiting from Spectrum, you must initialize the instrument using the procedure described on page 60.*

3. From the Start menu start **Spectrum**.

   The Spectrum window opens and the Spectrum software is loaded. The **READY** light on the indicator panel is illuminated.

   When a near infrared source is selected, scanning is disabled for 10 seconds; when a mid infrared source is selected, scanning is disabled for 90 seconds and the instrument stabilizes after approximately 20 minutes.

Initializing the Instrument

The instrument must be initialized after the PC connected to the instrument has been switched off.

If you switch off your PC, after switching on again, the first time you choose **Scan Sample**, **Scan Background**, **Monitor** or **Validate** from the Instrument menu or **Instrument** and **Instrument Validation** from the Setup menu; the message **Instrument is uninitialized do you want to initialize now?** is displayed. You must initialize the instrument before continuing.

If the instrument has been switched off but the PC has not, the instrument must be re-initialized when it is switched on. The instrument is initialized using the setup that it was using when it was switched off.

You can use the **Initialize** command to reinitialize the interferometer.

NOTE: *If a background or sample spectrum or interferogram is stored in the instrument, the data will be lost when the instrument is re-initialized.*

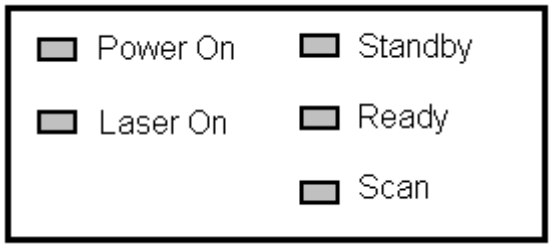
1. Display the Setup menu and choose **Instrument**.
   The Spectrum GX Instrument Setup tabs are displayed.

2. Click  .
   The Initialize Instrument dialog is displayed.

3. Choose **OK**.
   The instrument initializes. Progress messages are displayed during initialization.
   Choose **Halt** to stop the initialization.

Indicator Panel

The indicator panel, positioned on the lid of the optical module, consists of five LEDs. They are the **POWER ON**, **LASER ON, STANDBY, READY** and **SCAN**indicators.



Indicator	Color	Meaning
Power On	Green	The instrument is connected to the electricity supply and switched on.
Laser On	Green	The laser is operating.
Standby	Green	Initialization is in progress, or PC control has been switched to another instrument.
Ready	Green	The instrument is ready for further commands; the source has warmed up and optical components are stationary.
	Red	Error warning.
Scan	Green	The instrument is scanning.

Setting up the Instrument

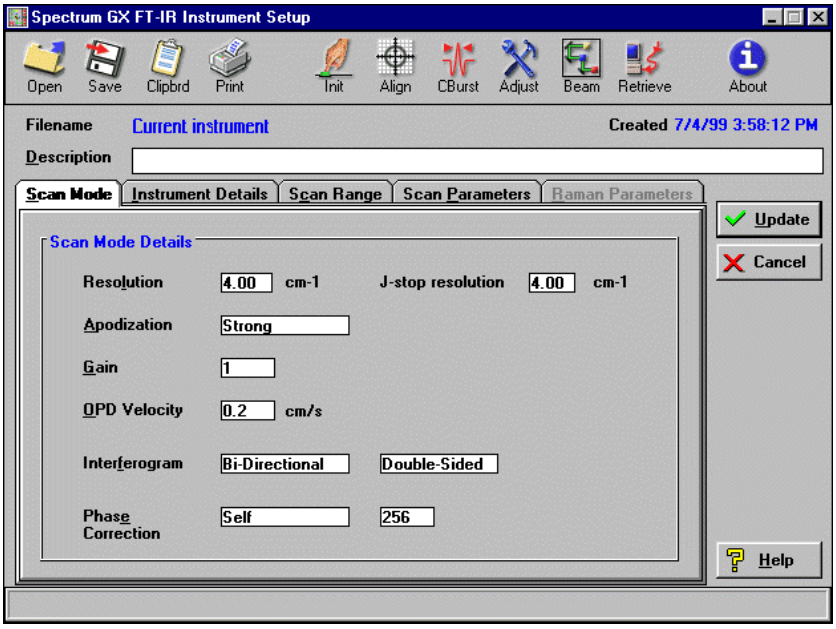
Instrument setup (.set) files contain information on the scan mode settings, scan parameters and instrument details. They enable you to save the current customized instrument settings for future use. You can also create new instrument setup files without changing the current instrument setup.

When you open a setup file, three items of information are displayed below the toolbar on the Spectrum GX Instrument Setup tabs:

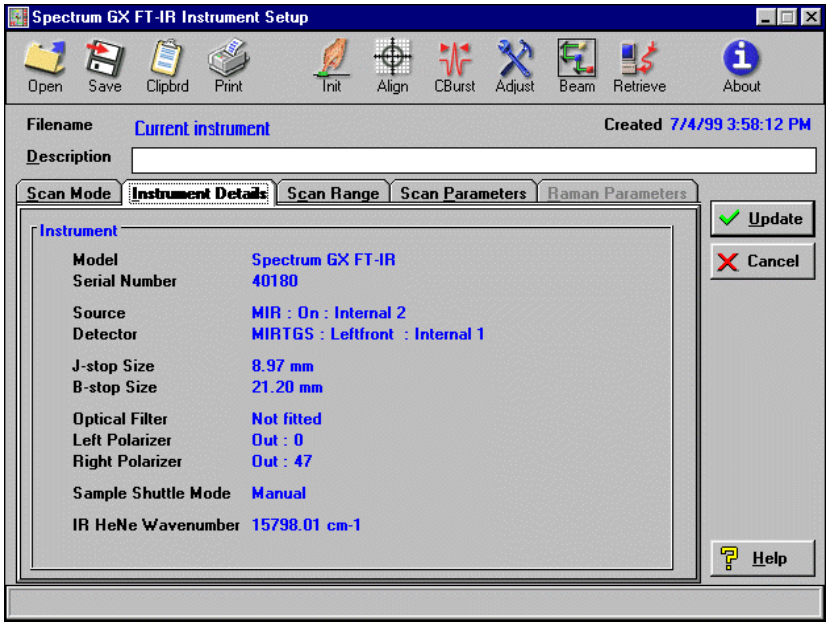
- The name of the current setup file.
- The date that it was created.
- The description that was entered when the setup was saved.

To setup your Spectrum GX to collect data, choose **Instrument** on the Setup menu. From here you can:

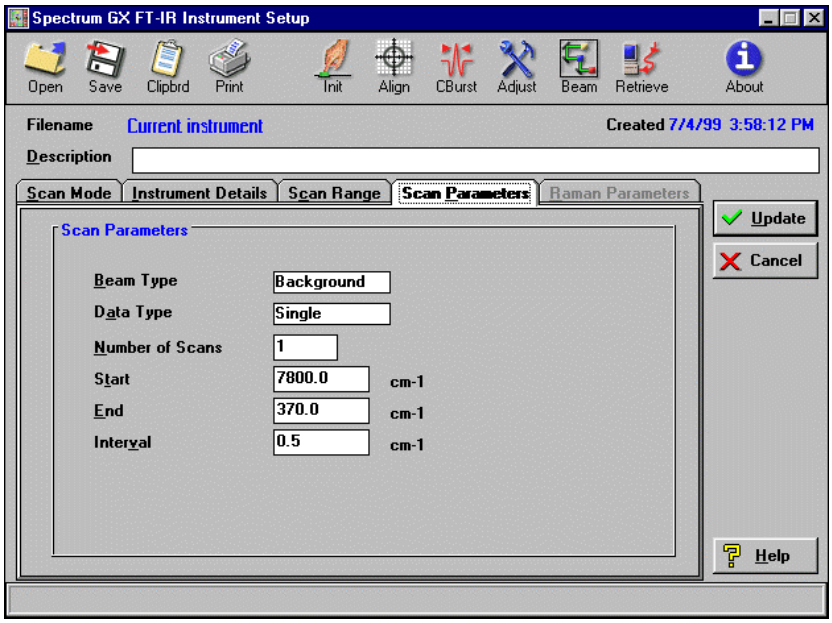
- Select the instrument resolution, J-stop resolution, apodization function, gain, OPD velocity, interferogram direction and phase correction.



- Display information about the version of firmware installed in your instrument and the instrument serial number. The Instrument Details tab also displays information on the source, detector, J-stop, B-stop, filter and polarizer currently fitted to your instrument.



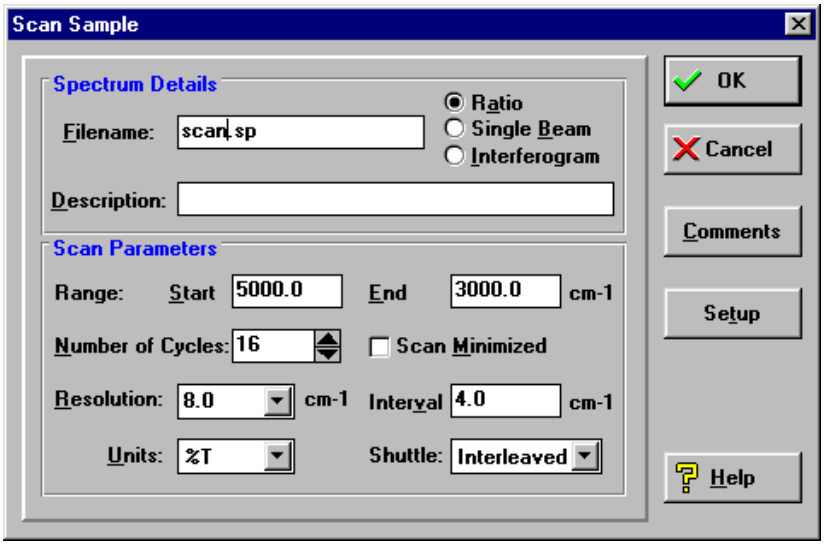
- Select the parameters for the scans collected. When you save the instrument setup file, the Scan Parameters are saved with the rest of the settings.



Scanning

To collect data from your Spectrum GX, choose either **Scan Background** or **Scan Sample** from the Instrument menu. From the dialog displayed you can:

- Enter the filename and a description.
- Enter a comment to be saved with the spectrum.
- Select the scan parameters.



Further information about controlling your instrument or processing the spectra and data from samples is given in the on-screen help files available in the software.

Adjustments Toolbox

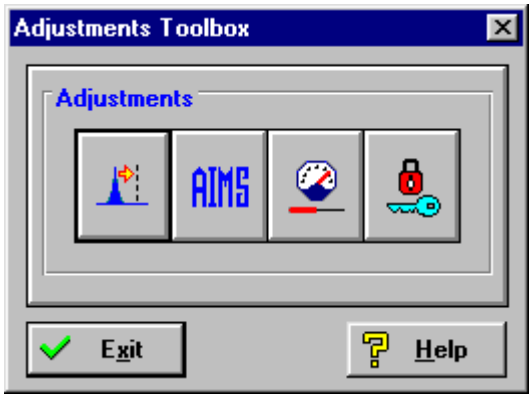
The Adjustments toolbox  enables you to:

- Perform wavenumber calibration.
- Use the Automatic Interferometer Management System (AIMS).
- Monitor energy.
- Set password protection for the Adjustments toolbox.

The Adjustments Toolbox

1. Display the Setup menu and choose **Instrument**.
   The Spectrum GX Instrument Setup tabs are displayed.

2. Click  .
   If the Adjustments Enter Password dialog is displayed, type the password.
   The Adjustments toolbox is displayed.

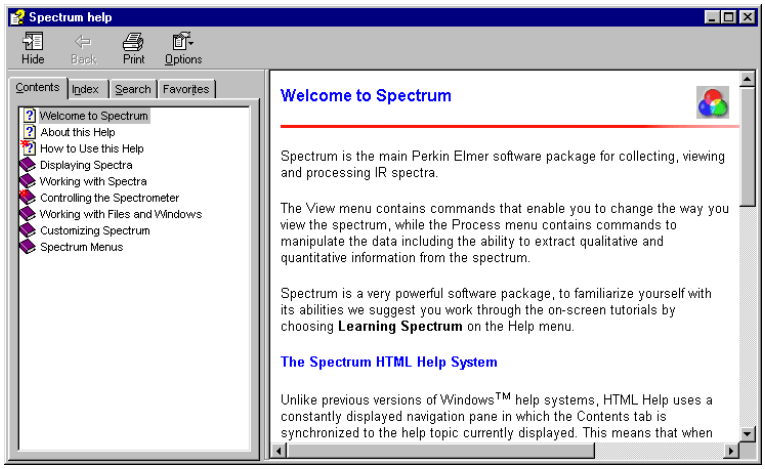


HTML Help

What is HTML Help?

HTML Help is the Microsoft standard format for Windows™ help systems introduced with the launch of Windows '98™.

HTML Help uses a window split into three sections (Tripane Window) to display help topics:



- Toolbar - across the top of the window is a series of tools that help you navigate, print and customize the help.

- Navigation Pane - on the left of the window are the Contents, Index, Search and Favorites tabs, which enable you to find your way around the help system.

- Main Window - the right side of the window is where the individual help topics are displayed.

What is so special about HTML Help?

Unlike previous versions of Windows ™ help systems, HTML Help uses a constantly displayed navigation pane in which the Contents tab is synchronized to the help topic currently displayed. This means that when you click on a jump that takes you to a different help topic, the Contents list also jumps to the new topic, enabling you to keep track of where you are within the help system.

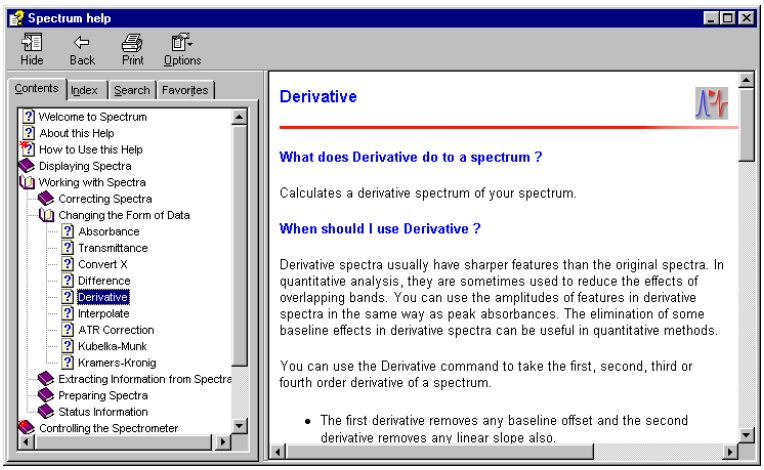
However, the major benefit of HTML Help is the ability to make the help more user-interactive and more visually interesting. Where possible, we have used stills, animations and interactive visuals to help get important ideas across.

How do I navigate around?

There are lots of ways to navigate around an HTML Help system:

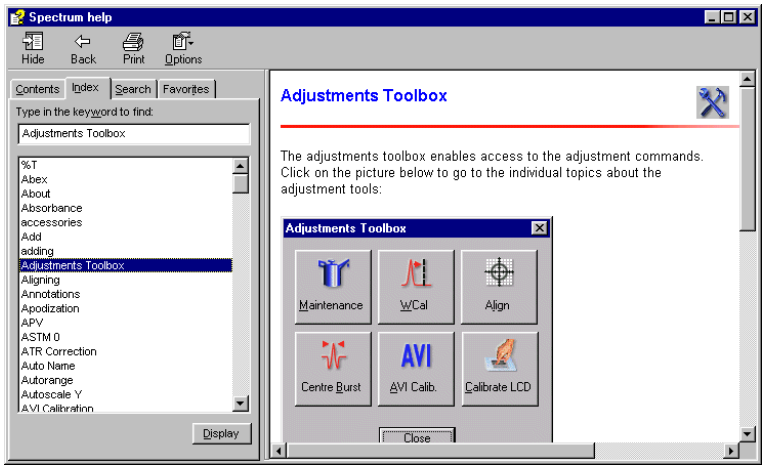
Contents

If you choose **Contents and Index** from the Help menu, the tripane window is displayed showing the opening page of the help system. Using the **Contents** tab in the navigation pane, clicking on a book icon ( ) will open ( ) the book and display the pages ( ) and sub-books inside it. Clicking on a book or a page also displays that help topic. It should be noted that unlike previous versions of help, books now have their own topics that in general give an overview of the topics in the book and/or a different way to navigate to the topic you require.



Index

Index enables you to look up topics that have been linked to a particular keyword by the help author.



Search

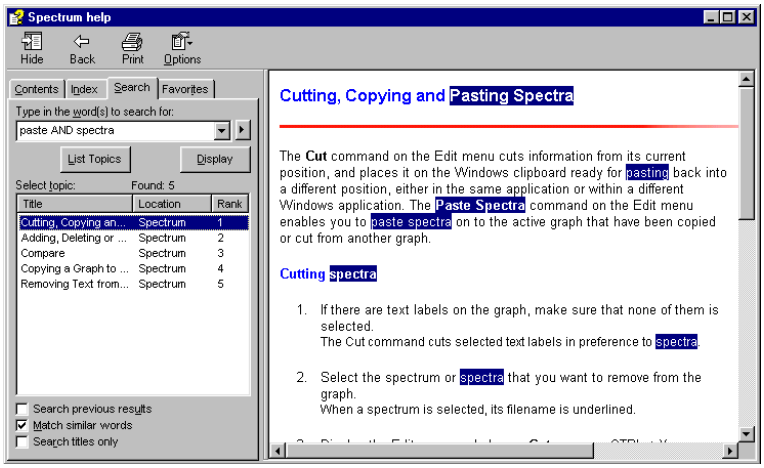
Search enables you to search the whole of the help for a word, phrase, or set of words.

This help file can use Boolean, wildcard and nested expressions to narrow down the search. For instance, the AND, OR, NOT, and NEAR operators enable you to precisely define your search by creating a relationship between search terms. The following table shows how you can use each of these operators.

If no operator is specified, AND is used. For example, the query “spacing border printing” is equivalent to “spacing AND border AND printing”.

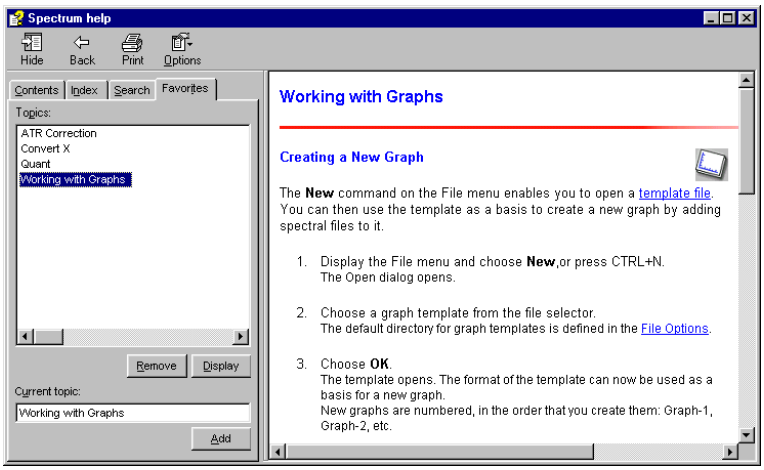
To search for	Use	For example	Will give
More than one term in the same topic.	AND	baseline AND correction	Topics that contain both the words "baseline" and "correction".
Either term in a topic.	OR	spectrum OR spectra	Topics that contain either the word "spectrum" or the word "spectra" or both.
The first term without the second term.	NOT	peak NOT table	Topics that contain the word "peak" but not the word "table".
Both terms in a topic, close together.	NEAR	third NEAR derivative	Topics that contain the word "third" within eight words of the word "derivative".

When the topic is selected, the specified words are highlighted.



Favorites

Favorites enables you to pick out topics that you want to be able to get to quickly.



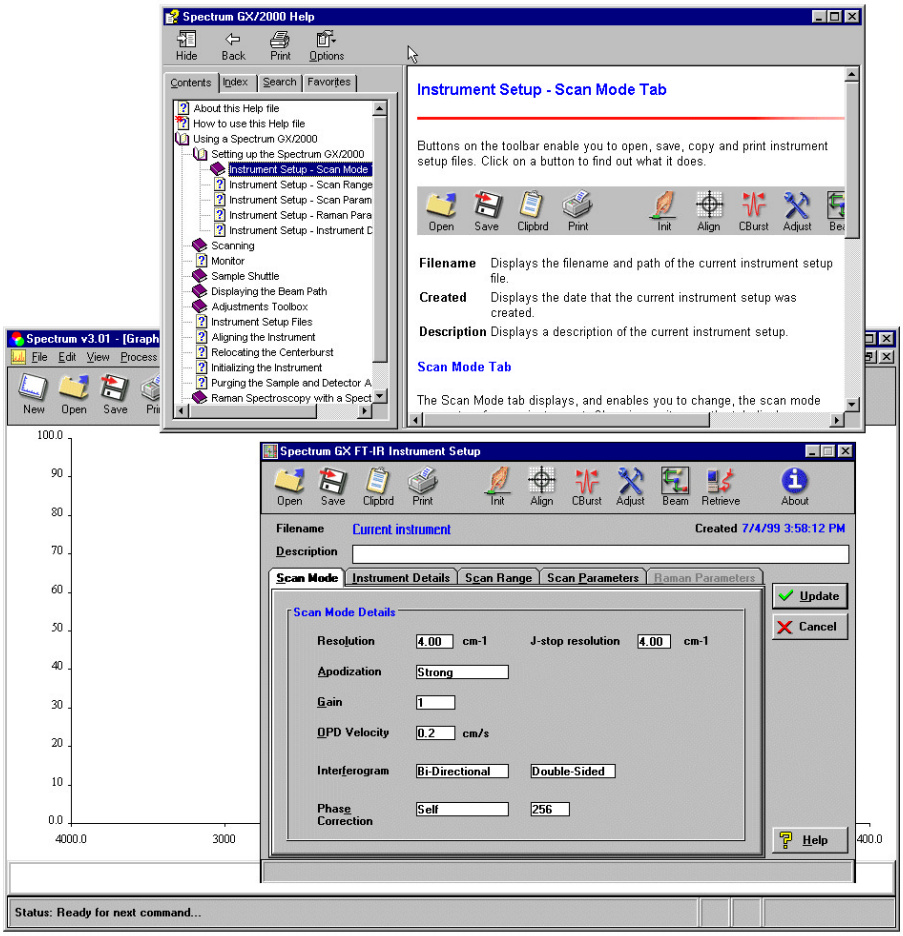
The Back button

At any time during the use of a help file you can click on the 

button to return to the previous page of the help.

Context sensitive help

You can also call the help file by clicking **Help** on a dialog. This will start the same help file but will immediately take you to the page of information most relevant to the help button you clicked.



Maintenance of the Spectrum GX 5

Introduction

The Spectrum GX will operate over long periods with minimum attention. If you are in any doubt regarding your ability to correct a malfunction of the instrument, consult the nearest PerkinElmer Service Department or Agent.

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. This includes windows such as the window between the optical module and the sample area, and the window between the sample area and the detector area (if fitted).*

System Requirements

Environmental Requirements

NOTE: *Read the* Warnings and Safety Information *in the front of this manual before using the Spectrum GX: it contains important information.*

Attention should be given to the following points before the instrument is installed.

Bench Space

The minimum width of bench required for the Spectrum GX is 910 mm. This is the space required for the optical module with a sample bench fitted on one side. The depth of the instrument is 630 mm and its height is 420 mm. Allow a space of at least 630 mm above the top of the instrument so that the lid can be opened.

The width of bench required may be more than this depending on which accessories are fitted and their configuration on the instrument (refer to the manual for the accessory).

Temperature

The temperature of the room in which the instrument is used must be within the range of 15 °C to 35 °C.

NOTE: *Do not position the Spectrum GX in direct sunlight because this may cause overheating.*

Humidity

The relative humidity of the room in which the instrument is used must not be more than 75% (non condensing).

Cleanliness and Ventilation

The room in which the instrument is used must be well-ventilated and free from dust and dirt.

Controlled EM Environments

This equipment is designed to operate in a controlled electromagnetic environment, that is where RF transmitters such as mobile telephones may not be used in close proximity.

NOTE: *If you are unsure about the environment in which you intend to use the Spectrum GX, contact your PerkinElmer Service Department.*

Electrical Requirements

A stable electrical supply is required with a frequency of 50 Hz or 60 Hz and at a voltage in the range 100 to 120 V or 220 to 240 V.

Electrical Connections

Fitting the Plug

The power cable for the electrical supply plugs into the back of the optical module. 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
Line	Black	Brown
Neutral	White	Blue

WARNING

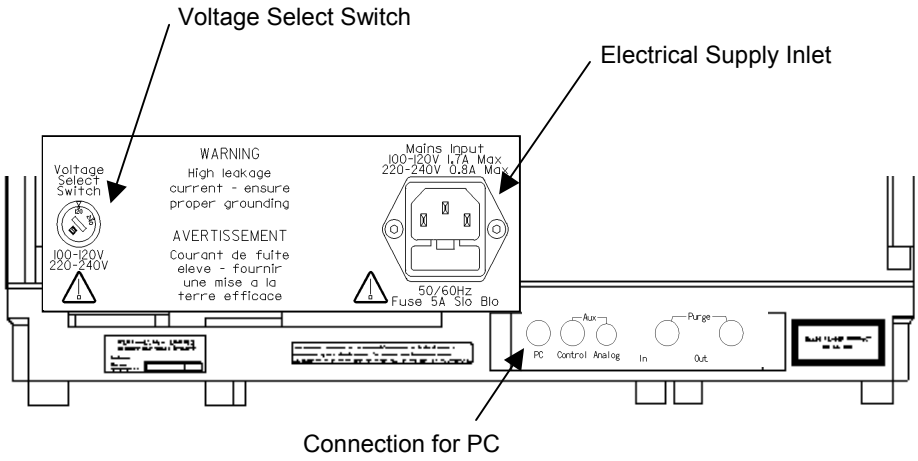
To ensure safe and satisfactory operation of the instrument, it is essential that the green or green/yellow ground (earth) wire of the power cord is connected to a ground that complies with the regulations of the local electricity supply authority (or equivalent body); ground circuit continuity is essential for safe operation of the equipment.

Connecting the Spectrum GX to the Electrical Supply

The instrument operates on an electrical supply with a frequency of 50 or 60 Hz and at voltages in the ranges 100 to 120 V or 220 to 240 V.

Set the **Voltage Select Switch** to the voltage of the electrical supply that you are going to use. The **Voltage Select Switch** is located on the back panel of the optical module, and is illustrated on the next page.

Fit the molded socket of the power cable into the electrical supply inlet at the back of the optical module. The location of the electrical supply inlet is illustrated on the next page.



Connecting the Spectrum GX to the PC

A cable (L136 5719) is provided for connecting the Spectrum GX to the PC. Both ends of the cable are fitted with the same type of connector. One end of the cable fits into the socket labeled **PC** at the back of the instrument (see above). The other end fits into a socket mounted on the transputer board fitted to the PC. To unplug the cable, pull back the metal sleeve that surrounds the connector.

Other Connectors

Analog

The **Analog** connector is not usually required. You will need it only if you want to use your own detector and pre-amplifier. For more information, consult your nearest PerkinElmer Service Department or Agent.

Control

Service use only.

Purge Connectors

For information about the connectors labeled **Purge In** and **Purge Out**, see *Purging Sealed Areas* on page 89.

Moving the Instrument

General

Disconnect the instrument from its electrical supply before moving it. Provided it is not subjected to large forces, the instrument can be moved short distances without removing the sample benches from the optical module. To move the instrument longer distances, we recommend that the sample benches are removed and the instrument is re-packed in its original packaging. This should be carried out by your PerkinElmer Service Department; please contact your local office for assistance.

Fitting the Shipping Clamp

The shipping clamp fits into the optical module to prevent optical components from moving while the instrument is being moved. If you have a fixed-range instrument, follow the instructions on page 82.

Fitting the shipping clamp in a variable-range instrument

To fit the shipping clamp:

1. Monitor the energy (this makes sure that the optical components are in the correct position to be clamped):
   a) Display the Instrument menu and choose **Monitor**.
      The Monitor dialog is displayed.
   b) Choose **Energy**.
   c) Click **OK**.
      Monitoring Starts.

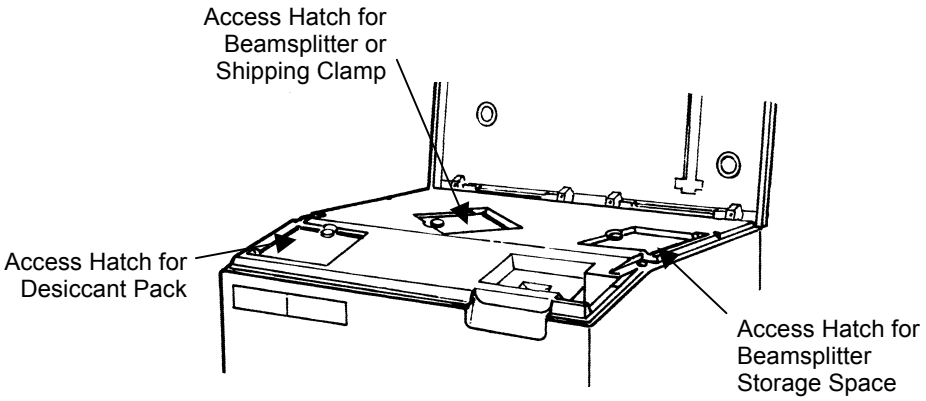
2. Switch off the instrument.

3. Undo the lock at the right-hand side of the optical module and raise the lid.
   There are three hatches in the cover beneath, which give access to the optical module.

4. Open the central hatch. To do this, press the knob and turn it counterclockwise.

5. Lift out the beamsplitter. Put it in the desiccated storage container in which it was supplied (see *Care and Storage of Beamsplitters* on page 101.)

6. Open the hatch on the right and remove the spare beamsplitter if there is one stored there (see *Care and Storage of Beamsplitters* on page 101.)



CAUTION *The instrument will be damaged if it is transported with a beamsplitter in the storage space in the optical module.*

7. Slide the shipping clamp into the beamsplitter compartment.

   The shipping clamp holds the lever in place and prevents the tilt table from moving.

8. Close the hatch immediately.

NOTE: *Because the optical module is sealed and desiccated, do not leave the hatch open for longer than necessary.*

CAUTION	*Failure to reactivate or replace the desiccant packs at the specified intervals may result in damage to sensitive optical components within the instrument. For more information, see* Desiccant Packs *on page 87.*

Lowering the shipping clamp in a fixed-range instrument

To lower the internal shipping clamp:

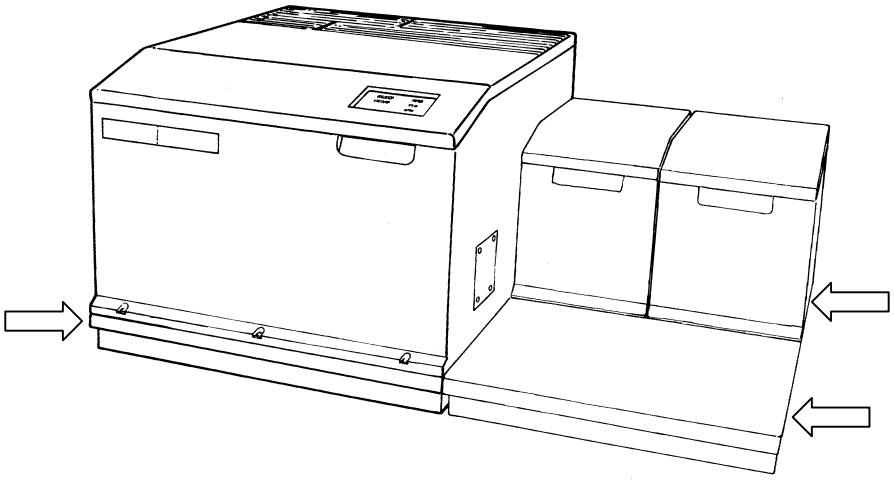
1. Monitor the energy (this makes sure that the optical components are in the correct position to be clamped):
   a) Display the Instrument menu and choose **Monitor**.
      The Monitor dialog is displayed.
   b) Choose **Energy**.
   c) Click **OK**.
      Monitoring starts.
2. Switch off the instrument.
3. Undo the lock at the right-hand side of the optical module and raise the lid.
   Monitoring stops, with the tilt table in a central position.
   There are three hatches in the cover beneath the lid (see page 80), which give access to the optical module.
4. On the right-hand side, there is a screw and a vertical plate – the shipping clamp. Loosen the screw until the shipping clamp drops; if necessary, push it down gently to make sure that it is clamping the optical components securely.
   When the shipping clamp drops into position, the screw is aligned with a small circular hole in the shipping clamp.
5. Tighten the screw.
6. Close the hatch immediately.

NOTE: *Because the optical module is sealed and desiccated, do not leave the hatch open for longer than necessary.*

CAUTION	*Failure to reactivate or replace the desiccant packs at the specified intervals may result in damage to sensitive optical components within the instrument. For more information, see* Desiccant Packs *on page 87.*

Lifting the Spectrum GX

The Spectrum GX can be lifted from underneath at its ends, as shown below. The combined weight of the optical module and sample bench is approximately 100 kg (218 lb), so you will need at least two people to lift it.



After the instrument has been moved to the position where it will be used, reverse the procedure you used above to raise or remove the shipping clamp so that the optical components can move freely.

Fitting Windows

There are four types of window that can be fitted into the ports in the optical module and in the detector module. Ports that are not used are fitted with blanking plates.

Window	Range
Quartz	Near Infrared
KBr	Mid and Near Infrared
CsI	Mid and Far Infrared
Film	Far Infrared

In addition, a far infrared filter window (L1365111) is supplied with all far infrared detectors, and must be fitted in the detector module when using these detectors. (A Film window should be used in the optical module.) A window is not usually required in the detector module when using near or mid infrared detectors.

To fit a window:

1. Remove the original window or the blanking plate by unscrewing the four screws at the corners. Retain the screws.

2. Fit the new window and its rubber seal.

NOTE: *The window must be oriented so that the alignment pin at the corner of the port fits into the corresponding hole on the window.*

3. Refit and tighten the four screws.

   After fitting windows in sealed areas of the instrument, purge these areas (see *Purging the optical module* on page 91).

Cleaning the Spectrum GX

You can clean the outside of the Spectrum GX using a damp cloth. Mild detergent may be used, if necessary. Always perform a patch test on an inconspicuous area of the instrument, before you clean the entire instrument.

Avoid spilling liquid into the instrument, especially into the top rear cover of the optical module, which contains a high-voltage supply. Clean all external spills immediately. If anything that is spilled enters the main body of the Spectrum GX, switch off the power and call 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. This includes windows such as the window between the optical module and the sample area, and the window between the sample area and the detector area (if fitted).*

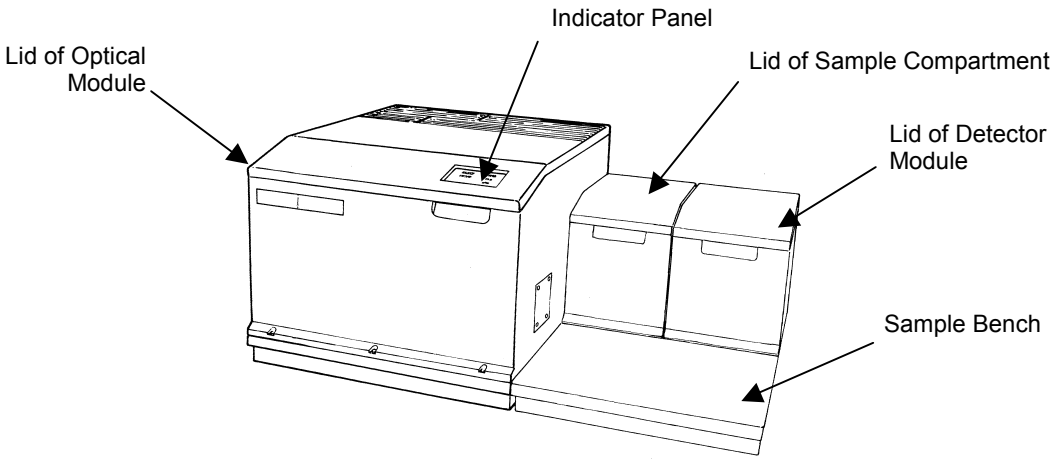
Removal of Covers

The lid of the optical module must be raised to gain access to the desiccant pack and beamsplitters. Also, if your instrument has a sealed and desiccated detector module, its cover must be removed periodically to gain access to the desiccant pack.

CAUTION *Other covers should not be removed, and doing so may result in contamination of the instrument.*

There is an interlock on the lid of the optical module. When this lid is lifted, the laser stops operating. After the lid has been closed, the instrument is automatically re-initialized.

WARNING *Always disconnect the instrument from the electrical supply before removing covers. Do not use the instrument with the covers removed or attempt to defeat the interlocks.*



Desiccant Packs

General

Some areas of the instrument are sealed and contain desiccant packs to reduce the amount of water vapor and carbon dioxide within them. At six-monthly intervals the desiccant packs must be reactivated, or replaced with new ones. We advise you to purge these areas with nitrogen or dry air when the desiccant packs are replaced.

Disposable bags of desiccant are also available from PerkinElmer, and can be used in the optical module instead of the desiccant packs that are supplied with the Spectrum GX. For more information see *Disposable Desiccant Packs* on page 93.

CAUTION	*Failure to reactivate or replace the desiccant packs at the specified intervals may result in damage to sensitive optical components within the instrument.*

NOTE: *The optical module is always sealed. The detector module can also be sealed, but it is normally open to the sample area. If the detector module on your instrument is not sealed, the instructions for re-activating the desiccant pack in the detector module and purging it do not apply.*

Removing the Desiccant Packs

Optical module

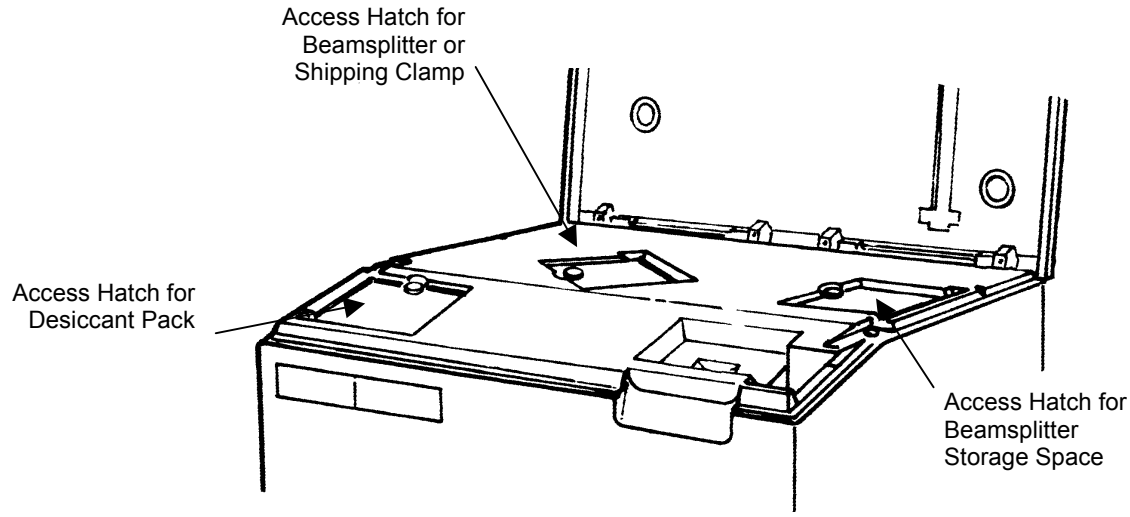
To remove the desiccant pack from the optical module:

1. Undo the lock at the right-hand side of the optical module and raise the lid, which is hinged at the back.
   There are three hatches in the cover underneath that give access to the optical module.

2. Open the hatch in the front left-hand corner of the cover. To do this, press the knob and turn it counterclockwise.

3. Lift out the desiccant pack (a blue rectangular box) and replace it with a new or reactivated one.

4. Shut the hatch immediately.



Detector module

The detector module is usually open to the sample area, but if it is sealed and desiccated (for example, if you use the instrument for studies in the far infrared), you will need to replace or renew the desiccant pack. To remove the desiccant pack from the detector module:

1. Remove and retain the screws that hold the cover of the detector module to the baseplate.

   There are four screws for a single detector cover and six screws for a double cover.

NOTE: *The two central screws for the double cover are captive. They are located at the bottom of long holes, which are hidden under the rear detector lid.*

2. Lift off the cover. The desiccant pack is the blue rectangular box.

3. Undo the single screw that holds the desiccant pack to the baseplate, and remove the desiccant pack.

4. Fit a new or re-activated desiccant pack, and refit the cover of the detector module.

Re-activating and Replacing the Desiccant Packs

If you have rechargeable desiccant packs, they 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. If you have disposable desiccant bags, see *Disposable Desiccant Packs* on page 93.

NOTE: *As an alternative to reactivating the desiccant packs, replacements are available from PerkinElmer. The part number is 04994506 for a desiccant pack for the optical module, and 04994507 for a desiccant pack for the detector module.*

Purging Sealed Areas

After new or reactivated desiccant packs have been fitted in the optical module and detector module, these areas should be purged with dry, oil-free nitrogen or air.

WARNING

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

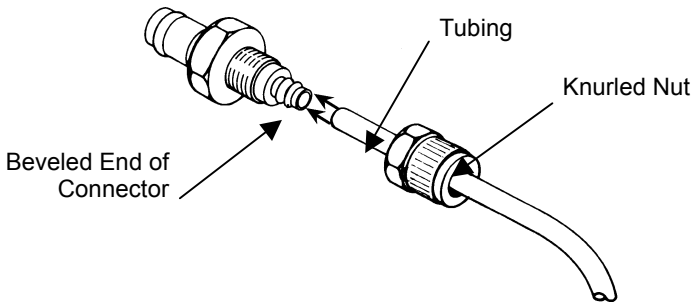
WARNING

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 pound per square inch (6.9×10^3 Pa) before you start the flow.

Purge connections

Use polyethylene tubing with a 6 mm external diameter and a 4 mm internal diameter to carry the gas to and from the instrument. Connectors are provided (04974265) that can be fitted to the ends of the tubes. To fit a connector to the tubing:

1. Unscrew the knurled nut from the connector.
2. Thread the tubing through the knurled nut and push it onto the beveled end of the connector.
3. Screw the knurled nut back onto the connector to clamp the tubing in place.



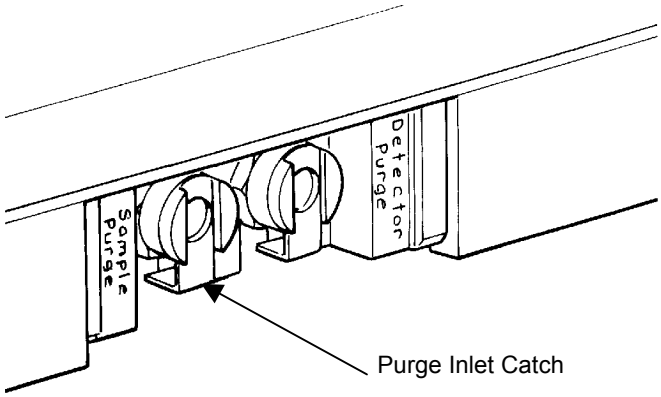
A tube fitted with one of these connectors can then be fitted to a purge inlet/outlet on the instrument. The purge inlet and outlet for the optical module is located at the back of the optical module. The purge inlets for the sample and detector areas are located on the side of the instrument.

Connecting the tubing

- Push the connector into the purge inlet until you hear a click.

Disconnecting the tubing

- Press the catch upwards, and pull out the connector.



Purging the optical module

The purge connectors for the optical module are located at the back of the optical module and are labeled **Purge In** and **Out**. The gas enters the optical module through the **Purge In** connector and escapes through the **Purge Out** connector.

1. Connect the gas tube to the purge inlet.
2. Fit a connector to the purge outlet.

WARNING

It is essential to fit a connector to the purge outlet on the optical module. The purge outlet is self-sealing and it is only by fitting a connector to it that it is opened.

3. Purge for 30 minutes at a pressure of approximately 1 lbf/inch^2 and at a rate of 5 l/min.

4. Disconnect the gas tube from the purge inlet.

Purging the detector module

The purging gas enters the detector module through the connector on the side of the sample bench that is labeled **Detector**. It escapes from the detector module through one of the holes that is provided for refilling cooled detectors.

NOTE: *If the detector module on your instrument is not sealed, these instructions do not apply. However, if you want to purge the detector module when you purge the sample area, see* Purging the Sample and Detector Areas *on page 113.*

1. Raise the lid of the detector module and raise the front edge of one of the rubber stoppers that is fitted in the cover below.

2. Purge for 15 minutes at a pressure of 1 lbf/inch^2 and at a rate of 2 l/min.

3. Disconnect the gas tube from the purge inlet, refit the rubber stopper, and close the lid.

Disposable Desiccant Packs

Disposable bags of desiccant are also available from PerkinElmer, and can be used in the optical module instead of the desiccant packs that are supplied with the Spectrum GX. The holder for those bags (L1362347), and a label for the holder, are supplied with the Spectrum GX; to obtain the disposable bags of desiccant, contact PerkinElmer and order two desiccant kits (N0171159).

Renewing the Disposable Desiccant in the Optical Module

1. Order two desiccant kits (N0171159). Each contains two bags of desiccant.

2. Inspect the plastic bags in which the spare desiccant packages are packed. If the plastic bag is not properly sealed, discard the desiccant pack.

3. Undo the lock at the right-hand side of the optical module and raise the lid, which is hinged at the back.

   There are three hatches in the cover underneath that give access to the optical module.

4. Open the hatch in the front left-hand corner of the cover. To do this, press the knob and turn it counterclockwise.

5. Lift out the desiccant pack or desiccant holder.

6. Remove the old desiccant bags from the holder and discard them.

NOTE: *Do not attempt to dry the disposable bags of desiccant for re-use. The temperatures needed to dry them will destroy the enclosing bag.*

7. Slide the four new bags into the holder.

8. With the open end of the holder at the top, lower the holder into the optical module.

9. Shut the hatch immediately.

Source Replacement

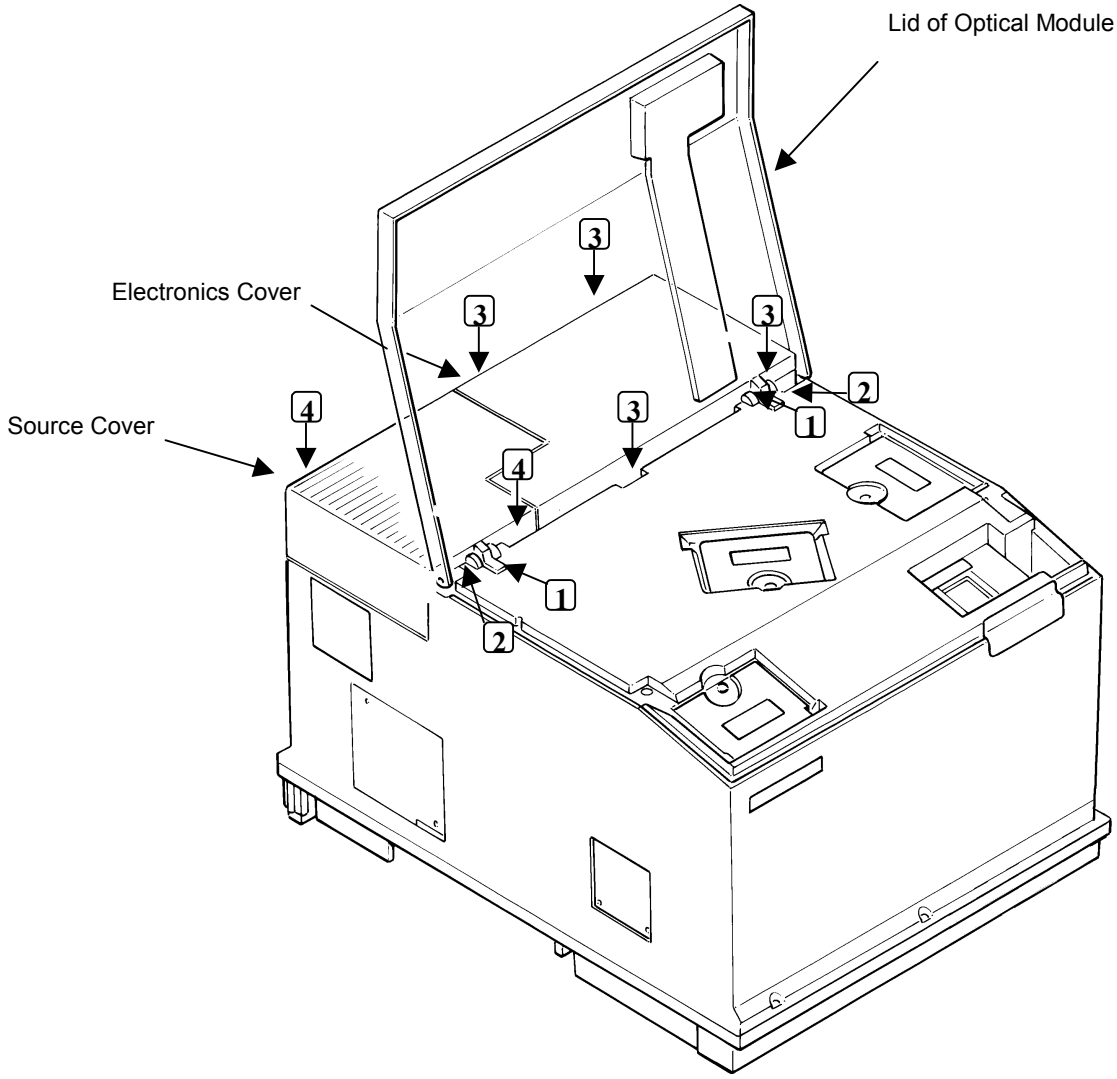
General

These instructions describe how to replace a source with a new one of the same type. Instructions are not given for replacing a source with one of a different type, for example, for replacing a mid infrared source with a near infrared source. If you want to do this, consult your nearest PerkinElmer Service Department or Agent.

NOTE: *You may have one source or a carousel containing one or two sources.*

Renewing a Single Source

1. Switch off the instrument.
2. Undo the lock at the right-hand side of the optical module and raise the lid.
3. Referring to the following diagram, remove the source cover as follows:
   a) Remove the electronics cover by taking out the four screws labelled **3**. (Two of these screws are concealed under the lid of the optical module.)
   b) Disconnect the ribbon cable from the electronics board.
   c) The ribbon cable connects the electronics board to the indicator panel in the lid of the optical module.
   d) Slacken the two nylon screws labelled **1**.
   e) Using pliers, pull the pins **2** out from the hinges.
   f) Remove the lid of the optical module.
   g) Remove the source cover by taking out the two retaining screws **4**.



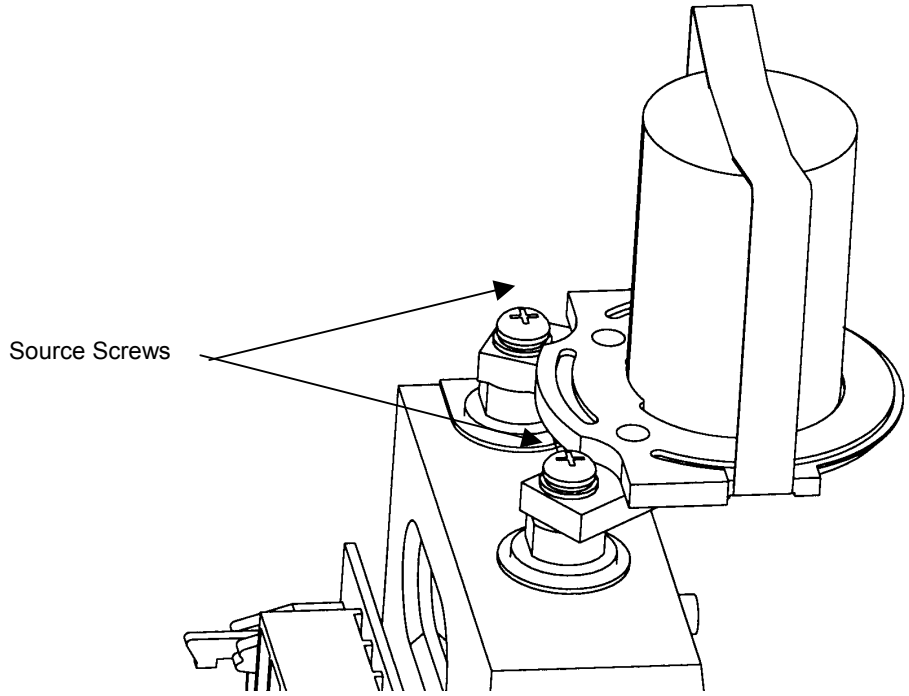
1 Screws (2)

2 Pins (2)

3 Screws in Electronics Cover (4)

4 Screws in Source Cover (2)

4. Remove the two source screws.



WARNING

If the source has recently been used, it will be very hot.

5. Remove the source.
6. Fit the new source and refit the screws.
7. Refit the source cover, the lid of the optical module and the electronics cover.

Before you use the instrument again, you must record the type and position of the source. You use the GX2000 application to do this: GX2000 enables you to use typed commands.

1. Switch on and initialize the Spectrum GX.
2. From Windows, open a DOS box or exit to DOS.
3. Change directory to pel_apps\GX2000.
4. Type **GX2000**.
   The GX2000 application starts.
5. For a mid infrared source, type **INSTALL SOURCE INT1 MIR**.
   For a near infrared source, type **INSTALL SOURCE INT1 NIR**.
6. Type **EXIT**.
   The GX2000 application closes.

Renewing a Source in the Source Carousel

The sources in the source carousel can each be renewed in the same way as one source.

The source that is to be renewed must be at the top of the source carousel, because the retaining screws are inaccessible when they are underneath. Before you switch off the instrument and remove the covers, make sure that the source that is to be renewed is at the top of the source carousel.

1. Display the Setup menu and choose **Instrument**.
   The Spectrum GX Setup tabs are displayed.
2. Click  .
   The Spectrum GX Beam Setup dialog is displayed
3. Make sure that the source that is to be renewed is not selected. If it is selected, click the other source, then click **OK**.
   The Spectrum GX Beam Setup dialog closes.
4. Click **OK**.
   The Spectrum GX Setup tabs close.

5. Wait until the source has moved into position.

Now you can renew the source:

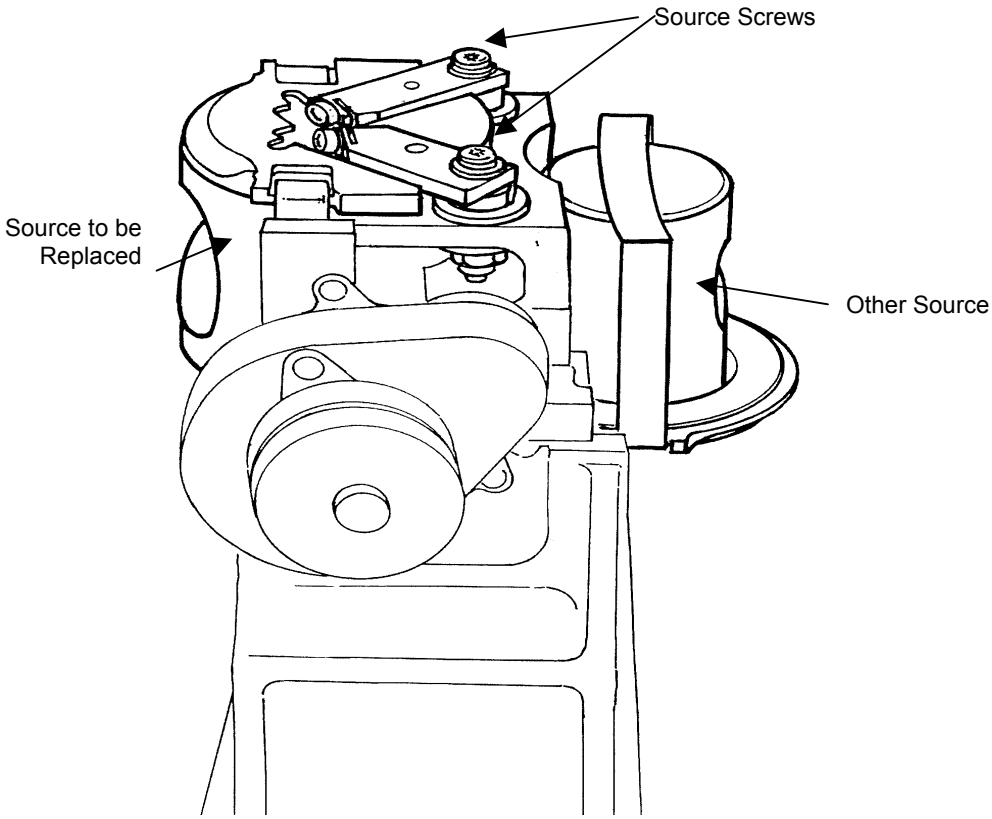
6. Switch off the instrument.

7. Undo the lock at the right-hand side of the optical module and raise the lid.

8. Referring to the diagram in *Renewing a Single Source* on page 94, remove the source cover as follows:
   a) Remove the electronics cover by taking out the four screws labelled **3**. (Two of these screws are concealed under the lid of the optical module.)
   b) Disconnect the ribbon cable from the electronics board.

      The ribbon cable connects the electronics board to the indicator panel in the lid of the optical module.
   c) Slacken the two nylon screws labelled **1**.
   d) Using pliers, pull the pins **2** out from the hinges.
   e) Remove the lid of the optical module.
   f) Remove the source cover by taking out the two retaining screws **4**.

9. Remove the two source screws.



WARNING

If the source has recently been used, it will be very hot.

10. Remove the source.
11. Fit the new source and refit the screws.
12. Refit the source cover, the lid of the optical module and the electronics cover.

Before you use the instrument again, you must record the type and position of the source. You use the GX2000 application to do this: GX2000 enables you to use typed commands.

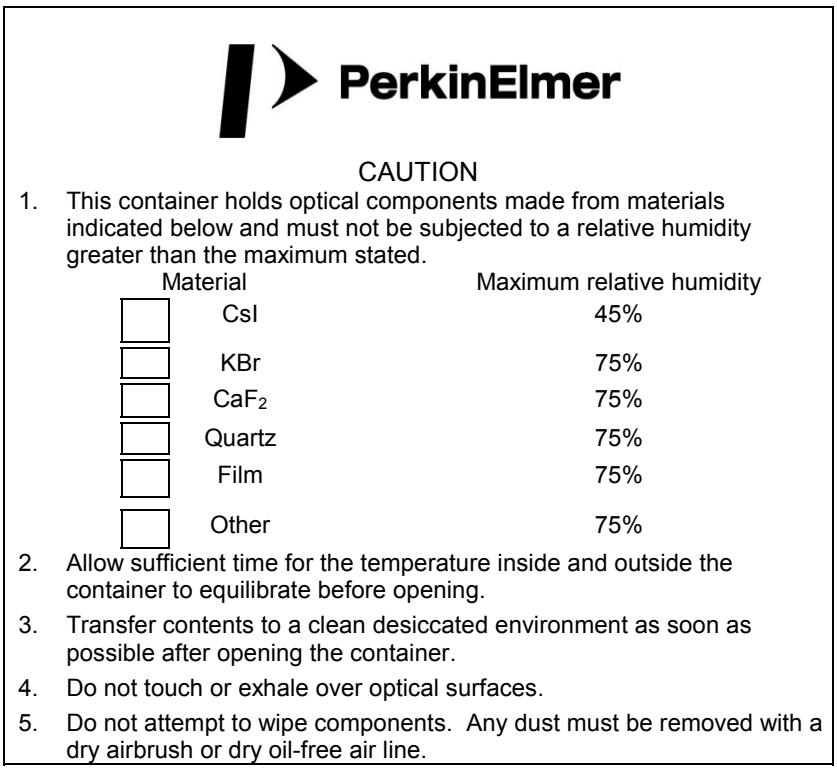
1. Switch on the Spectrum GX.
2. From Windows, open a DOS box or exit to DOS.
3. Change directory to pel_apps\GX2000.
4. Type **GX2000**.
   The GX2000 application starts.
5. For a mid infrared source, type **INSTALL SOURCE INT2 MIR**.
   For a near infrared source, type **INSTALL SOURCE INT1 NIR**.
6. Type **EXIT**.
   The GX2000 application closes.

Care and Storage of Beamsplitters

Beamsplitters must be stored in an environment that is free from water vapor. When a beamsplitter is in use, it is in the correct environment because the optical module is sealed and desiccated. There is a storage compartment in the optical module where a second beamsplitter can be stored.

If you have more than two beamsplitters, the additional ones should be stored in the containers in which they were supplied. These containers are sealed and desiccated, and are suitable for the long-term storage of beamsplitters. Make sure that when handling beamsplitters, you follow the instructions that are printed on the label on the storage container.

NOTE: *Make sure that the storage containers are kept properly closed. If they are not opened often, the desiccant packs in the containers need only be replaced with re-activated ones every six months. If the containers are opened often, we advise you to renew the desiccant packs more often.*



PerkinElmer

CAUTION

1. This container holds optical components made from materials indicated below and must not be subjected to a relative humidity greater than the maximum stated.

Material	Maximum relative humidity
☐ CsI	45%
☐ KBr	75%
☐ CaF_2	75%
☐ Quartz	75%
☐ Film	75%
☐ Other	75%

2. Allow sufficient time for the temperature inside and outside the container to equilibrate before opening.
3. Transfer contents to a clean desiccated environment as soon as possible after opening the container.
4. Do not touch or exhale over optical surfaces.
5. Do not attempt to wipe components. Any dust must be removed with a dry airbrush or dry oil-free air line.

Fuse Replacement

WARNING

Disconnect the instrument from the electrical supply before removing the fuse.

To replace the fuse:

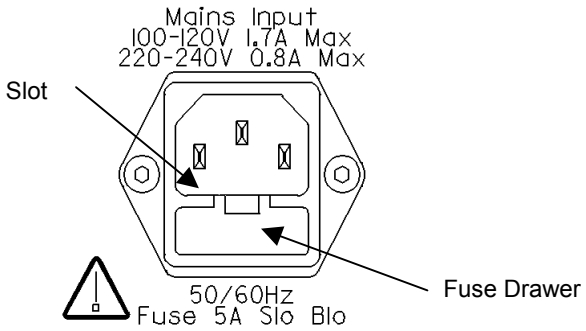
1. Insert a screwdriver into the slot, and lever out the fuse drawer.
2. Insert a new fuse, and close the fuse drawer.

WARNING

Use only the fuse specified in the table below.

NOTE: *Replacement fuses are available from PerkinElmer.*

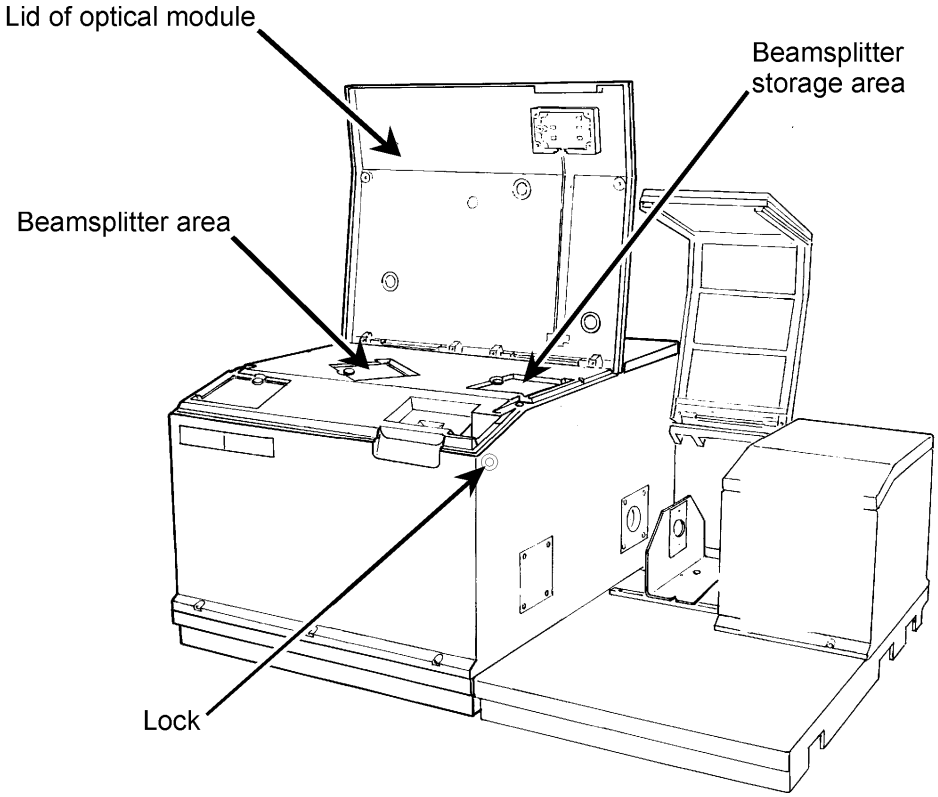
Location	Fuse	Part Number
Electrical Supply Inlet	5 Amp Slo-Blo	0C974333



Changing a Beamsplitter

NOTE: *You cannot change the beamsplitter if you have a fixed-range instrument.*

The beamsplitters are easily interchangeable and there is a storage compartment for a spare beamsplitter in the optical module.



NOTE: *For information on beamsplitter care and storage see page 105.*

To minimize the need to re-purge the optical module, change the beamsplitter as quickly as possible. If a small positive pressure of purge gas is applied when the beamsplitter is being changed, the purge is preserved (see *Purging Sealed Areas* on page 89). The desiccant packs must be removed and reactivated or replaced when they become saturated (see *Desiccant Packs* on page 87).

1. To open the lid of the optical module, undo the lock on the right-side of the optical module and raise the lid (see illustration on the previous page).

   There is an interlock on the lid of the optical module, and when this lid is raised the laser stops operating.

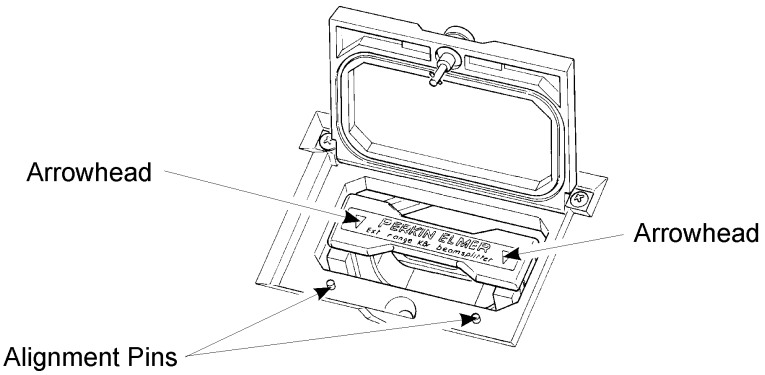
2. Open the beamsplitter area lid by pushing down the black knob and turning it counter-clockwise.

3. Lift out the current beamsplitter, taking care not to touch any optical surface.

4. Place the beamsplitter in the storage area in the optical module or in a desiccated container.

   Beamsplitters are supplied in desiccated containers that are suitable for long-term storage if the desiccant is still active. We recommend that you store additional beamsplitters in these containers.

5. Hold the new beamsplitter so that the arrowheads point towards the front of the instrument.



6. Insert the beamsplitter into the beamsplitter area, with the arrowheads pointing towards the alignment pins.

NOTE: *Make sure that the beamsplitter handle is pushed down firmly against the stops.*

7. Close the beamsplitter area lid and the lid of the optical module.
   The instrument re-initializes.

8. Always re-align the optical system.

Care and storage

The beamsplitter can be removed and replaced very easily. It is important to follow these guidelines when changing the beamsplitter:

- Never touch the surface of the beamsplitter.
- Never leave the beamsplitter out on the bench.
- Never drop the beamsplitter.
- Do not leave a hygroscopic beamsplitter in an instrument that is switched off.
- Always purge the optical module after changing the beamsplitter.

Beamsplitters made from hygroscopic materials must be stored in a warm, dry environment. In the optical module there is a storage area for a beamsplitter that is not being used. This will only preserve hygroscopic beamsplitters if the instrument remains switched on. Beamsplitters are supplied in a box containing desiccant to preserve them when not in use.

Calibration

Wavenumber calibration is provided by the 632.99 nm HeNe laser. Also, the laser is used to provide directional information about the motion of the interferometer. The laser beam path through the interferometer is offset from the infrared beam path.

Cooled Detectors

CAUTION	*These detectors must not be irradiated by the source when they are not cooled because this may prevent them from operating correctly when cooled. Do not select any cooled detector until it has been cooled, and block the beam or deselect the detector when the detector is not in use.*

If you are changing to an uncooled detector in the instrument, the low liquid nitrogen message is displayed when you choose **Update** on the Spectrum GX Beam Setup dialog. A dialog is displayed that enables you to **Cancel** and return to the Spectrum GX Beam Setup dialog or **Override** and continue with the change (overriding may damage the detector).

InSb

A better signal-to-noise ratio for accumulated scans may be achieved by changing the OPD velocity to 1.0 cm/s under high-energy conditions (≥ 0.1% of maximum throughput), and to 0.2 cm/s at lower energies.

These detectors may be damaged if they are irradiated by the maximum beam energy, and may also be temporarily impaired by visible or ultraviolet radiation. Therefore, we recommend that:

- A filter that blocks visible and ultraviolet radiation is used at all times, for example, the Near-infrared Anti-aliasing Filter (L1304540).
- You do not set the J-stop image size to greater than 6.3 mm.

Cooling the Detector

WARNING

The extremely low temperature of liquid nitrogen can burn skin and eyes. Avoid exposure by wearing protective gloves and safety goggles whenever you work with it.

WARNING

When liquid nitrogen warms to room temperature, nitrogen gas vaporizes so rapidly that resulting pressures can send a funnel or detector cap suddenly and forcefully shooting upward from the top of the dewar.

1. Open the lid of the detector area.
2. Remove the plug from the dewar.

CAUTION

Stand where you can see the inside of the funnel as you pour the nitrogen in. Pour slowly, so that neither the funnel nor the dewar overflows. Take care not to overfill the funnel and splash liquid nitrogen onto the instrument covers.

3. Insert a dry plastic funnel into the top of the detector area and slowly fill the detector dewar with liquid nitrogen.

CAUTION

Make sure that the detector dewar is filled to the top with liquid nitrogen before selecting the detector. Prevent radiation from reaching the detector by closing the B-stop or obstructing the beam path in the sample area.

WARNING

Be sure to wait the specified time when filling the funnel and before replacing the detector cap. This enables the bubbling nitrogen to settle down and the pressure to dissipate. In addition to wearing safety goggles at all times, stand back from the instrument after each time you fill the funnel.

4. Stand back and wait two minutes.

   This nitrogen also vaporizes as the dewar continues to cool. The two-minute wait enables the bubbling to settle down and the pressure of the vaporizing nitrogen to dissipate.

5. Continue to pour liquid nitrogen into the funnel, adding a little more each time the funnel empties.

   The funnel takes longer to empty as the dewar fills. This happens after two to three more funnels of liquid nitrogen.
   Because the dewar has now cooled, the liquid nitrogen does not vaporize, but instead fills the dewar.

6. Remove the funnel and wait two minutes.

   The liquid nitrogen settles down and bubbling slows.

7. When the nitrogen stops bubbling, refit the detector cap.

8. Close the lid of the detector area.

   When the detector dewar has been filled, it will remain at its operating temperature for approximately eight hours.

NOTE: *Cooled detector Dewars require pumping down after approximately 12 months operation. When the boil-off rate of liquid nitrogen becomes excessive (that is the liquid nitrogen level is low after 3 - 4 hours operation), consult the nearest PerkinElmer Service Department or Agent.*

Purging the Sample and Detector Areas

Sealed and Desiccated Areas

The optical module is sealed and desiccated. When the intensity of the water vapor and carbon dioxide peaks becomes unacceptably large, remove the desiccant pack and re-activate or renew it. Usually the detector area is open to the sample area, but it can be sealed and desiccated. For studies in the far infrared the detector area is always sealed and desiccated.

The desiccant pack should be removed and re-activated or renewed every six months. The sealed areas should also be purged at this time because they must be opened to access the desiccant packs (see *Desiccant Packs* on page 87).

Unsealed Areas

In normal circumstances, the instrument can be operated satisfactorily without purging the sample or detector areas.

If the instrument is to be operated in the far infrared, we recommend that you purge the sample area and use a sample shuttle to eliminate water vapor bands present in this region of the spectrum. The detector module is sealed and desiccated when a far-infrared detector is installed.

If the instrument is to be operated in the mid or near infrared, purging of the sample and detector areas is not usually necessary, although for critical applications in the mid infrared it may be required.

Purge Gas

Dry, oil-free nitrogen or air can be used as the purge gas.

WARNING

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

For measurements in the far infrared, or critical applications in the mid or near infrared, the detector and sample areas must be purged with gas at a pressure of 1 lbf in^{-2} (6.7 kPa) and a flow rate of about 2 l/min.

Purge Connections

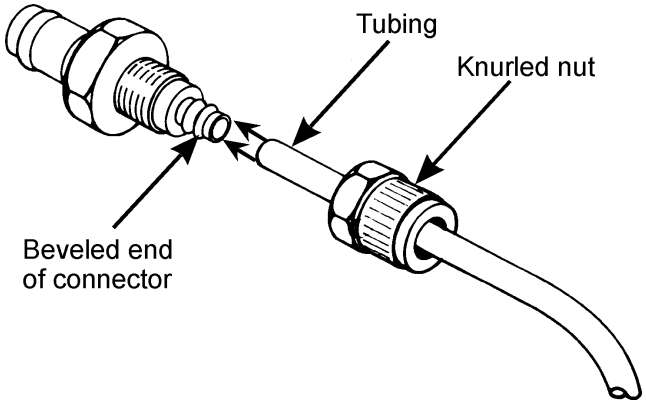
WARNING

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 lb in^{-2} (6.9x10 kPa) before you start the flow.

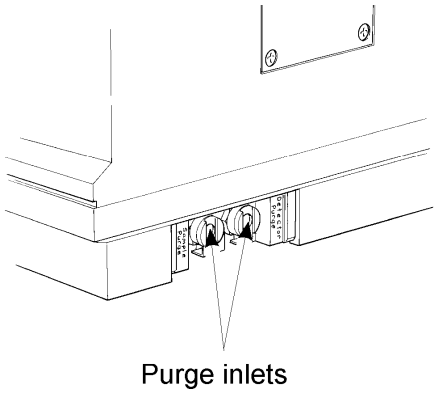
Polyethylene tubing with a 4 mm internal diameter and a 6 mm external diameter must be used to carry the gas to the purge inlets on the instrument. Purge connectors are provided (04974265) that can be fitted to the end of the tubing and then inserted into the purge inlets on the instrument.

Fitting a connector to the tubing

1. Unscrew the knurled nut from the connector.
2. Thread the tubing through the knurled nut and push it onto the beveled end of the connector.
3. Screw the knurled nut back onto the connector to clamp the tubing in place.



The purge inlets for the sample and detector areas are located on the outer edge of the sample area baseplate, below the external detector area window.

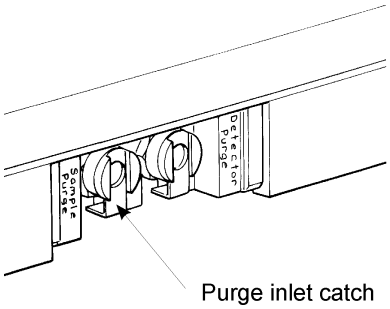


Fitting the tubing to the purge inlet

➢ Push the connector into the required purge inlet until a click is heard.

Detaching the tubing from the instrument

1. Press the catch upwards. The catch is located under the purge inlet.



2. Pull the connector out of the purge inlet.

Purging

Purging the sample area

1. Close the sample area lid.
   Note that it is only necessary to purge the sample area that you are using.

2. Fit the tubing connector into the appropriate purge inlet labeled Sample Purge (as described earlier).

3. Purge the sample area.
   The gas will escape around the edges of the sample area cover and through one of the holes that is provided for refilling cooled detectors.

Purging the sample and detector areas

1. Close the sample area lid.
   Note that it is only necessary to purge the sample area that you are using.

2. Fit the tubing connector into the appropriate purge inlets labeled **Sample Purge** and **Detector Purge** (as described earlier).
   Even if there is not a window between the sample and detector areas, both areas must be purged separately.
   You can either purge both areas or only the detector area.

CAUTION	*If there is a window between the sample and detector areas, the detector area should **always** be desiccated. Purging may be necessary when the desiccant pack is replaced. (For instructions, see* Purging Sealed Areas *on page 89.)*

3. If there is not a window between the sample and detector areas, purge one or both of these areas at a pressure of 1 lb in^{-2} (6.9 kPa) and a flow rate of 2 l/min for 10 minutes then maintain a bleed of 0.5 l/min during data collection.
   The gas will escape around the edges of the sample area cover and through one of the holes that is provided for refilling cooled detectors.

NOTE: *The sample area must be flushed each time the lid is opened and closed again.*

Sample Carrier

Installing the Sample Carrier or Accessory

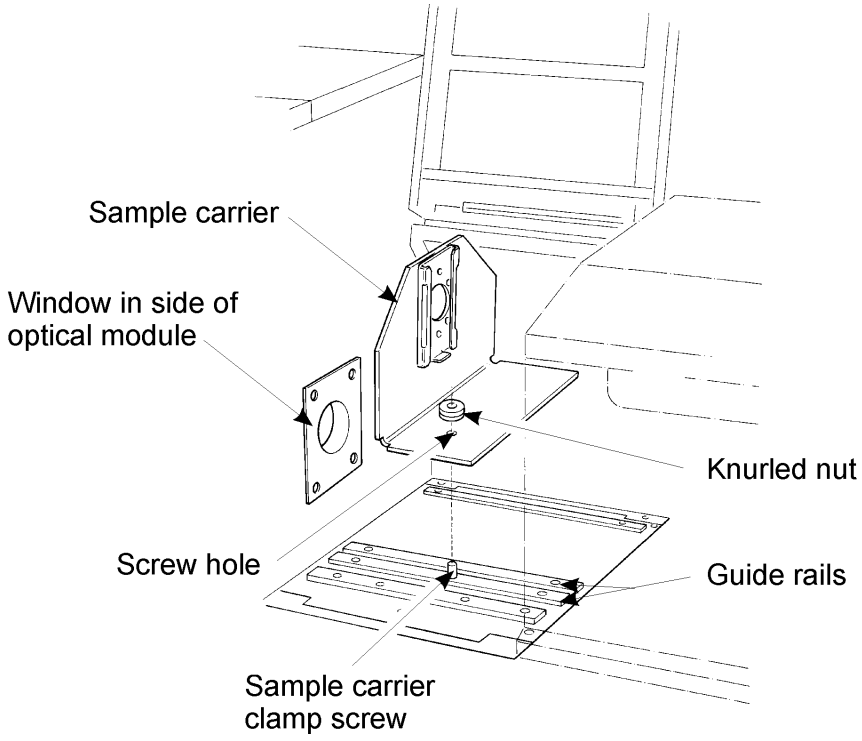
1. Hold the sample carrier in the sample area, with the vertical sample holder towards the window in the side of the optical module.

2. Align the screw hole with the sample carrier clamp screw.

3. Lower the sample carrier onto the guide rails, positioning the dowels (on the underside of the sample carrier) between the guide rails.

4. Place the knurled nut on the sample carrier clamp screw, with the flat face of the knurled nut uppermost.

5. Tighten the screw a few turns so that the sample carrier moves freely on the guide rail.

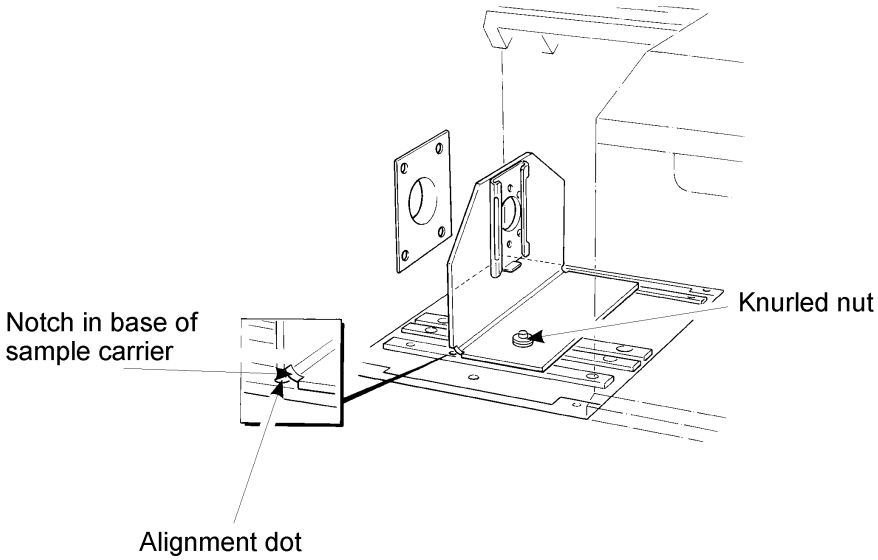


Aligning the Sample Carrier

There are two pairs of white alignment dots on the sample area baseplate. The dots closer to the optical module (the other set of dots can be ignored) enable you to locate the sample at the J-stop image position by aligning the notches in the base of the sample carrier with the white alignment dots on the sample area baseplate.

1. Move the sample carrier so that the notches on the base of the sample carrier are aligned with the white dots on the guide rails.

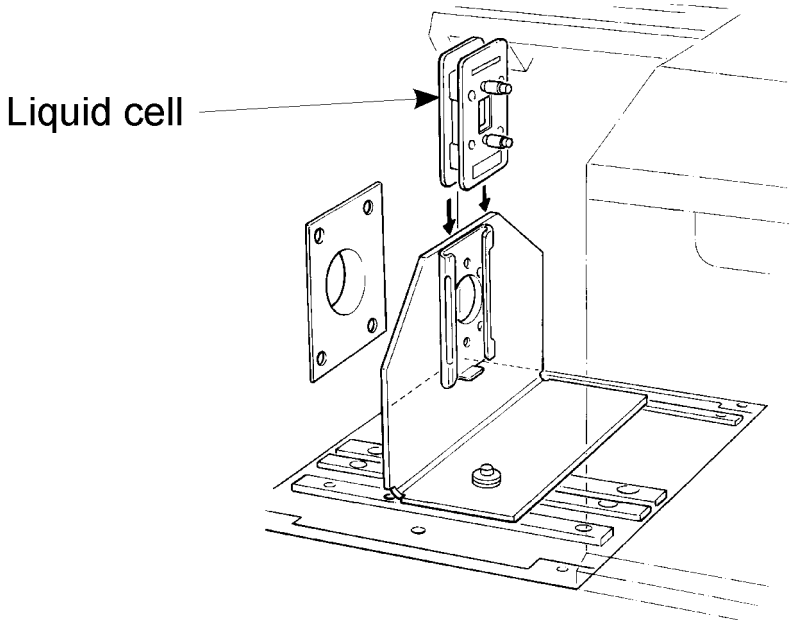
2. Tighten the knurled nut.



Installing Sampling Accessories in the Sample Carrier

The sample carrier can accommodate all the standard carrier-mounted sampling accessories. The liquid cell is used here as an example.

➢ Lower the sample holder or sampling accessory into the sample carrier.



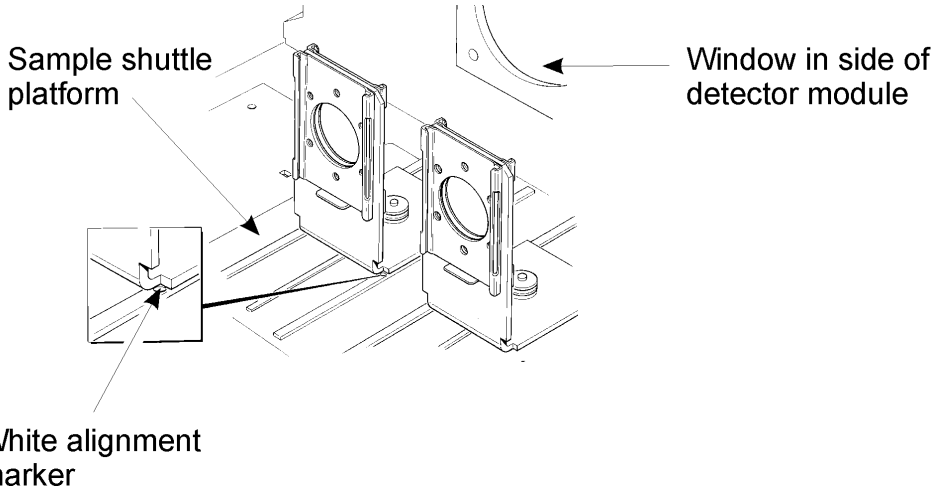
Installing and Aligning the Sample Shuttle

The sample shuttle baseplate is fitted in place of the standard sample area baseplate and a ribbon cable is used to connect the shuttle to the optical module. For details of the installation procedure, see the leaflet *Sample Shuttle User's Guide* supplied with the sample shuttle.

Aligning the Sample Shuttle

There are two pairs of white alignment marks on the sample shuttle platform. The pair of white alignment marks closer to the optical module enables you to locate the sample at the J-stop image position.

Align the notches in the base of the sample slide with the white alignment marks on the sample shuttle platform in order to locate the sample at the J-stop image position. The dual sample slide is aligned in the same way as the two single sample slides.



Theory 6

OPD Velocity

In the classical Michelson interferometer with a linearly scanning mirror, the OPD (Optical Path Difference) velocity is twice the mirror velocity. This is because the infrared beam passes from the beamsplitter to the moving mirror and back again. If the mirror travels at a velocity of x cm/s, the infrared beam travels at $2x$ cm/s.

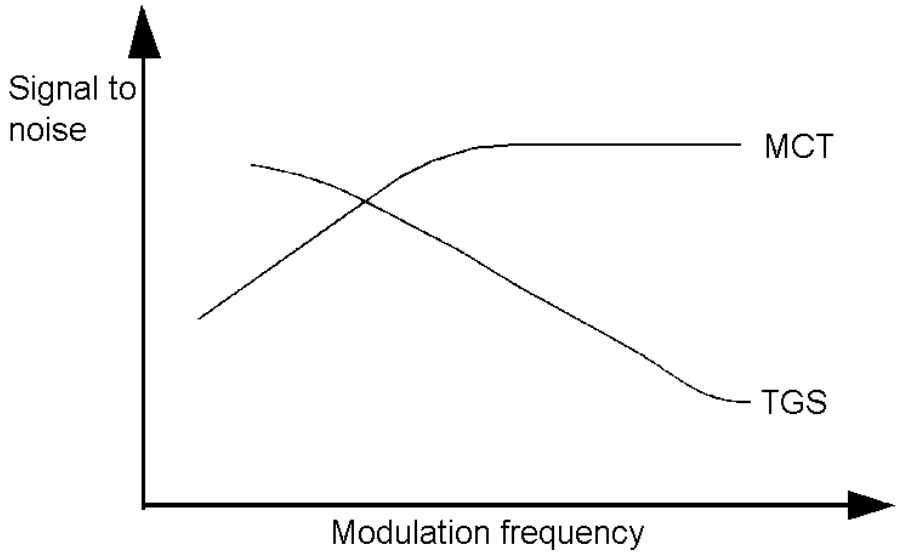
The interferometer modulates the source energy as a function of wavenumber (see *The Principle of the Michelson Interferometer* on page 30) and mirror velocity. The modulation frequency is given by:

$$f = 2V.\tilde{\nu}$$

where V is the mirror velocity, therefore the OPD velocity is $2V$
$\tilde{\nu}$ is the wavenumber of the source emission.

For an OPD velocity of 1 cm/s and a typical scan range of 4000 - 400 cm^{-1}, the modulation frequency on the detector ranges from 4 kHz to 400 Hz. For any detector there is an optimum modulation frequency range that gives the best signal-to-noise ratio in a given time.

In general, the signal-to-noise ratio of thermal detectors (that is, TGS or photoacoustic) improves as the modulation frequency decreases, while that of photoelectric detectors (for example MCT) improves as the modulation frequency increases. In each case, the improvement in signal-to-noise reaches an optimum limit. The graph below shows typical signal-to-noise versus frequency curves for two commonly used detectors.


Signal to
noise
MCT
TGS
Modulation frequency

Apodization

The process of Fourier Transformation (FT) only generates a perfect spectrum if the interferogram extends from +∞ to -∞, clearly an impossible condition. In practice, the interferogram has to be truncated at some point that corresponds to a selected maximum optical path difference. If the true energy spectrum contains transitions that are sharper than the resolution corresponding to the actual maximum OPD, then artifacts occur in the FT spectrum. These artifacts may be in the form of sidelobes or ripple. In the extreme case of a narrow *spike* in the spectrum, the response is in the form of a mathematical sine function:

$$\frac{\sin ax}{ax}$$

where x is the distance from the position of the *spike* (in wavenumbers)
a is determined by the maximum OPD
($a = 2\pi \times$ maximum OPD).

Apodization functions

If the data are gradually attenuated or apodized instead of terminating abruptly at the maximum OPD, then the magnitude of the outlying sidelobes can be reduced at the expense of broadening the central peak, that is, by degrading the spectral resolution. The form of the attenuation curve, or apodization function, determines the relative magnitude of three factors:

1. The loss of resolution.

2. The reduction of the largest sidelobes.

3. The rate of attenuation or convergence of ripple far from the central peak.

Because each of these factors can only be improved at the expense of one or both of the others, the optimum choice of apodization function depends on the relative importance of the three factors in a particular spectral measurement.

Note that, except at the ultimate resolution of the instrument, factor 1, loss of resolution, can be compensated for by selecting a better resolution setting. This in turn necessitates a longer scanning time to achieve the same signal-to-noise ratio. So, in effect, there is a direct trading of improvement in factors 2 and 3 against scan time. Some typical examples are given below.

	Relative Width*	**Largest Sidelobe****	**Attenuation Rate of Ripple*****
Boxcar	0.603	0.217	$1/\Delta\tilde{\nu}$
Weak	0.724	0.058	$1/\Delta\tilde{\nu}$
Medium	0.844	0.014	$1/\Delta\tilde{\nu}$
Raised cosine	0.907	0.0073	$1/\Delta\tilde{\nu}$
Strong	0.965	0.0037	$1/\Delta\tilde{\nu}$
Kaiser-Bessel	1.19	0.0005	$1/\Delta\tilde{\nu}$
Triangle	0.885	0.047	$1/(\Delta\tilde{\nu})^2$
Filler	1.16	0.0009	$1/(\Delta\tilde{\nu})^3$

* On this scale, a relative width of 1.0 corresponds to a width at the half height equal to the reciprocal of the maximum optical path difference.

** Sidelobes can be positive or negative. The magnitude of the largest is given.

*** $\Delta\tilde{\nu}$ = Distance in cm^{-1} from the peak.

Function	Feature
Boxcar	Best resolution
Weak	Good Resolution
Medium	General Purpose
Raised cosine	General Purpose
Strong	General purpose, low ripple
Kaiser-Bessel	High accuracy, low ripple
Triangle	Good convergence
Filler****	High accuracy, high convergence

**** Use an apodization function with high convergence and/or very low ripple for background or sample spectra when working in a region of low spectral energy in the presence of a strong, abrupt spectral feature. An example of such a situation is when working in the very near infrared with a quartz beamsplitter, which inherently has an abrupt spectral cutoff.

J-stop

The rays of the collimated beam in an interferometer are not all parallel to the optical axis but are spread over a range of angles. This can be thought of as being equivalent to a cone of radiation emanating from each point on the beamsplitter. The function of the J-stop is to limit the angle of this cone.

The need to limit the angle arises because the optical path difference (OPD) for a ray at an angle θ to the axis is effectively less than that for an axial ray by a factor of cosθ. If this difference at maximum OPD is greater than the shortest wavelength of the radiation being measured, there will be severe degradation of line shape and resolution. When expressed as a wavenumber, it is known as the J-stop wavenumber and is the highest wavenumber at which good resolution can be obtained. For wavenumbers less than half the J-stop wavenumber, the effect on resolution is insignificant. The J-stop wavenumber ($\tilde{\nu}$) is given by:

$$\tilde{\nu} = \frac{\Delta\tilde{\nu}}{1-\cos\theta} \approx \frac{2\Delta\tilde{\nu}}{\theta^2} = \frac{2}{\theta^2 D} \qquad 1$$

where $\Delta\tilde{\nu}$ is the nominal resolution.
D is the maximum OPD (in cm).

The angle θ is directly proportional to the diameter of the J-stop and its image in the sample area (d in mm) and, for this instrument:

$$\theta = \frac{d}{280} \qquad 2$$

Combining equations *1* and *2*:

$$\nu = \frac{2x\,2\theta^2}{d^2 D} = \frac{156\,800}{d^2 D} \qquad 3$$

There are two further effects of the J-stop that are interrelated and must be taken into account.

Firstly, because of the shorter effective OPD, off-axis rays experience an OPD velocity slightly less than that experienced by axial rays. Therefore, features in the spectrum calculated from such off-axis rays appear to be at a slightly longer wavelength (lower wavenumber) than that calculated from the on-axis ray of the same wavelength. Rays at an angle θ are subject to a wavelength calibration error $\Delta\lambda$, where:

$$\Delta\lambda = \lambda\frac{\theta^2}{2} \qquad 4a$$

or a wavenumber calibration error $\Delta\tilde{\nu}$, given by:

$$\Delta\tilde{\nu} = \tilde{\nu}\frac{\theta^2}{2} \qquad 4b$$

The average error, $\Delta\lambda'$ or $\Delta\tilde{\nu}'$ for all rays from axial to angle θ, as defined by the J-stop, is given by:

$$\Delta\lambda' = \lambda\frac{\theta^2}{4} \qquad 5a$$

$$\Delta\tilde{\nu} = \tilde{\nu}\frac{\theta^2}{4} \qquad 5b$$

So long as no part of the radiation – either axial or extreme rays – is obstructed by the sample or sampling accessory, the above error is easily corrected by the instrument software because the J-stop size is known.

Secondly, because the usual sample position is located at a point in the optical path where there is an image of the J-stop, the sample or sampling accessory itself tends to act as a J-stop when its effective size is smaller than the current J-stop. Conversely, when a small J-stop is in use a smaller sample can be used without loss of energy. In any situation where the sample or sampling accessory is serving as the effective J-stop, or is obstructing some part of it, a calibration error can occur. The maximum possible value of this error is given by equations 5a and 5b.

B-stop

The B-stop is a variable aperture positioned in the optical path near to an image of the beamsplitter. Reducing the aperture size provides a convenient method for reducing the intensity of radiation passing through the instrument. This has two primary applications: firstly, it enables you to avoid overloading high sensitivity detectors in situations where the attenuation of the sample or sampling accessory is small; and, secondly, it restricts the angle of the cone of radiation passing through a sample at the usual sample position (the J-stop image).

For critical measurements of absolute transmission, for example, of optical filters, reduction of the B-stop size is recommended because this reduces the effect of optical beam distortion created by the sample. Reducing the B-stop size may also improve the wavelength accuracy of certain optical filter measurements. Of course, if the detector is not overloaded when the B-stop aperture is large, more scans will be required with the smaller B-stop aperture to achieve the same signal-to-noise ratio.

CAUTION	*Certain sampling accessories obstruct the center of the beamsplitter image and, with these, there will be a certain B-stop aperture size below which all signal will be lost.*

Phase Correction

In an ideal interferometer, zero optical path difference for all wavelengths of interest would occur at the same point in the scan of the moving mirror, resulting in a symmetric interferogram. In such an instrument, the cosine transform would generate the correct spectrum.

In order to achieve this simple condition, three conditions would have to be met:

- The zero OPD reference point from which the transform is calculated would have to be exactly at zero OPD.
- The beamsplitting surface would have to introduce no wavelength-dependent phase change.
- The optical thicknesses of the beamsplitter and compensator plates would have to be precisely equal.

In practice, these three conditions are not met and, in particular, the use of a high efficiency, multi-layer beamsplitter surface inherently generates wavelength dependent phase effects.

To overcome the difficulty, both the cosine and sine transforms of the interferogram are calculated and combined, in proportions that vary with wavelength, to give the correct final result. The true spectral data can be thought of as having been rotated through an angle A from the ideal zero position, which corresponds to the cosine transform. For any wavelength, the cosine and sine transforms produce the projections of the real value on to the two axes. The true value of the spectrum at that wavelength can then be generated by multiplying the cosine projection by cos -A and the sine projection by sine -A, and adding them. In the case of calculating A for every calculated wavelength, this is equivalent to squaring both the cosine and sine transforms, adding them, and taking the square root. This latter method is *magnitude* phase correction.

The alternative is to generate what is known as a *phase curve* which is, in effect, a smooth curve defining A for all wavelengths. Inherently, the phase curve is simple, continuous and not rapidly changing, and can be defined by a few values. This can then be used to generate a true spectrum from the cosine and sine transforms as described above, interpolating values for A as required.

The usual method of generating the phase curve is to perform a low resolution transform of the interferogram and calculate the values of A from the relative values of the cosine (c) and sine (s) transforms using $A = \tan^{-1} s/c$.

There are four possible sources for the phase curve data:

- Self, where each spectrum, whether background or sample, is used to generate its own phase curve.
- Background, where the background data are used to create the phase curve used for both the background and sample spectra.
- Self Locked, where the phase curve used for correcting background spectra is the one obtained from the background that is current at the time of locking, and the phase curve used for correcting sample spectra is the one obtained from the last sample from which data were collected before locking.
- Background Locked, where the phase curve used for both the background and sample spectra is the one obtained from the background that is current at the time of locking.

The optimum choice from these four depends, firstly, on the completeness of the spectral data for sample and background; and, secondly, on the possibility that, in the interval between collecting the data used to create the phase curve and measurement of the spectrum of interest, something may have occurred that could alter the phase curve.

Under most circumstances, self-phase correction is the optimum choice. However, in spectral regions where sample absorption is such that the signal is almost buried in noise, the phase curve will usually be strongly affected by the noise and give inaccurate data. In such cases, it may be better to use background phase correction because calculation of the background phase curve will not have been affected by the absorption. However, background phase correction is susceptible to any changes in the instrument that occur between scanning of the background and of the sample. Thus, it may be less accurate if, for example, there is a long delay between collection of the background and sample spectra.

Locked (Self or Background) can be of advantage in cases where, for any reason, the background spectral data contains extensive regions of low spectral energy.

The phase correction step in processing the interferogram can be avoided by calculating the magnitude spectrum. The disadvantage of this procedure is that, while noise in spectra can have negative as well as positive values, the result will always be treated as positive. Thus, the effect will be to *rectify* noise and create an offset error in low transmittance values. Also, the magnitude calculation is not suitable for single-sided interferograms where complete data is not available from both sides of the centerburst.

Glossary

This glossary contains definitions of the terms used in this manual and terms related to FT-IR spectroscopy in general. The terms are listed in alphabetical order. Where a definition makes reference to another entry in this glossary, the entry referred to is shown in italics.

Abscissa

The horizontal axis of a spectrum, along which wavelength or wavenumber is usually plotted.

Alignment

The adjustment of the interferometer mirror angles to optimize the interferogram centerburst amplitude. This is achieved by aligning one interferometer mirror.

Apodization

A mathematical operation that reduces unwanted oscillations on either side of narrow bands in the spectrum. The oscillations are reduced by multiplying the interferogram by a function that decreases steadily as it approaches the maximum path difference. Application of an *apodization function* causes some loss of resolution, or line broadening. However, the overall noise level in the spectrum is reduced, in an analogous fashion to spectral smoothing.

Apodization function

The various apodizing functions give different compromises between line broadening and reduction of oscillations on either side of narrow bands in the spectrum. See also *Boxcar apodization* and *Norton-Beer apodization functions*.

Background spectrum

The background spectrum is a single-beam spectrum recorded without the sample in the beam. It is used by the instrument in a ratio calculation that eliminates the instrument response and features introduced into sample spectra by atmospheric absorption, or possibly by using a cell or sampling accessory.

Background phase correction

If phase errors are suspected with low transmitting samples the correction results may be improved by selecting background phase correction, whereby the correction routine is calculated from the current background spectrum.

Beamsplitter

A beamsplitter is a plate with approximately equal transmittance and reflectance, used to generate and recombine the two beams of an interferometer. The intensity of the beams emerging from the interferometer depends upon the product of the transmittance and reflectance of the beamsplitter and on the OPD between the two internal beams. The choice of beamsplitter material depends upon the wavelength range to be covered.

Bi-directional interferogram

The interferometer collects data in both scanning directions. In interferogram-combined mode, the interferometer collects data when moving in both directions and the two sets of data are added. In separate mode, the interferometer scans as in combined mode but data from each direction are stored separately and not added together.

Boxcar apodization

Boxcar, or no apodization, is used to enable the highest possible resolution to be obtained. When Boxcar is used, all points in the interferogram are given equal weight. If the resolution is not better than the narrowest linewidth in the spectrum, oscillations appear in the baseline on either side of the peaks.

B-stop

The size of the B-stop aperture defines the area of the beam passing through the interferometer. Reducing the size of the aperture limits the energy from the source that passes into the interferometer, and may thus protect sensitive detectors from becoming saturated or damaged.

Centerburst

The region of the interferogram around zero path difference, where the amplitude is greatest.

Co-added scans

A number of spectra or interferograms can be combined during monitoring to improve the signal-to-noise ratio, but the monitored spectrum or interferogram is updated less rapidly.

Continuing a scan

Add a number of scans to the last spectrum you collected in order, for example, to improve the signal-to-noise ratio. The resultant spectrum is the average of the total number of both original and added scans.

Data interval

The data interval, or digital resolution, refers to the *abscissa* spacing of data points in a spectrum or interferogram. The unit for the spectral data interval is the wavenumber (cm^{-1}) and for interferogram data it is the number of interferogram points collected.

Data range

The data range of the instrument is the wavenumber range over which data collection is requested by the user. The data range must be compatible with the operating range of the components of the beam path, for example, the *beamsplitter* and detector.

Double-sided interferogram

The instrument starts scanning the interferogram at one side, the interferogram extends through the centerburst and out to an equal distance on the other side.

Dynamic range

The ratio of the intensity of the maximum signal near zero path difference to the r.m.s noise level in the interferogram. For signal averaging to function properly, the dynamic range of the signal channel must exceed that of the interferogram so that no significant part of the signal is lost.

Energy

In energy mode, the instrument scans continuously about the center of the interferogram and displays the relative energy in the *centerburst*.

Filter wheel

The filter wheel accessory enables various filters and attenuators to be positioned in the beam. The introduction of a filter enables you to optimize the system for a particular *scan range*.

Fourier transformation

The mathematical process by which the interferogram is analyzed into its component frequencies with their corresponding amplitudes.

Gain

The detector signal is amplified before being digitized. The gain of the amplifier can be changed to ensure that the analog to digital converter is not overloaded by highly transmitting samples, and that it is used efficiently for strongly absorbing samples.

Initialization

The process by which the instrument is prepared for use - tests are performed to ensure that the instrument is working correctly and the *instrument setup* is implemented.

Instrument setup

The instrument setup defines the settings of optical and electronic components in the interferometer module and the instrument operational parameters.

Interferogram

A recording of the detector signal obtained as the path difference between the two beams of an interferometer is varied. An interferogram usually consists of a strong signal at zero path difference (the *centerburst*), decaying rapidly towards the sides.

Interleaved scan cycle

When a *sample shuttle* is installed, the instrument can perform a series of interleaved sample and background scans, so that each sample is ratioed against an effectively simultaneously recorded background.

J-stop

The circular J-stop (Jacquinot-stop) aperture defines the angle at which rays pass through the interferometer and thus restricts the beam divergence to the maximum acceptable for the required *resolution*.

J-stop image size

The size of the J-stop image at the focal point in the sample area.

J-stop resolution

The best *resolution* that can be achieved up to the *J-stop wavenumber* for a given J-stop size.

J-stop wavenumber

The upper wavenumber limit at which the J-stop resolution is achieved.

Magnitude phase correction

The phase correction step in processing the interferogram can be avoided by calculating the magnitude spectrum. Magnitude spectra are not affected by phase errors but are subject to ordinate errors in regions of low transmittance. If used, it must be applied to both the background and sample spectra.

MCT detector

The MCT (Mercury Cadmium Telluride) detector is a high sensitivity, photoconductive device operated at liquid nitrogen temperature. It has a much better response at high modulation frequencies than the *TGS detector*, so faster scan speeds are used. For the highest sensitivity, narrow band MCT detectors, which cut off at about 700 cm^{-1}, are used. MCT detectors are saturated on exposure to full beam energy, so attenuation may be needed with highly transmitting samples.

Monitoring

The instrument scans continuously and displays the result of each scan on the screen. A background spectrum, a sample spectrum, an interferogram, or the *energy* incident on the detector can be monitored.

Norton-Beer apodization

The three apodization functions described by Norton and Beer as Weak, Medium and Strong are provided. They give the best functions compromise between reduction of sidelobes and increase in spectral bandwidth.

OPD

The OPD (optical path difference) is the difference in optical path between the two beams of the interferometer. The maximum OPD defines the range scanned on each side of the interferogram for double-sided scanning, or the OPD scanned to the longer side for single-sided scanning and is approximately the reciprocal of the resolution value. The maximum OPD is independent of the apodization function used.

OPD velocity

The OPD velocity, or scan speed, for an interferogram is the rate at which the *OPD* changes during a scan.

Optical filters

They are located on the *filter wheel*. The introduction of a filter enables you to optimize the system for a particular *scan range*. For example, if you want to collect spectra in the near infrared region using a cooled detector, the introduction of a filter reduces the amount of mid and far infrared energy that reaches the detector.

Ordinate

The vertical axis of a spectrum, along which % Transmittance, Absorbance or % Reflectance are plotted.

PAS detector

In Photoacoustic Spectroscopy (PAS), sample absorption causes heating, which creates a pressure wave in a sealed cell. The pressure wave can be detected by a sensitive microphone. This technique is used for the study of certain solids.

Phase correction

This is used to compensate for frequency-dependent phase variations caused by the *beamsplitter* and signal amplification, which produce asymmetry in the interferogram. The information used for phase correction is obtained from the central region of the interferogram by a procedure called the Mertz method. The most accurate results are obtained with *double-sided interferograms*.

Phase correction source

The type of spectrum or interferogram that is used as the source for *phase correction*. The phase correction source can be *self*, *background* or *magnitude*.

Polarizer

This is used to polarize the output beam of the interferometer. The polarizer can be moved in and out of the beam and rotated through 180° in one degree increments. The introduction of a polarizer enables orientational and structural studies to be performed.

Purging

A procedure designed to remove unwanted gases (typically water vapor and carbon dioxide) from a specific area of the instrument. The optical module, the sample and detector areas can be purged.

Resolution

See *Spectral resolution*.

Ratio spectrum

The most common spectrum to collect. The sample spectrum is divided by a background spectrum, to remove the instrument characteristics.

Sample shuttle

The sample shuttle provides a means of positioning either of two sample slides in the optical beam of the spectrometer. The primary function of the sample shuttle is to enable the use of an *interleaved scan cycle*. An alternative, and less common, use of the shuttle is to enable an accessory to be switched in and out of the beam without disturbing the alignment of the accessory.

Scan range

The maximum wavenumber range over which data can be collected.

Scan speed

See *OPD velocity*.

Self phase correction

The sample spectrum is phase corrected from the sample interferogram and the background spectrum is phase corrected from the background interferogram.

Setup

See *Instrument setup*.

Signal averaging

Performing several scans and averaging them improves the *signal-to-noise ratio* in the final spectrum. This is because noise, which is a random signal, decreases as a result of the averaging process, whereas the detector signal is reinforced. The improvement in *signal-to-noise ratio* is proportional to the square root of the number of scans averaged.

Signal-to-noise ratio

This is a measure of the relative magnitudes of the detector signal and the noise in a spectrum. It is usually measured in the region where the optical system responds most strongly, and must be quoted for a particular resolution and scan time.

Single-beam spectrum

Dispersive infrared spectrometers measure double-beam spectra: the background and sample spectra are measured together and ratioed as the instrument scans through the wavenumbers.

FT-IR spectrometers, however, measure single-beam spectra: all the wavenumbers of the background spectrum are measured at once, and then all the wavenumbers of the sample are measured at once.

Single-sided interferogram

Scanning starts at the required distance on the longer side, progresses through the *centerburst* and finishes close to the centerburst.

Spectral resolution

Spectral resolution describes the ability of the instrument to distinguish between adjacent frequencies in the spectrum.

TGS detector

The TGS (TriGlycine Sulfate) detector is a pyroelectric (thermal) device operated at room temperature and is the most commonly used detector in FT-IR spectroscopy.

Uni-directional interferogram

The interferometer collects data in only one direction and returns to the starting point before collecting the next interferogram.

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