OPERATION MANUAL

DW-530 FTIR SPECTROMETER

DRAWELL
Artist of Science

Please read operating manual before installation and operation.

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WARNING AND CAUTION

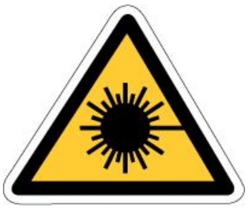
1. Installation attempt that any user does without our special personnel may cause parts protection invalid; installation indications described in the manual cannot replace the installation work done by special personnel.

   There are some sensitive optical components included in the FTIR main unit. Room temperature balance about 24 hours is needed after the instrument arrives. During the period, please do not uncover the instrument. Remain the instrument and the spare parts in the packing case until the special personnel arrives.

2. Before our special personnel finish installing the instrument, please do not run interferometer, or optical components may be broken. During using period, user should keep proper humidity and temperature in the lab. Damage of KBr beamsplitter and window plate caused by high humidity is not in our warranty range.

3. If source should be opened for some reason, its high temperature surface must not be touched to avoid user being hurt.

4. Please do not envisage the laser by all means!



Laser Warning Label

Contents

Chapter 1 Introduction

ModelDW-530 FT-IR spectrometer is a new generation of FTIR spectrometer, developed and manufactured by Shanghai Drawell Scientific Instrument Co.,Ltd. with independent property right. It features simple operation, complete accessories and rich software functions etc. It is a necessary analytical instrument used for research and production in the field of petroleum, medicine, chemical industry, environment protection, university education, agriculture, public security, and national defense etc.

1.1 FTIR History

The story of FTIR (Fourier Transform Infrared) spectrometry began in 1891 when a device called the two-beam interferometer was invented by the U.S. physicist, Albert Abraham Michelson. The interferometer splits and recombines a beam of light such that the recombinant light produces a wavelength-dependent interference pattern. Michelson knew that the interference pattern, or interferogram, contained information from which a spectrum could be obtained, but at the turn of the century, only atomic spectra were of any interest to the scientific community. On invention therefore, the interferometer was largely a fascinating tool awaiting the discovery of a more useful application.

Around 1950 there were two discoveries that suggested that this “more useful application” might be IR spectrometry. At that time, most IR analysis was done by Dispersive spectrophotometers which beamed IR radiation through a sample, separated the exiting light, and then examined each wavelength at the detector separately. The first of the two discoveries, made by the British astrophysicist, Peter Fellgett, was that the interferometer produces and sends to the detector information from all wavelengths of the incident IR beam simultaneously. This simultaneous measurement of incident energy is known as the multiplex advantage. The second discovery, made by Jacquinot, was that more energy reaches the sample and detector when using an interferometer than when using a conventional Dispersive device. This increase of throughput energy is known as Jacquinot’s advantage. Fellgett’s and Jacquinot’s discoveries showed that from an energy point of view, an interferometer in combination with an IR source and detector could provide tremendous advantages over then-current Dispersive instruments. In 1949 Peter Fellgett used an interferometer for astronomical spectroscopy and transformed the interferogram into a spectrum by means of a mathematical algorithm called the Fourier transform. Basically, the components of FTIR analysis were all in place.

There was only one problem: The transformation of the raw interferogram into a spectrum was extremely time consuming. Even with the help of computers in the early sixties, a Fourier transform could take hours and could easily take longer if the interferograms had to be transported to a computer center. In 1964, the Fast Fourier transform was discovered (or rediscovered) by Cooley and Tukey, and instead of taking hours, transforms were completed in a matter of minutes. By the middle seventies, the final pieces had fallen into place. Minicomputers allowed spectra to be computed in the laboratory immediately after measurement of the interferogram, and small gas lasers were found to be ideal clocking mechanisms for the interferometer.

Today's FTIRs combine the tremendous computational power of a microcomputer with the precision and accuracy of elegant IR instrumentation. FTIR is by far the preferred technique of measuring high quality IR spectra. If it can be said that a technology epitomizes the concept of having one's cake and eating it too, that technology is FTIR.

1.2 Basic Principal of FTIR

An IR spectrometer is an analytical instrument that passes IR radiation through a substance and measures its absorbance (or transmittance). Because each substance has a characteristic absorbance pattern—absorbing some wavelengths and not others—the substance can be qualitated or identified. And because the amount of the substance is proportional to the amount of absorbance, the substance can also be quantitated.

As mentioned above, the first types of IR spectrometers were dispersive instruments. These instruments passed an IR beam through a sample and then broke it up into discrete wavelengths before it entered the detector. Each wavelength was examined in turn by the detector and "reported' to a plotter that slowly traced out the spectrum. FTIRs, on the other hand, do not separate the IR beam before it passes to the detector. The interferometer sends all wavelengths to the detector simultaneously and the detector reports its information in the form of an interferogram. A computer must then transform the interferogram into a spectrum by means of the Fast Fourier transform. (A Fourier transform is the remapping of a sine or cosine function in the time domain to the frequency domain, or vice versa.) In essence, the interferogram reports the total absorbance, and the computer discerns the individual absorbance for each wavelength.

There are many types of interferometers, but most are based on the design of Michelson's original 1891 model. Since the theory of all interferometers is the same and the Michelson interferometer is the simplest, we will use it to illustrate the basics of FTIR theory.

The simplest form of the Michelson interferometer is shown in Figure 1-1.

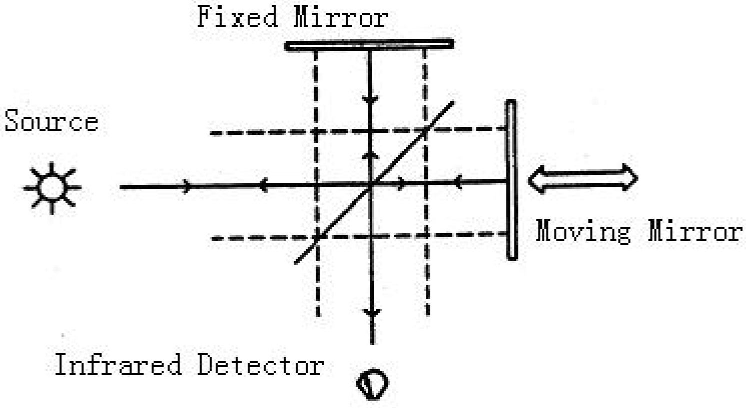


Figure 1-1 A Simple Michelson Interferometer

It consists of a source, two perpendicular mirrors, a beam splitter, and a detector. One of the mirrors is fixed and the other moves along an axis perpendicular to its plane. A beam of radiation from the source is directed to the beam splitter where half of it is reflected to the fixed mirror and the other half is transmitted to the moving mirror. Because the moving mirror causes a pathlength difference in one of the beams, the beams interfere when they recombine at the beamsplitter. This interference causes a variation in the intensity of the recombinant beam which is again split, half on average going to the detector and half going back to the source. The beam passing to the detector produces the interferogram and ultimately yields the spectrum. The beam that returns to the source contains the same information as that going to the detector, but is 180°out of phase. It is rarely of interest because of the difficulty of separating it from the input beam.

We will be able to understand how the interferometer operates if we start with an example of the way it effects a monochromatic light source (consisting of a single wavelength). When a single wavelength of light hits the beamsplitter, half goes to the fixed mirror and half goes to the moving mirror. If the mirrors are equidistant from the beam splitter, the beams will return to the beamsplitter in phase and interfere constructively. With an ideal beamsplitter, all the returning light will be sent to the detector and none will go back to the source. (None returns to the source because the returning source beam actually destructively interferes due to phase delays on reflection.) The point at which the fixed and moving mirrors are equidistant from the beamsplitter is called the Zero Pathlength Difference (ZPD).

If the moving mirror is moved 1/4 the wavelength of the incident light, the total pathlength of the beam that travels to the moving mirror will be 1/2 wavelength longer. The pathlength difference between the fixed and moving mirror is called the optical retardation. The beam of light traveling back to the beamsplitter will be 1/2 wavelength out of phase with the beam coming from the fixed mirror and the beams will destructively interfere on recombination. No energy will be sent to the detector and all of it will go back to the source.

If the moving mirror is moved 1/4 wavelength further to 1/2 the wavelength of the incident beam, the optical retardation will be 1 wavelength and the beam from the moving mirror will return to the beamsplitter exactly in phase with the fixed mirror beam. Again, the maximum beam intensity will go to the detector. As the mirror is moved further away from the beamsplitter, the pattern continues: If the mirror is moved at constant velocity, the detector records a cosine wave with a maximum intensity each time the optical retardation is an integral multiple of the source wavelength. Figure1-2 shows the relative intensity of the detected beam as the moving mirror is displaced.

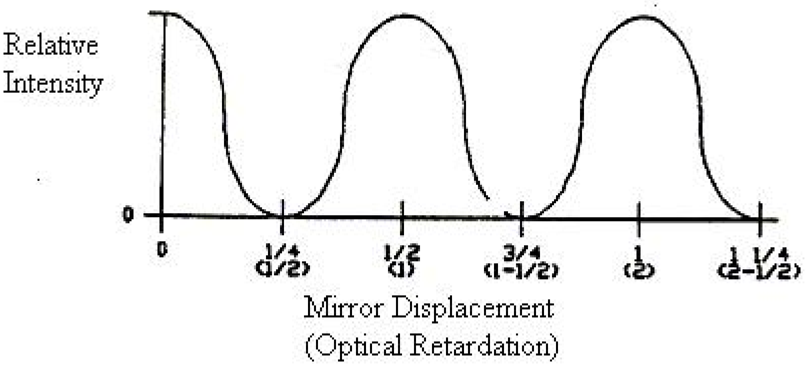


Figure 1-2 Relative Intensity of a Monochromatic Light Source as the Moving Mirror is displaced

This cosine wave of signal intensity versus mirror displacement is the interferogram produced by a single wavelength.

By extension, when a broadband light source (consisting of multiple wavelengths) goes through the interferometer, each wavelength of the incident beam constructively and destructively interferes at different mirror displacements. The signal going to the detector at any one time is the "composite" cosine wave of the individual waves at the corresponding mirror position. At the ZPD point (0 optical retardation), all wavelengths interfere constructively and the composite wave is at a maximum. As the mirror moves further and further away from the beam splitter, the composite waves gradually flatten out. Fig. 1-3 shows a very simple interferogram.

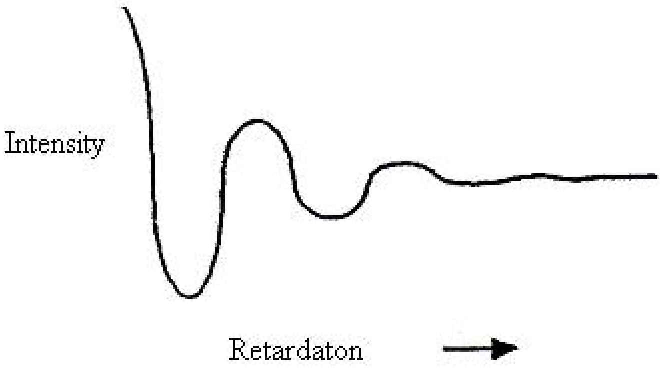


Figure 1-3 A Simple Interferogram

The interferogram shows the signal intensity of all wavelengths as a function of mirror displacement (or time). The Fast Fourier transform produces the spectrum by remapping this signal intensity as a function of individual wavelength (or frequency).

In practice, the moving mirrors are positioned in such a way that the signal intensity can be measured at points both before and after the ZPD. This allows the interferometer to "stabilize" before collecting data and also gives the computer data with which to correct instrument artifacts.

Theoretically, the mirror can be moved an infinite distance, but in real life this is neither practical nor possible. In a real spectrometer, the moving mirror moves a finite distance. We will see that putting a limit on the optical retardation affects the resolution and peak profile of the resulting spectrum.

RESOLUTION

The resolution of a spectrometer is the measure of its ability to distinguish between the peaks produced at two different wavelengths. In a dispersive instrument, resolution is dependent mainly upon the slit width and the Dispersive element (a prism or grating); when the slit is narrowed, a narrower range of frequencies passes to the detector. Since the slit width is also varied to maximize the signal at both ends of the frequency range, resolution is not constant. In an FTIR, the resolution depends on the maximum retardation of the moving mirror: The greater the retardation of the moving mirror, the better the resolution. Therefore, for a given retardation, resolution is constant over the entire frequency range. In general, a doubling of the mirror pathlength reduces the resolution by half (from 2 to 1 wavenumber, for instance). A spectrometer with 2 cm^{-1} resolution has the ability to distinguish peaks 2 wavenumbers apart.

Let's take the case of an IR beam consisting of only two wavelengths. Each wavelength will produce a cosine wave and the signal at the detector will be the sum of the two waves. If these wavelengths are far apart, the mirror will have to travel only a short distance for the separate waves to go out of and come back into phase, producing a maximum signal at the detector. If the incident wavelengths are close together (having almost identical wavelengths), the mirror will have to travel a much longer distance for the individual cosine waves to go out of and come back into phase. Figure 1-4 shows two widely separated wavelengths of equal intensity and their individual and combined signals at the detector. Figure 1-5 shows two closely spaced wavelengths similarly.

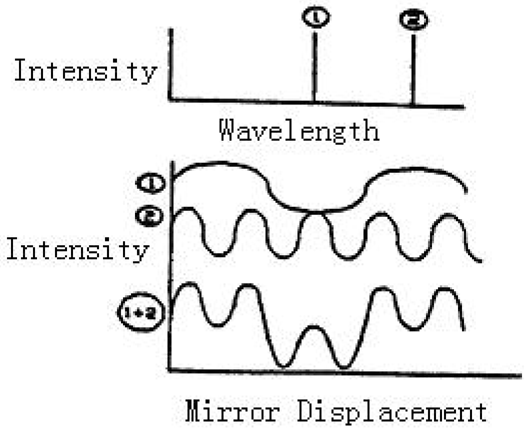


Figure 1-4 Detector Signal of Two Widely Separated Wavelengths

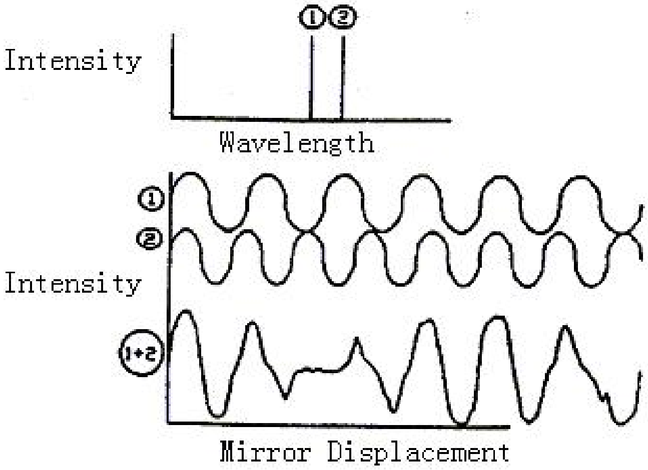


Figure 1-5 Detector Signal of Two Closely Spaced Wavelengths

APODIZATION

The finite travel of the moving mirror leaves a sharp truncation of the data at both ends of the interferogram. The Fourier transform of this cutoff results in the formation of “feet” around the absorption peaks of the spectrum that are simply instrument artifacts. The process of applying a weighting function that reduces these feet is called apodization. The apodization function weights the data at the center of the interferogram most heavily and decreases the weight of data at the ends. Since the end of the interferogram contains the high resolution data, the tradeoff for removal of the feet is a reduction in resolution. Apodization functions deform the true peak contours of the spectrum in a specific way, therefore all spectra used to perform quantitative measurements (such as subtraction) must be processed using the same apodization function. Figure 1-6, below shows the results of using a triangular apodization function. The top curve is the unapodized or "boxcar" apodized peak. The triangular apodized peak below it is much broader.

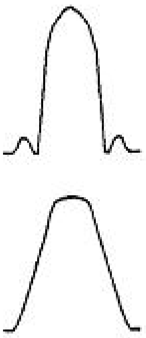


Figure 1-6 A Boxcar Apodized Peak (Top), and the Same Peak After Triangular Apodization

PHASE ERRORS AND PHASE CORRECTION

Due to optical, electronic and sampling effects, a funny thing always happens to the data on the way to the interferogram: the cosinusoidal components are subjected to phase shifts that cause the interferogram to be asymmetrical around the ZPD or centerburst. The interferogram is said to be "chirped" when this occurs and the process that corrects the chirping is called phase correction. In a sense, phase correction molds the interferogram back into shape after inevitable instrumental errors have been introduced. Two common types of phase correction methods are the Mertz method and the Magnitude method.

SAMPLING THE INTERFEROGRAM

We know that an interferogram can be obtained from the interferometer when the moving mirror is moved away from the beamsplitter. But we need some kind of clocking mechanism that tells the system when to sample the signal at the detector so that we can actually "see" or record the interferogram. This clocking mechanism is the He-Ne (helium-neon) laser. It too is passed through the beamsplitter; the system is able to assess the position of the moving mirror by counting the interference fringes of the detected laser beam. At certain fringe intervals a signal is sent to the analog-to-digital converter (ADC) which samples the detector signal, digitizes it, and sends it to the computer for storage and processing. Each sampling or reading of the detector represents a data point in the interferogram. When the computer has determined that is has received all the data points needed for a scan, it instructs the interferometer to go back to point 0 and prepare for the next scan. A single scan corresponds to the collection of data for one interferogram.

An individual scan takes less than a second with an FTIR. Because of the precise clocking of the He-Ne laser, the scan can easily be "overlayed" and averaged with other scans whose data are taken at identical intervals. This averaging, called Connes' advantage, has the effect of drastically increasing the signal-to-noise ratio (SNR) and constitutes another of the great advantages of FTIR over dispersive IR. The practice of averaging like scans is called coaddition.

ZERO FILLING

Since sampling of the interferogram cannot take place at infinitely small intervals, there is a linear interpolation of data between each data point of the resulting spectrum. This produces an obvious steeping effect and an apparent loss in accuracy because the actual transmission or absorbance of the beam may be much above or below this linear interpolation. In order to get a better idea of the true spectral shape, the end of the interferogram is "padded" with zerovalued data points. These extra points are then transformed along with the sampled data points and become interpolated points as determined by the apodization function. (These points are not apodized, however.) The practice of increasing the data point input of the interferogram in this way is called "zero filling." The result is a smoothing of the resulting spectrum without loss of resolution. Zero filling is very time consuming, with each order of zero filling more than doubling the computation time. Therefore, the benefits of accuracy and precision must always be weighed against the drawbacks of computation time.

1.3 Anatomy of an FTIR Scan

Now that we know a little bit about FTIR theory, let's take a look at an actual scan to see what's happening when we test a sample. Let out sample be a film of polyethylene. We will need to do two types of scans: a scan of the polyethylene itself, and scan of the “background.” Remember that the IR beam travels through a medium of “air” on the way to the detector. This air may contain absorbing substances such as CO_2 and water vapor that must be “subtracted” from the sample. This subtraction process is done by taking a background scan and ratioing it against the sample scan.

The basic sequence of any scan is shown in Figure 1-7. The scan consists of the data collection, apodization, FFT transform, and phase correction. Usually the background scan is obtained first.

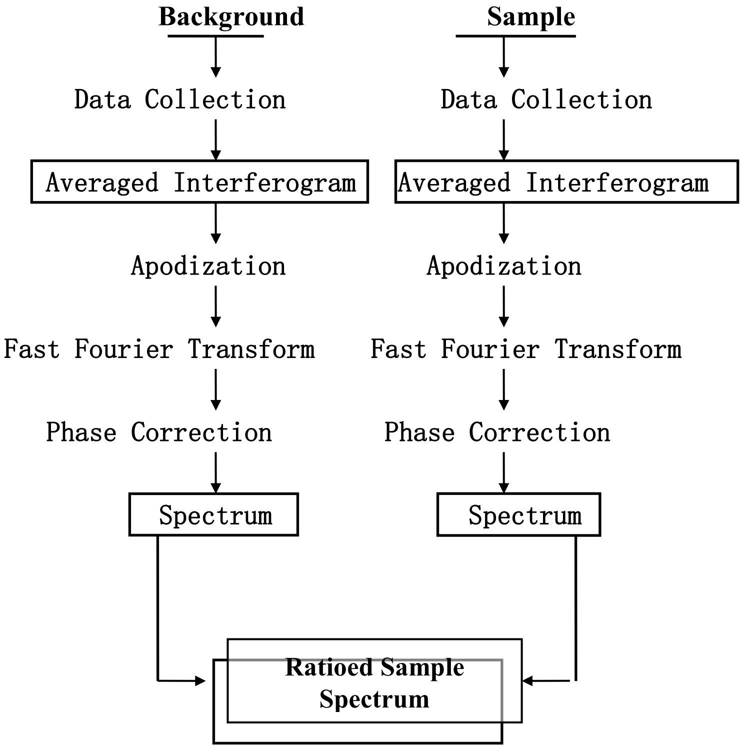


Figure 1-7 The Basic FTIR Scan Sequence

The background scan (sometimes called a single-beam or open-beam scan) is simply a scan done with no sample in the sample holder. When the command to start the scan is received, the ADC reads the detector at preset intervals and sends each data point in turn to the computer. This is repeated until all interferograms have been collected and cumulatively averaged. The averaged interferogram is then apodized, transformed, and phase corrected to provide the background spectrum. (The interferogram may also have a refractive index correction of the X axis in the case of Transept interferometers. See Some Laser Precision

Analytical Innovation, below.)

The sample scan is obtained similarly: The ADC reads the detector and sends an array of data points comprising the interferogram to the computer. Interferograms are averaged as they are collected, and the averaged interferogram is apodized (using the same function as the background scan), transformed, and phase corrected (also using the same correction method as the background scan). The spectrum is the ratioed against the background spectrum to produce the final sample spectrum in transmittance. A simple calculation converts transmittance results to absorbance if desired.

1.4 Transparent materials

Material	Chemical composition	Spectral Range (cm-1)	Water solubility（g/100mL）	Refractive index
Sodium chloride	NaCl	5000-625	35.7	1.54
Potassium bromide	KBr	5000-400	53.5	1.56
Cesium iodide	CsI	5000-165	44.0	1.79
KRS－5	TlBr,TlI	5000-250	0.02	2.37
Silver chloride	AgCl	5000-435	not soluble	2.0
Silver bromide	AgBr	5000-285	not soluble	2.2
Barium fluoride	BaF2	5000-830	0.17	1.46
Calcium fluoride	CaF2	5000-1100	0.0016	1.43
Zinc sulfide	ZnS	5000-710	not soluble	2.2
Zinc selenide	ZnSe	5000-500	not soluble	2.4
Diamond (Ⅱ)	C	3400-2700;1650-600	not soluble	2.42
Germanium	Ge	5000-430	not soluble	4.0
Silicon	Si	5000-600	not soluble	3.4

1.5 Some Innovations

The theory of all interferometers is the same: They all produce an interference pattern by introducing a pathlength difference between the two components of a split beam. But there are some basic design differences in interferometers that accomplish the split and recombination in a way that allows for higher precision and accuracy and reduces drawbacks inherent in the Michelson design.

The spectrometer we produce adopts a cube-corner type Michelson interferometer, which uses ninety-degree, cube-corner reflector instead of flat mirrors in traditional Michelson interferometer. (as shown in figure 1-8).

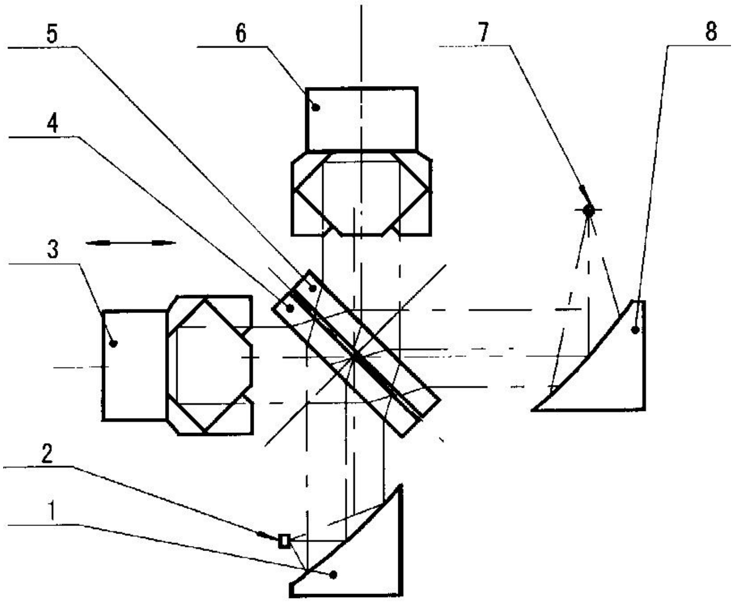


Figure 1-8 The Cube-corner Type Michelson Interferometer
1. Collimating mirror 2. Detector 3. Moving mirror 4. Beamsplitter 5. Compensator
6. Fixed mirror 7. Source 8. Collimating mirror

The difference between Cube Corner Type Interferometer and traditional Michelson Interferometer is that fixed and moving mirrors are cube-corners. The principle of cube-corner interferometer is: A beam of radiation from the source after collimating mirror is a parallel beam of light, and is directed to the beam splitter where half of it is reflected to the moving mirror and the other half is transmitted to the fixed mirror. Because the moving mirror causes a pathlength difference in one of the beams, the beams returning from cube-corner moving mirror and fixed mirror, which are parallel with the incidence light, interfere when they recombine at the beamsplitter. As cube-corner Michelson interferometer uses cube-corner mirrors, interference caused by outside factors are reduced. And stability is improved evidently. Because this kind of interferometer changes pathlength difference by moving the cube-corner, the distance the moving mirror needs to move is shorter than that of the refraction interferometer with the same resolution. Thus this interferometer can realize fast scan more easily. It also has the same advantages as Michelson interferometer featuring small volume, compact structure etc.

Chapter 2 Summary of DW-530 FTIR Spectrometer

2.1 General structure of DW-530 FTIR

DW-530 FTIR spectrometer consists of the following parts: interferometer, sample chamber, detector, electrical system and data system. At the general layout, small module structure is adopted in the spectrometer: proper arrangement and combination of modules can satisfy needs with different testing conditions; this kind of building block structure can be extended and upgraded easily, thus to improve operation flexibility of the equipment greatly.

Blocking optical design boosts up operation flexibility, and also improves energy throughput, as shown in figure 2-1. The optical system consists of individual modules, such as interferometer, detector and sample compartment etc, linked by standard optical path interfaces in a building blocks design.

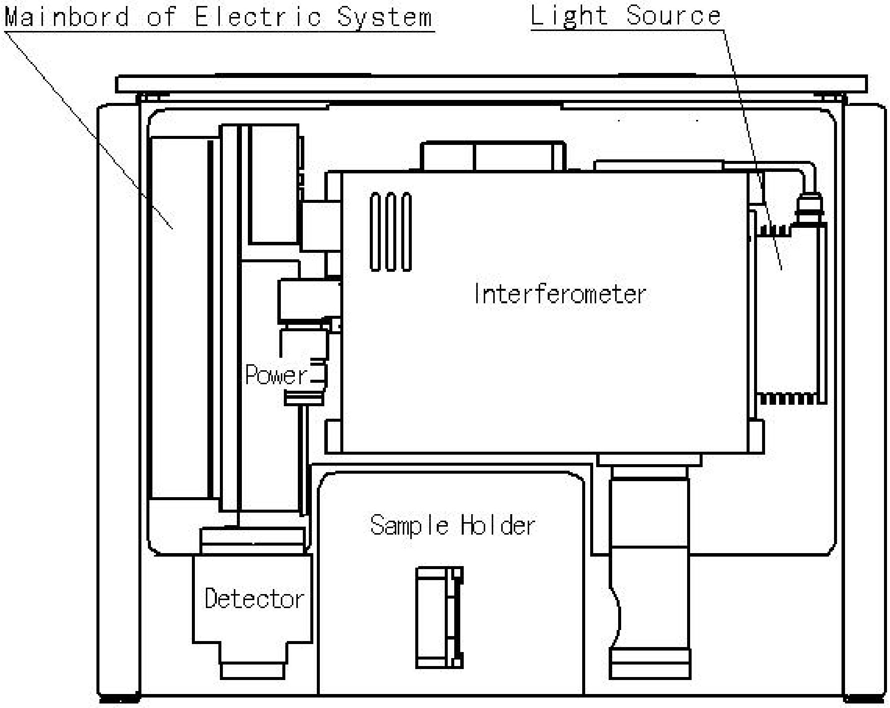


Figure 2-1 General Layout ofDW-530 FTIR Spectrometer

Optical path interface is precise optical transfer element. It is through flat mirror or parabolic mirror to make transformation and switching of infrared beam of light among function blocks come true. The performances and features of optical path interface system are mainly represented to be following two aspects: 1. following with a proper mode, use parallel and confocal optical forms alternatively, and change beam directions periodically, to eliminate halo effect and make effective output always staying at the highest level; 2. through adopting different optical path interface components, proper transformation among modules can be ensured, and there is no need for user to carry out any adjustment.

2.2 Main Features of DW-530 FTIR Spectrometer

2.2.1 Interferometer

DW-530 FTIR spectrometer adopts cube-corner Michelson interferometer (as shown in Figure 2-2). The Michelson interferometer consists of a source, a beamsplitter, a compensator, two perpendicular mirrors and a detector. The beamsplitter and the compensator are plane types. The two perpendicular plane mirrors in traditional Michelson interferometer are replaced by cube-corner reflectors in cube-corner interferometer. The cube-corner moving mirror moves along the direction perpendicular to beamsplitter's coating-film surface. When an infrared beam from the source is directed into the interferometer, it is split by the beamsplitter, and half transmitted and half reflected to the two cube-corner mirrors. Beams coming back from the two cube-corners are parallel with the incidence beams, and when the two beams recombine, interference will happen. Because the cube-corner moving mirror causes a pathlength difference in one of the beams, the interferogram will be obtained.

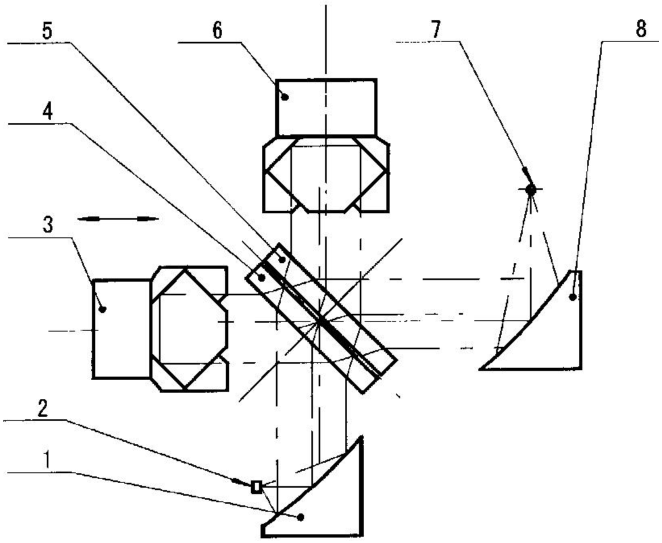


Figure 2-2 Interferometer

1. Collimating mirror 2. Detector 3. Moving mirror 4. Beamsplitter 5. Compensator 6. Fixed mirror 7. Source 8. Collimating mirror

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Interferometer ofDW-530 FTIR spectrometer is made fully sealed and moisture-proof. It is sealed with outside optical path by KBr window plate and lock ring. Deliquescence of KBr beamsplitter and compensator can be avoided effectively. Thus requirements for operation environment are reduced.

2.2.2 Electrical System

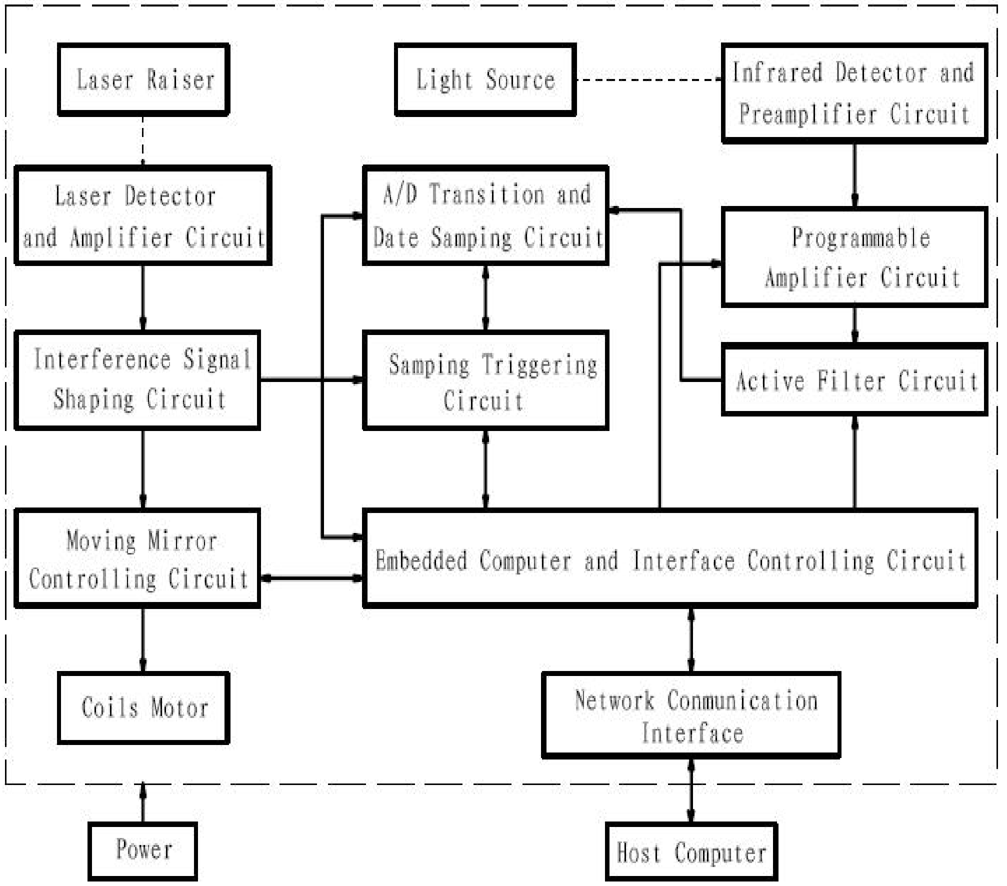


Figure 2-3 Principle Graph ofDW-530 FTIR Spectrometer Circuit System

ToDW-530 FTIR spectrometer, its interferometer is controlled by its own microcomputer, dependent with main computer as data system. The two parts are connected by cable with RJ45 plugs to realize data communication. Main function ofDW-530 FTIR spectrometer circuit system is: interferometer servo control, data collection & processing, data communication etc. The principle graph of whole circuit system is shown in figure 2-3, which mainly comprised of one electric board and periphery circuit.

2.2.3 Data System

Common compatible computer is adopted in data system ofDW-530 FTIR spectrometer. The software can work together with third-party software under the WINDOWS operating system. At the same time, user can develop new spectrometer data operating program himself based on his own demands. Standard operating software of DW-530 FTIR supplies all routine analysis operating functions of infrared spectrum.

2.3 Main Specifications of DW-530 FTIR Spectrometer

The main specifications of DW-530 FTIR spectrometer are as follows:

1. Wavelength range: 7800 cm^{-1} ~ 350 cm^{-1}

2. Resolution: better than 1cm^{-1}

3. Wavenumber precision: ±0.01cm^{-1}

4. Transmittance repeatability: 0.5%T

5. 100%T line SNR: better than 20,000:1 (RMS value, at 2100cm^{-1}, 4 cm^{-1} resolution, DTGS detector, 1 minute data collecting)

6. 100% line T inclining:

Wavelength (cm^{-1})	100%T line (%T)
500 ~ 800	98.0 ~ 102.0
1900 ~ 2200	99.5 ~ 100.5
2800 ~ 3200	99.5 ~ 100.5
4000 ~ 4400	98.5 ~ 101.5

7. Scan speed: High speed、Intermediate speed、Low speed, selectable;

8. Detector: DTGS(Standard configuration).

2.4 Configuration

Standard configuration includes:

1. High performance IR source with air-cooled high-efficiency reflex sphere;
2. Cube-corner Michelson interferometer system;
3. Electrical system;
4. External optical path sampling system;
5. DTGS infrared detector system;
6. All-purpose computer data system.

Optional FTIR Accessories:

1. Temperature control detector components;
2. Wireless communication module
3. Single-reflect ATR;
4. Diffuse/Specular Reflectance;
5. Horizontal ATR ;
6. Liquid ATR;
7. Various Gas Cells and Various Liquid Cells;
8. Agate mortar;
9. Hydraulic press;
10. Dehumidifier.

Chapter 3 Environment Requirement & Installation

Our special personnel will be responsible for installing instrument system. In fact, there is no need of user to do initial installation. But you had better be familiar with system installation and environment requirements. Please read the following content to know how to choose installation site and what you should do before installing the instrument.

Notice: installation attempt that any user does without our special personnel may cause parts protection invalid; installation indications described in the manual cannot replace the installation work done by special personnel.

There are some sensitive optical components included in the FTIR main unit. Room temperature balance about 24 hours is needed after the instrument arrives. During the period, please do not uncover the instrument. Remain the instrument and the spare parts in the packing case until the special personnel arrives.

Notice: before our special personnel finish installing the instrument, please do not run interferometer, or optical components may be broken. During using period, user should keep proper humidity and temperature in the lab. Damage of KBr beamsplitter and window plate caused by high humidity is not in our warranty range.

During the typical installation process, special personnel from Shanghai Drawell Scientific Instrument Co.,Ltd. or its agent will supply following services:

1. Open the instrument main unit to prepare for running the interferometer;
2. Open and install data system and other accessories; connect all cables; electrify the system to make sure each part can work normally;
3. Check “background spectrum” of the equipment;
4. Check system running;

After making sure that the instrument runs normally, special personnel will show you following basic operations:

1. Set data collection parameters;

2. Collect "background" and "polystyrene" spectra;
3. Process, display and output spectrogram;
4. Analyze one sample;
5. Show operations when using all accessories and sample spare parts;

To ensure correct run of the system, following descriptions supply you dimension and weight of each part of the system.

Dimension of DW-530 main unit is shown in figure 3-1 and 3-2:

Height	Length	Width	Weight
27cm	52cm	44cm	25kg

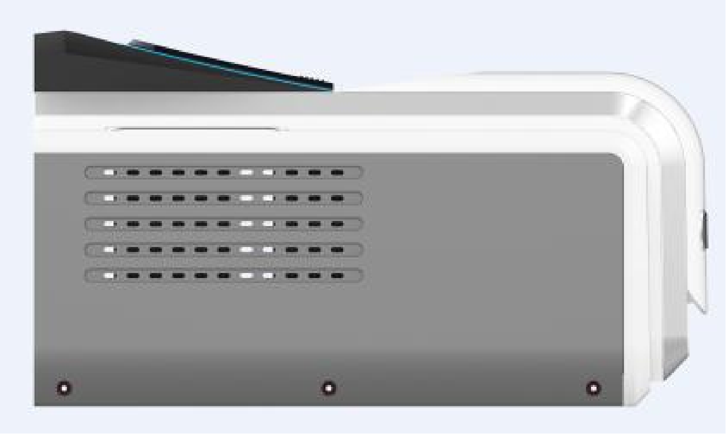


Figure 3-1 Side-view of DW-530 FTIR Spectrometer

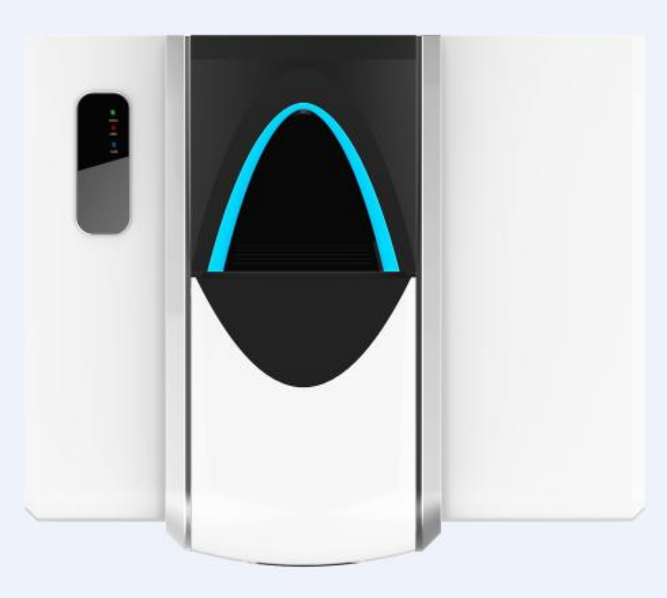


Figure 3-2 Top-view of DW-530 FTIR Spectrometer

There, in the data system, all-purpose computer is adopted. The dimension will be different along with different supplier's products.

To provide high efficient work, data system should be placed near the DW-530 FTIR spectrometer main unit and display.

3.1 Site Requirements

Work environment, where DW-530 FTIR spectrometer locates, should be kept clean and orderly. Any dunghill, dust and smog will affect system's work. Smoking is also forbidden.

DW-530 FTIR spectrometer includes laser. Laser radiation exists when opening cover of the interferometer; laser power is 2mW, and it will not be harmful to human's body. **But please do not envisage the laser by all means!**

Ambient Conditions and Ventilation

The room temperature must be in the range of 15 ℃~ 30℃. Relative humidity should be less than 60%.

Optical components, especially beamsplitter, have strict demands to environment humidity. Maintenance of optical system should be noticed. Optical head is crucial to the performance of your system and is relatively expensive to replace, so it pays to be cautious in a humid environment. Vapor condensation phenomenon may occur when cold equipment is opened and exposes in humid air. When the equipment is used for the first time or after being laid aside for a long period of time, warm-up for several hours should be carried out first.

It is also imperative that the environment surrounding your spectrometer be free of corrosive vapors or of any other type of materials that may affect the instrument. We'll not be responsible for problems caused by these. The amount of halogenaled hydrocarbon vapor in the environment of the instrument should be less than 25ppm to avoid premature IR source failure and corrosion from generated halogen acides.

Optical components and power supply can all give out heat, so normal work of ventilation hole and window should be ensured for the convenience of heat dispersion. Around the equipment at least 10cm space should be left to keep good ventilation.

Source inside the interferometer is a high temperature part. Interferometer must not work in the environment with flammable and explosive gas. **If source should be opened for some** reason, its high temperature surface must not be touched to avoid user being hurt.

IR source should be replaced after being used for a period of time. Replaced period decided by operating frequency. Otherwise material volatilized from IR source will spread onto nearby optical components' surfaces, which may cause system energy reduced.

Vibration

The optical bench and peripheral systems have been designed to withstand general vibrations. However, the equipment should be shielded from severe vibration or shocks. Ideally, the spectrometer should be placed on a separate stable surface, isolated from fans, motors and other constantly vibrating equipment.

Power supply & Cable

DW-530 FTIR spectrometer system uses 220V(110V) AC power supply, and it must be grounded reliably.

Momentary disturb, like electrophoresis and electric-cutoff, overpass and dispersion of voltage, can cause problems, such as data loss, exceptional result, system lock & close etc. Regular current change of huge electric device near the instrument will also affect its normal running. So we advise that you adopt following protection steps:

1. Ensure power stable in the range of 220±10%(110V±10%);
2. If power problems often happen, a power regulator should be configured.
3. Special power socket for the spectrometer system should be used, and it can not be shared with other electric devices;
4. If the carpet is spread around, put a piece of electrostatic-proof robber cushion;
5. Spectrometer power supply should be grounded; do not cancel the protection ground or use outspread cable without grounding conductor. Three-electrode outspread cable and

socket must be used.

3.2 Installing explanation

If you have not read through section 3.1, please read relative content carefully. Following installing explanation do not mean user can install spectrometer system himself without agreement of Shanghai Drawell Scientific Instrument Co.,Ltd..

User's attempt to install any part of the system means that he gives up quality guarantee of our factory automatically.

When unpacking, please check with the packing list to confirm that all the items are included and in good conditions. User should keep well the documents provided with the instrument for later use.

Your system had been tested and adjusted strictly in the factory before delivery and some cables had been connected well.

Installing process includes two parts: installing data system and display; installing interferometer and its accessories.

Installing data system and display

1. Put the computer main unit on proper and stable workbench (the surface should be no less than 1.5m×1m), leave some space for the convenience of connecting cables;
2. Connect the display, keyboard and mouse, to corresponding sockets at the rear of the computer;
3. If you have a printer, connect it to printer interface on the computer;
4. Take out cable with RJ45 plugs from the sample compartment of the spectrometer, connect the computer with the spectrometer;
5. Plug in the power cables of computer and display to power switchboard with filter;

Installing interferometer and its accessories

1. Remain the spectrometer unpacked in the room for temperature balance for at least 24

hours;

2. Open the package, take out the spectrometer and put it on prepared proper workbench.
3. Connect the power cable of the spectrometer and the cable with RJ45 plugs (in the package) between spectrometer and computer;
4. Check the connection; if there is no mistake, electrify and start the spectrometer to carry out test;
5. If accessories are chosen, unpack them; install them to their installation positions according to their instruction manuals.

Chapter 4 Basic Operation

4.1 Brief introduction of spectrometer operation

This section will introduce operating procedures briefly.

FTIR spectrometer is perfect combination of complex spectrometer and computer technology. Interferometer can get infrared energy through some kind of medium, but this kind of data cannot be used directly in spectroscopy analysis, so a powerful "brain" is needed to transform initial data to a spectrum that can be recognized, and the brain is "computer".

Furthermore, computer and its application on spectrometer is the key of spectrometer operation. Spectrometer operation is as easy to learn as to send commands to computer. Commands are inputted through keyboard or mouse; commands inputted are in fact commands sent to the spectrometer.

Summary of computer's role

Computer data system of the spectrometer is all-purpose computer. The function of spectrometer operating system is managing the system resource, which is totally the same with that of PC. It will read commands from keyboard, display relative information on the display and printer, and run spectrometer operating software and other programs. Moreover, it manages disk space and main memory, carries out all kinds of file processing commands. Without operating system, no PC can work. DW-530 FTIR spectrometer system uses popular Windows XP /VISTA/7/8/8.1/10 standard operating system.

Programs or collection of relative data stored on the computer disk are called file. When running the program, you will create and store data files. Each file has its own file name, and these files will be stored according to an order, that is, catalog.

4.2 Brief introduction of data collection

Collecting "background" spectrum

Each obtained sample scan will be ratioed against background scan. The more accumulative total background scan, the higher the SNR, the bigger safety coefficient that random noise is controlled to be lower than sample signal. Generally, when carrying out sample scan, background scan more than twice should be accumulated. If a certain background will be used for several samples or for a long period of time, The times of background scan should at least double of that of sample scan. Time taken on collecting background at the beginning is worthy, as it can improve SNR. When changing sample accessory or changing data collection parameters, a new background signal should be collected.

Placing sample and obtain sample scan

In a general way, sample is put on the sample holder in the sample compartment. If ATR, diffuse reflection or mirror reflection analysis is needed, sample should be put on corresponding accessory and then the accessory is placed into the sample compartment. Please refer to the manuals of the accessories for details.

After your system is preheated and signal check has been done, background spectrum has been obtained, you can open sample compartment and put sample on the holder, then cover the lid and begin sample scan.

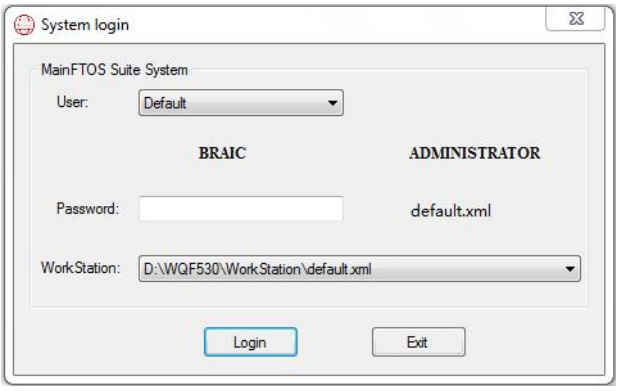
4.3 Simple operation exercise

Start、test、preheat:

1. Electrify 220V power source, turn on DW-530 FTIR spectrometer and then computer.
2. Double click the icon MainFTOS Suite on the desktop, or click the program from the Windows Start menu. The software will be launched, the user login dialog box (Fig. 4-1) will be shown as follows:

   Select the User ID from the drop-down list, and enter the User Password in the password textbox. (The predefined password of user ID "Default" is "FTOS".) You can always select those workspaces from the drop-down list. Choose the instrument model corresponding to the workspaces "WQF530", or the standard workStation "Default".

   Click the Login button. The MainFTOS Suite user main window opens.



User: Default

BRAIC ADMINISTRATOR

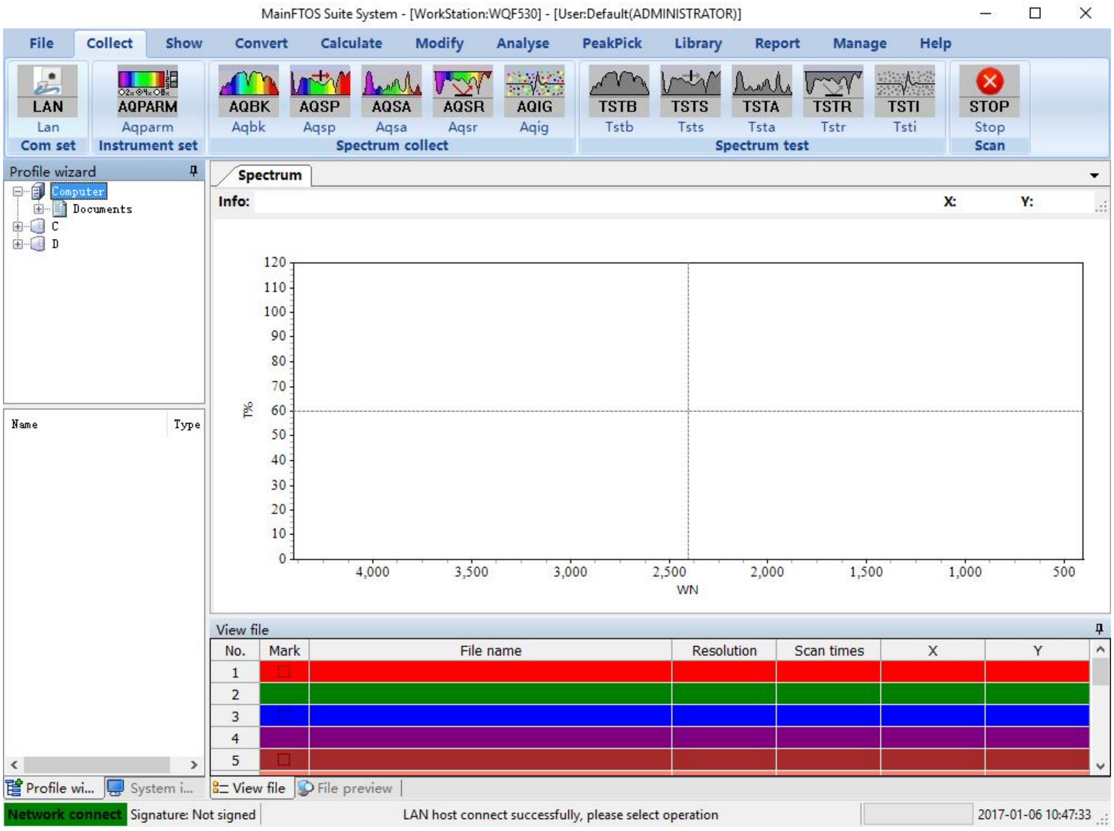
Password:

default.xml

WorkStation: D:\WQF530\WorkStation\default.xml

Fig. 4-1

3. The main window of the program will be shown as in Fig. 4-2



MainFTOS Suite System - [WorkStation:WQF530] - [User:Default(ADMINISTRATOR)]

No.	Mark	File name	Resolution	Scan times	X	Y
1	☐					
2	☐					
3	☐					
4	☐					
5	☐					

Network connect | Signature: Not signed | LAN host connect successfully, please select operation | 2017-01-06 10:47:33

Fig. 4-2

4. The main menu includes following information:

Title bar

Located at the top of MainFTOS Suite, including the name of the software, workStation, user name and group and the control button.

Menu bar

MainFTOS Suite supplies ten menus including all functions of spectrum operations.

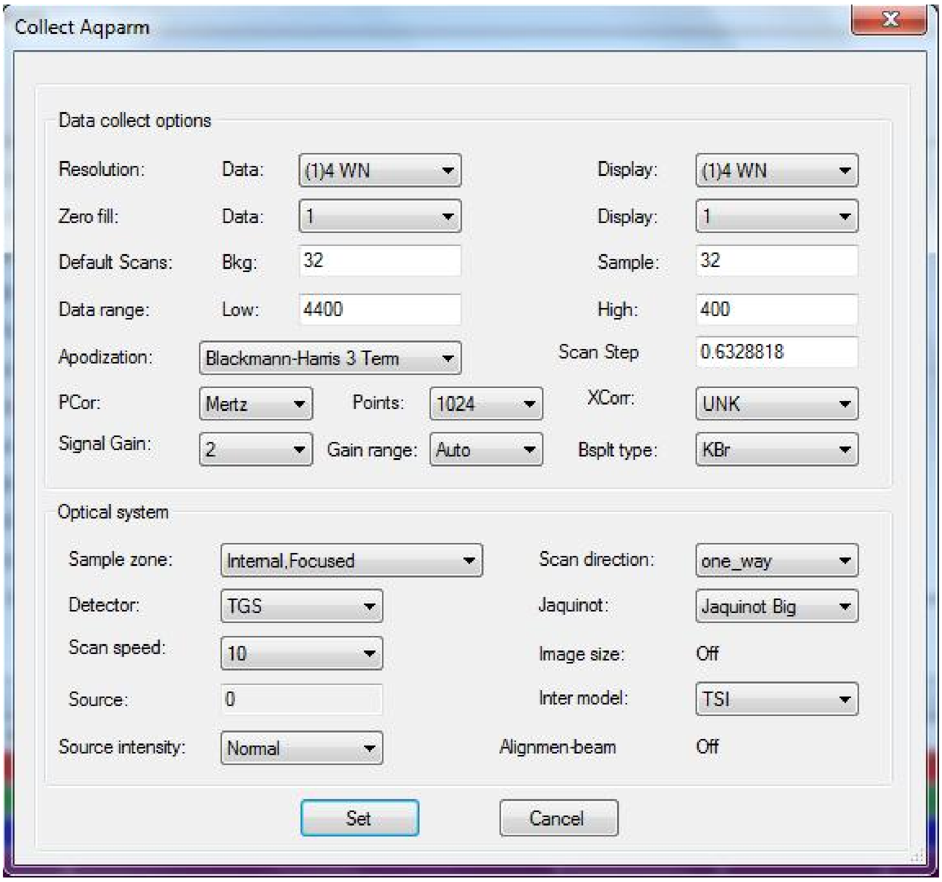
Window

Including Profile window, System info window, View file window, File preview window and Spectrum window.

Status bar

In the bottom of MainFTOS Suite, which in turn shows: the network status of the instrument, the signature information of the current spectrum, the on-line state of the instrument, the current progress of the current spectrum and the current time of the system.

5. Click "Collect" in the menu bar; click "Aqparm", following System parameter setting dialog box will be shown as in Fig. 4-3. Such parameters as, scan times, apodization、scan speed etc can be set here. Set the parameters to the followings, Signal Gain:2, Speed:10. After parameters are set, click "Set" button to exit.


Collect Aqparm

Data collect options

Resolution: Data: (1)4 WN Display: (1)4 WN
Zero fill: Data: 1 Display: 1
Default Scans: Bkg: 32 Sample: 32
Data range: Low: 4400 High: 400
Apodization: Blackmann-Harris 3 Term Scan Step 0.6328818
PCor: Mertz Points: 1024 XCorr: UNK
Signal Gain: 2 Gain range: Auto Bsplt type: KBr

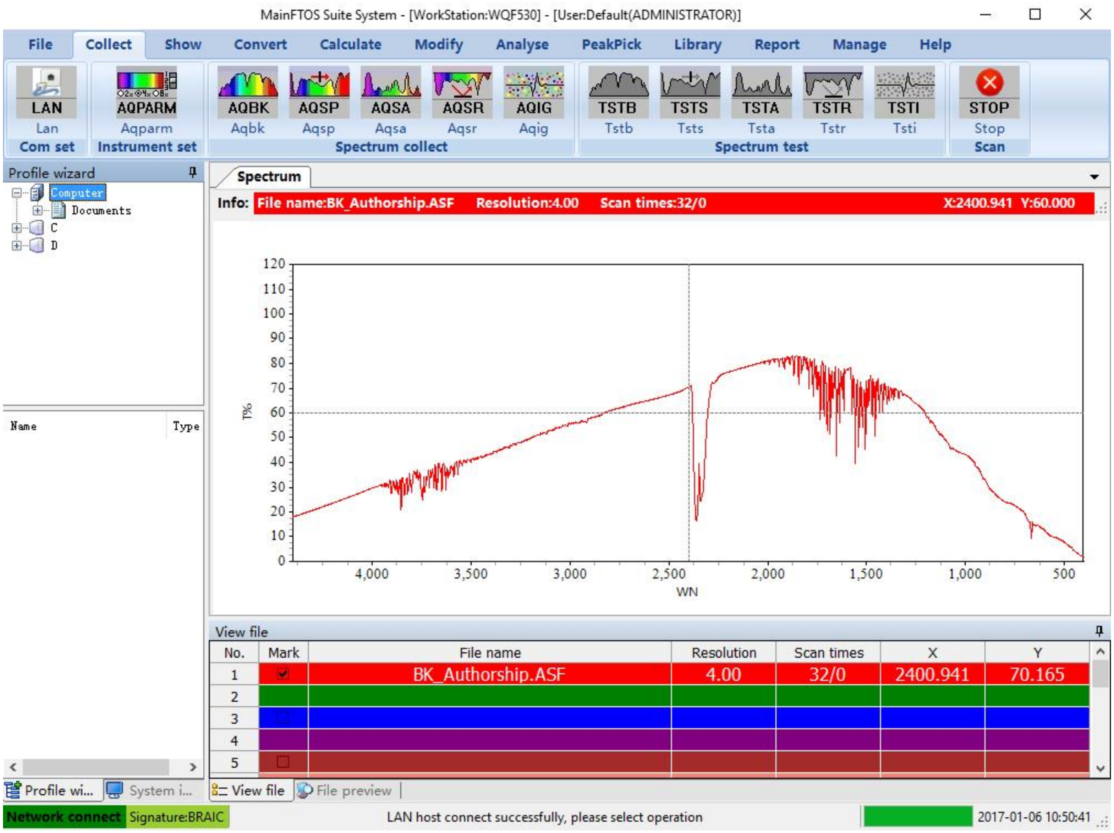
Optical system

Sample zone: Internal,Focused Scan direction: one_way
Detector: TGS Jaquinot: Jaquinot Big
Scan speed: 10 Image size: Off
Source: 0 Inter model: TSI
Source intensity: Normal Alignmen-beam Off

Fig. 4-3

6. Click "Collect" in the menu bar; click "Tstb" (Test Background). Program will enter into

Air Testing Collection process, and the background spectrum will be displayed in spectrum display window, as is shown in Fig. 4-4.



Info: File name:BK_Authorship.ASF Resolution:4.00 Scan times:32/0 X:2400.941 Y:60.000

No.	Mark	File name	Resolution	Scan times	X	Y
1	☑	BK_Authorship.ASF	4.00	32/0	2400.941	70.165
2						
3	☐					
4						
5	☐					

LAN host connect successfully, please select operation

2017-01-06 10:50:41

Fig. 4-4

7. If above six operations are normal, and the spectrometer has been preheated for 20 minutes, sample collection can be carried out.

Collect sample spectrum

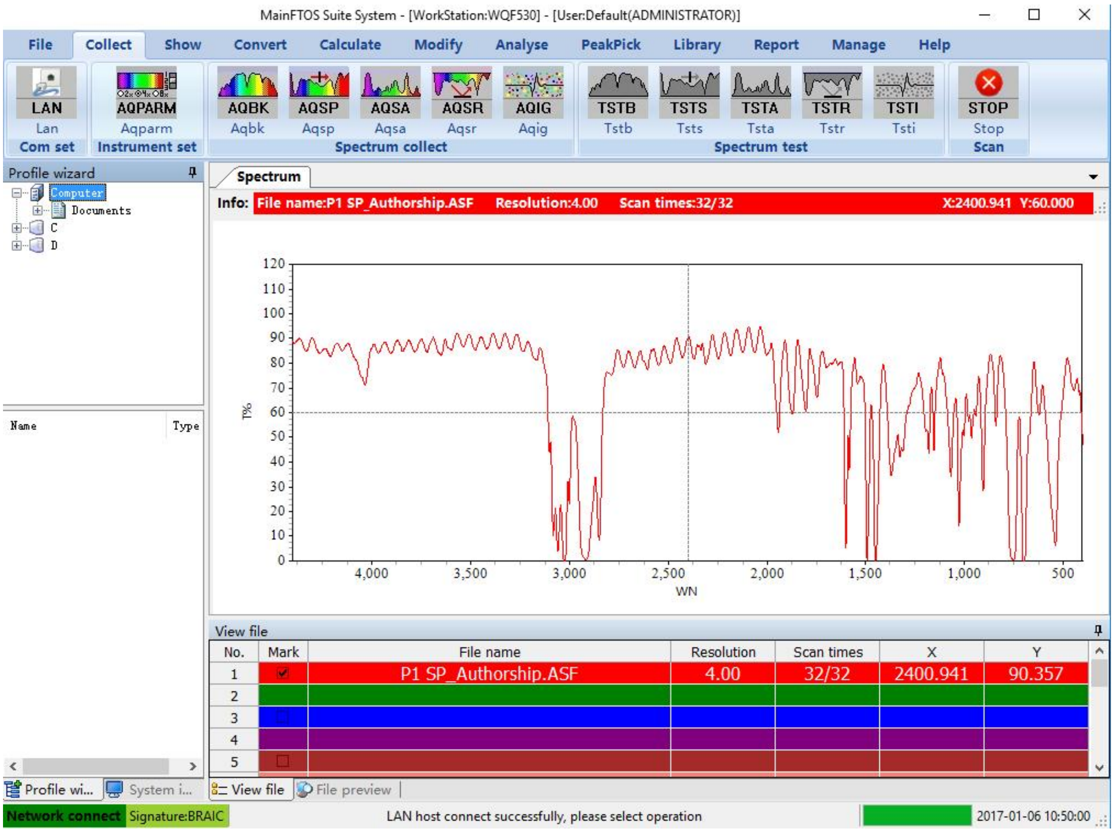
1. Click “Collect”; then click “Aqbk” show Collect Background spectrum dialogue box. Enter a file name, scan times, title, Description1 and Description2. Then click “Collect” to start background collection. After collection, next program will be carried out.

(Background to be collected is usually an air spectrum or a spectrum of blank KBr plate pressed by the hydraulic press.)

2. Put the sample to be measured or the plate pressed of KBr and sample mixture onto the sample holder in the sample compartment.

3. To collect a transmittance spectrum,

Click "Collect"; then click "Aqsp"; click "Collect" in the shown dialog box after inputting a file name, scan times, title, Description1 and Description2. When data colleting is finished, a transmittance spectrum can be obtained, as is shown in Fig. 4-5.



Info: File name:P1 SP_Authorship.ASF Resolution:4.00 Scan times:32/32 X:2400.941 Y:60.000

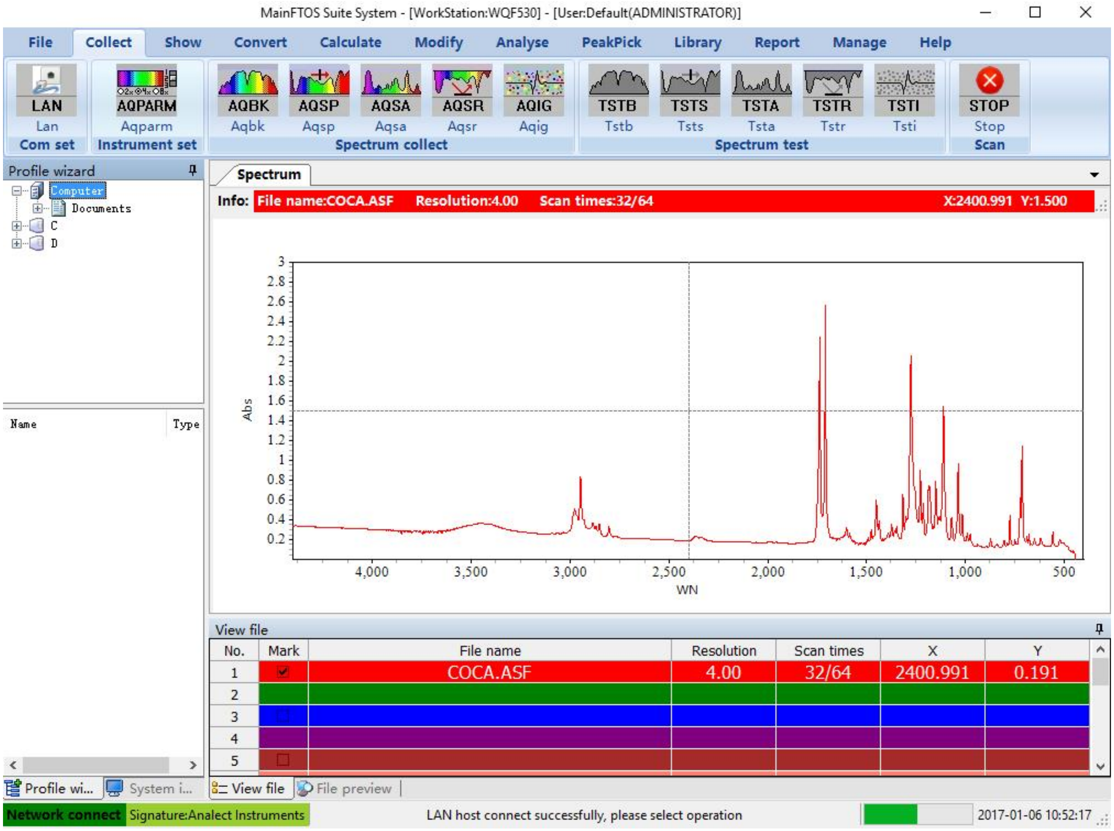
No.	Mark	File name	Resolution	Scan times	X	Y
1	☑	P1 SP_Authorship.ASF	4.00	32/32	2400.941	90.357
2						
3	☐					
4						
5	☐					

Network connect Signature:BRAIC LAN host connect successfully, please select operation 2017-01-06 10:50:00

Fig. 4-5

To collect an absorption spectrum:

Click "Collect"; then click "Aqsa"; click "Start" in the shown dialog box after inputting a file name, scan times, the title, Description1 and Description2. When data colleting is finished, an absorbance spectrum can be obtained, as is shown in Fig. 4-6.



MainFTOS Suite System - [WorkStation:WQF530] - [User:Default(ADMINISTRATOR)]

Info: File name:COCA.ASF Resolution:4.00 Scan times:32/64 X:2400.991 Y:1.500

No.	Mark	File name	Resolution	Scan times	X	Y
1	☑	COCA.ASF	4.00	32/64	2400.991	0.191
2						
3	☐					
4						
5	☐					

Network connect Signature:Analect Instruments LAN host connect successfully, please select operation 2017-01-06 10:52:17

Fig. 4-6

Print out sample spectrum

Click "File" on the menu bar; click "Print". Program will enter into special print program.

Shutdown operation

After using, first click stop (*STOP*), then close the software, and shut down the instrument.

Other operations

MainFTOS Suite application has rich functions; so the operation is complicated. We will explain them in detail in MainFTOS Suite software manual.

Spectrometer maintenance guidelines

When spectrometer cannot start normally:

(1) Please restart WQF series instrument, and restart MainFTOS Suite program.

(2) Observe the lamp on the instrument shell light up or flashing normally.

(3) Check if there are red spots in the sample compartment, thus to conclude if the laser is lit.

(4) Check if software runs normally.

(5) Record error information and get contact with your local agent or directly to us.

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