

# ***FTIR*** ***Quick Start Manual***

Keck Interdisciplinary Surface Science Center  
NUANCE, Northwestern University  
Room 1149, Cook Hall  
2220 Campus Drive  
Evanston, IL, 60208

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## I. Sign up

Before starting your experiment, please sign up in the login-in computer.

## II. Sample preparation

The details of sample preparation can be seen in our website:

<http://www.nuance.northwestern.edu/keckii/ftir4.htm>

- Preparing liquid samples for transmission analysis.
- Preparing solid samples for transmission analysis.
- Preparing liquid samples for ATR measurement.
- Preparing solid samples for ATR measurement.
- Preparing samples for PM-IRRAS measurement.

Also, please read the "**help**" files in the "**OMNIC**" software such as "[\help\sampling techniques\transmission sampling techniques](#)", "[\help\sampling techniques\ATR sampling techniques](#)" and "[\help\sampling techniques\ARK multibounce HATR](#)".

## III. Transmission and ATR measurement


**Precaution:** Avoid scratching ATR crystals. Avoid the use of materials that attack ATR crystals.


1) Select a detector.

There are two detectors in the spectrometer, *i.e.*, "DTGS" (deuterated triglycine sulfate) and "MCT" (mercuric cadmium telluride). Both of them cover the mid-infrared range from 4000 to 400  $\text{cm}^{-1}$ . The "DTGS" detector is used for the acquisition of regular transmission spectra. The "MCT" detector has higher sensitivity than "DTGS". It is usually used for the acquisition of ATR spectra. If you use the "MCT" detector, you must fill the "MCT" detector with about 1 liter liquid nitrogen (liquid nitrogen is available in Rm. 1154. Please fill out the login-sheet when you pick up the liquid nitrogen). Before you start an experiment, please wait 30min to let the detector fully cool down.


2) Start the " OMNIC" software.

3) Watch the bench status indicator on the upper right of "OMNIC" window.

If the indicator is a green check mark " Bench Status", the spectrometer has passed all the diagnostic tests. Please go to Step 4.

If the indicator is a yellow circle "", a cooled detector has become warm.

If the indicator is a red "X", the spectrometer has failed a diagnostic test. Any you have to run the following two functions.

**Reset bench:** Open the "**experiment set-up**" window under the "**collect**" menu. In the "**diagnostic**" page, click the " button.

If the interferogram becomes fine, you don't need to further run the following the function.

**Alignment of bench:** It is important that the sample compartment is clear of all accessories

when this task is performed.


Open the "**experiment set-up**" window under the "**collect**" menu. In the "**diagnostic**" page, click the "**Align...**" button.

- 4) Make sure the base plate in the sample compartment of the spectrometer is correct. The base plate for an ATR experiment is different from the one for a transmission analysis. When installing the ATR kit, don't forget to connect the purge tube.
- 5) Select an experimental file from the drop-down list box of **Experiment: Transmission E.S.P** so that you can quickly set all the software parameters for different types of data collection. For example,
  - "**Transmission E.S.P.**" for regular transmission spectroscopy
  - "**MCT 4cm-1 ARK**" for attenuated total reflection (ATR) spectroscopy
- 6) Open the "**experiment set-up**" window under the "**collect**" menu. And set up the parameters as shown in the following table.

<b>Experimental parameters</b>	<b>Transmission measurement</b>		<b>ATR measurement</b>
In " <b>collect</b> " page			
<b>No. of scan</b>	Around 32		64~128
<b>Resolution</b>	4, <b>8</b> , 16cm <sup>-1</sup>		4, <b>8</b> , 16cm <sup>-1</sup>
<b>Final format</b>	Absorbance or %transmittance		Log(1/R) or %Reflectance
<b>Correction</b>	None		None
<b>Background handling</b>	Collect background after 0 min		Collect background after 0 minutes
In " <b>bench</b> " page			
<b>Gain 1</b>	Auto gain		Auto gain
<b>Sample compartment</b>	Main		Main
<b>Detector</b>	DTGS TEC		MCT/A*
<b>Accessory</b>	Transmission E.S.P.		"ARK E.S.P flat" for films; "ARK E.S.P trough" for liquid;
<b>Window material</b>	"None" for solid	"KBr", "BaF <sub>2</sub> " for liquid	ZnSe or Ge
<b>Spectral range</b>	4000-400	depend on window material	depend on window material


- 7) Watch the live display of interferogram in the "**bench**" page.

The maximum voltage should be within the acceptable range: 5.6~9.8. If the peak-to-peak voltage is in the acceptable range, please go to Step 8. If the peak-to-peak voltage is out of the acceptable range, adjust the “Aperture” value in the “bench” page.

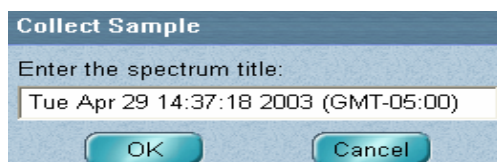
- 8) Under the “**window**” menu, choose “new window”.
- 9) Click the “collect background” button to collect the background. And then a single beam will appear. Subsequently click the  button on the upper right of window to start the acquisition of background.

(**Attention:** In case of the transmission analysis of liquid samples, a background single beam must be obtained from the IR window. In case of the ATR analysis, a background single beam must be obtained from the ATR crystal).



- 10) Load your sample.

- 11) Click the “collect sample” button  for data collection.

The collect-sample window appears and then a dialogue box shows the default title for the sample spectrum. You can type a desired title, too. This title is not a file name.



If you specify that a background should be collected before every sample, a message appears to ask you to remove the sample for a background collection. After collecting the background spectrum, then put your sample into the sample compartment. Please follow the instruction to do it.

When all the sample data have been collected, a message window will pop up. You can click  to see a summary of all problems. You can click  to add the acquired spectrum to the spectral window.

- 12) Choose “**save as**” under the “**file**” menu to save the spectrum to the folder “C:\user\”. Please select “**.SPA**” format to save all the information of raw data.

#### IV. PM-IRRAS measurement

If you don’t run a PM-IRRAS experiment, please skip this section.

The basic principle of PM-IRRAS measurement can be found in Buffeteau’s paper, which is published in *Applied Spectroscopy*, Vol 45(3), (1991), 380~389.

- 1) For PM-IRRAS measurement, please use the “MCT/A” in the tabletop optics module (TOM) box. You must fill the “MCT” detector with liquid nitrogen (liquid nitrogen is available in

Rm. 1154). Before you start an experiment, please wait 30min to let the detector fully cool down.

- 2) Switch on the power of “**PEM-90**” and “**GWC Instruments**”. And then set up them as follows:

For “PEM-90”, “Unit” = WAV

“PRESETS” =  $\lambda/2$

“SYSTEM STATUS” = LOC

For “GWC Instruments”, “local/exit” switch = “local”

“SUM/DIFF” switch = “SUM”

“input gain” = 2

“output gain” = 2

“phase adjust” = 3.86

- 3) Make sure the half-wave-retardation frequency at the specific wavenumber.

For example, to set the frequency to  $1500\text{cm}^{-1}$  as follows:

- On the panel of “PEM-90” controller, switch the “wavelength” unit to “**nm**” by pressing the button.
- Press the “**set**” button twice, and then the “**nm**” indicator will blink.
- Press “**Δ**” or “**∇**” button to set the wavelength to 6666.6nm, which is corresponding to  $1500\text{cm}^{-1}$ . (3846.2nm corresponding to  $2600\text{cm}^{-1}$ )

- 4) Wear gloves and adjust the angles of two mirrors on the sample stage to select the incidence and reflectance angles of IR beam.

- 79-83 degrees-- commonly for studying films on metals.
- 74-76 degrees-- commonly used for studying air/water interface
- 72 degrees-- commonly used for studying films on glass substrates.
- 67 degrees-- commonly used for studying films on dielectric substrates.

- 5) Put a reference sample on the sample stage (**Caution: don't touch the mirror on the sample stage**).

- 6) Start the " **OMNIC**" software.

- 7) Select the experimental file of “**PEM1**” from the drop-down list box of .

- 8) Under the “**collect**” menu, open the “**experiment set-up**” window. Set up the experimental parameters as follows:

In the “**Collect**” page:

Number of scans: 2048 or 1024 recommended (512~3072)

Resolution:  $8\text{cm}^{-1}$  or  $4\text{cm}^{-1}$

Final Format: Single beam

Correction: None

Background handling: collect background after 0 minutes.

File handling: save interferogram

In the “**Bench**” page:

Gain: gain 2

Aperture: 8-12 for small samples; any values for large samples

Sample compartment: right AEM

Detector: MCT/A

- 9) **Adjust the sample height:** put a white paper on the top of the reference sample, and then put the aperture-mask on the white paper. Then you should see a red spot inside the aperture. Subsequently adjust the height knob to move the red spot until the red spot is aligned to the white line on the horizontal sample holder. After this task is done, remove the white paper and the mask.
- 10) After adjusting the sample position, watch the live display of interferogram in the “**bench**” page. Please check the maximum voltage. If the maximum voltage is out of the recommended range (the recommended maximum voltage is 5.5~9.5; around 8 is the best), further adjust “**aperture**” or “**gain**” in the “**bench**” page. (*Don’t align any other optical part in the TOM box by yourself*).
- 11) If your sample is quite large (larger than 25mm× 50mm), skip this step.  
If your sample is small (smaller than 25mm× 25mm), please put the aperture-mask on the surface of the sample. (The IR beam spot should be located at around the center of the aperture).
- 12) Under the “**SST**” menu, click “**photoelastic modulation**”. And then a “**photoelastic modulation**” page will pop up. Check the “**A**” amplitude and the “**B**” amplitude. The “**B**” amplitude should be 30~80 percent of the “**A**” amplitude. If not, adjust either the “**input gain**” knob or the “**output gain**” knob on the panel of “GWC Instruments”. After finishing examination, click the “**OK**” button to close this page.
- 13) Under the “**SST**” menu, click “**collect sample**”. And then you will get two spectra labeled with “input A” and “input B”, respectively.
- 14) Remove your reference sample and put your thin film sample onto the sample stage (**Caution: don’t touch the mirror on the sample stage**). And subsequently repeat Step 11 and 13.
- 15) Under the “**view**” menu, click “**stack spectra**”.
- 16) Ratio spectra  
In order to obtain the differential reflectivity spectrum, you need to ratio the spectra three times, as expressed by:

$$\text{differential reflectivity spectrum} = \frac{\text{spectrum of Sample B} / \text{spectrum of Sample A}}{\text{spectrum of Reference B} / \text{spectrum of Reference A}}$$

The above equation represents:

$$\frac{\Delta R}{R} = \frac{R_p - R_s}{R_p + R_s}$$

Where  $R_p$  is the  $p$ -polarized reflectivity and  $R_s$  is the  $s$ -polarized reflectivity

For example, select two spectra as active (Hold down the **Ctrl** key while clicking with the mouse on the second spectrum). And then check “**ratio spectra**” under the “**SST**” menu.

- 17) Choose “**save group**” under the “**file**” menu to save all the spectra to the folder of “C:\user\”.
- 18) You can copy and paste the final spectrum to a new window. Under the “**view**” menu, click “**full scale**” to see the peak.
- 19) Turn off the power of “PEM-90” and “GWC Instruments” after you finish your experiment.


## V. Grazing-angle reflectance measurement


The following operation instructions are based upon the fact that you have hands-on experience in transmission and ATR measurements.

A variable angle specular accessory is used for FTIR specular reflectance measurement. If you set the incidence angle at  $80^\circ$  (typically  $74\sim 83^\circ$ ), you can use it to measure very thin films or adsorbed species on the substrate. The recommended sample dimension is  $>20\text{mm}\times >50\text{mm}$ .

- 1) Select a detector.

In case of thick films or strongly reflected species, use the “DTGS” detector. In case of very thin films or monolayers, use the “MCT” detector and you must fill the “MCT” detector with liquid nitrogen.



- 2) Insert the grazing-angle reflectance baseplate into the sample compartment.
- 3) Wear gloves, and then adjust both the incidence and the reflectance angles to  $80^\circ$ .
- 4) Put a reference sample on the sample stage (**Caution: don't touch the mirror on the sample stage**).
- 5) Start the “ OMNIC” software. Select the experimental file of “**Grazing Angle\_IR**” from the drop-down list box of **Experiment: Transmission E.S.P**.
- 6) **Adjust the sample height**: put a piece of white paper on the top of the reference sample (please ensure the intimate contact between the white paper and the reference sample). Then you should see a red spot on the white paper. Subsequently adjust the height knob to move the red spot until the red spot is aligned to the white line on the sample stage. After this task is done, remove the white paper.

- 7) In the “**bench**” page, select the corresponding detector from the drop-down menu of “detector”
- 8) Watch the live display of interferogram in the “**bench**” page. Please check the maximum voltage. If the maximum voltage is out of the recommended range (the recommended maximum voltage is 5.5~9.5), further adjust “**aperture**” or “**gain**” in the “**bench**” page.
- 9) Click the “collect background” button to collect the background.
- 10) Remove your reference sample and put your thin film sample onto the sample stage, and then click the “collect sample” button  for data collection.

## VI. DRIFTS measurement

The following operation instructions are based upon the fact that you have hands-on experience in transmission measurements.

The DRIFTS (Diffuse Reflectance Infrared Fourier Transform Spectroscopy) measurement is suitable for powder samples or rough surfaces.

- 1) Select a detector.  
Generally, use the “DTGS” detector. If the signal is too weak or the IR spectrum is too noisy (the signal-to-noise ratio is too small), you can use the “MCT” detector (you must fill the “MCT” detector with liquid nitrogen).
- 2) Insert the DRIFTS accessory into the sample compartment (don’t close the cover of the sample compartment)
- 3) Load a reference sample into the sample stage.
- 4) Start the “ OMNIC” software. Select the experimental file of “**DRIFTS-Nexus Smart Collector**” from the drop-down list box of .
- 5) Under the “**collect**” menu, open the “**experiment set-up**” window. Set up the experimental parameters as follows:  
In the “**Collect**” page:  
Number of scans: 128 or 256  
Resolution:  $8\text{cm}^{-1}$  or  $4\text{cm}^{-1}$   
Final Format: Log (1/R)  
Correction: None  
File handling: save interferogram  
Background handling: collect background after 0 minutes.


In the “**Bench**” page:

Gain: Autogain

Sample compartment: Main

Detector: either DTGS or MCT/A


Accessory: smart collector

- 6) Click the “collect background” button to collect the background.
- 7) Load your sample into the sample stage, and then click the “collect sample” button  for data collection.
- 8) After you get the DRIFTS spectrum, you can make “kubelka-Munk” correction of the DRIFTS spectrum. Click “**other conversions**” under the “**process**” menu, Select “**kubelka-Munk**”.

## VII. NIR measurement

The following operation instructions are based upon the fact that you have hands-on experience in Mid-IR transmission measurements.

The default setting of the spectrometer is for Mid-IR. You have to swap the beam-splitter and the detector for near-infrared (NIR) measurement. For NIR measurement, select the quartz-halogen source (25,000~2,000 $\text{cm}^{-1}$ ), Silicon on  $\text{CaF}_2$  beam-splitter (13,500~1,200 $\text{cm}^{-1}$ ), either InGaAs (12,000~3,800 $\text{cm}^{-1}$ ) or InSb (10,000~1,850 $\text{cm}^{-1}$ ) as detector. **After you have finished your NIR experiments, please return the “KBr” beam-splitter and the “MCT/A” detector to the spectrometer.**

- 1) Install the black “C-series” screen into the optical port on the right side of the sample compartment. You can also select other screens such as “B-series” or “D-series”.
- 2) Plug out the detector from the location marked as “MCT”. Plug either InGaAs or InSb detector into the spectrometer (For the InSb detector, please fill it with liquid nitrogen and then wait for 30min before starting data acquisition). **Handle detectors with care. Avoid any collision.**
- 3) Swap the beam-splitter to “ $\text{CaF}_2$ ”. And store the “KBr” beam-splitter at the spare lot **inside the spectrometer. Handle beam-splitters with care. Avoid any collision (scratch).**
- 4) Start the “ OMNIC” software. Select the experimental file of “**NIR- $\text{CaF}_2$ -transmission**” from the drop-down list box of .
- 5) Under the “**collect**” menu, open the “**experiment set-up**” window. Set up the experimental parameters as follows:

In the “**Collect**” page:

Number of scans: 32, or 64

Resolution: 8 $\text{cm}^{-1}$  or 4 $\text{cm}^{-1}$

Final Format: Absorbance

Correction: None

File handling: save interferogram

Background handling: collect background after 0 minutes.

In the "**Bench**" page:


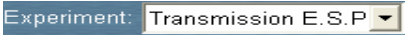

Gain: gain 1

Sample compartment: Main

Detector: either InGaAs or InSb

Source: white light

Spectral range: 10,000~4,000 $\text{cm}^{-1}$  for InGaAs detector, 10,000~2,000 $\text{cm}^{-1}$  for InSb detector


- 6) Open the "**experiment set-up**" window under the "**collect**" menu. In the "**diagnostic**" page, click the "**Align...**" button. It is important that the sample compartment is clear of all accessories when this task is performed.
- 7) Watch the live display of interferogram in the "**bench**" page. Adjust "**aperture**" or "**gain**" to optimize the maximum voltage (3.0~9.8).
- 8) Click the "collect background" button to collect the background.
- 9) Load your sample into the sample stage, and then click the "collect sample" button  for data collection.
- 10) If you want to change the X-axis unit to "nanometer" from " $\text{cm}^{-1}$ ", firstly click the desired spectrum curve to make it active, and then click "**other conversions**" under the "**process**" menu, subsequently select "**nanometer**".
- 11) Option: A blue square optical filter can be used to cut off the optical signal with the wavenumber  $>6500\text{cm}^{-1}$ .
- 12) After you have finished your NIR experiments, please do the following:
  - a) Swap the detector to "MCT/A"
  - b) Swap the beam-splitter to "**KBr**". Store the "**CaF<sub>2</sub>**" beam-splitter at the spare lot **inside the spectrometer**.
  - c) Remove the black screen from the optical port on the right side of the sample compartment.
  - d) Select the experimental file of "**Transmission E.S.P**" from the drop-down list box of .
  - e) Open the "**experiment set-up**" window under the "**collect**" menu. In the "**diagnostic**" page, click the "**Align...**" button. It is important that the sample compartment is clear of all accessories when this task is performed. After this task is done, click the "**OK**" button.
  - f) Exit the " **OMNIC**" software
  - g) Return all the stuff to the original location.

## VIII. Visible measurement

The following operation instructions are based upon the fact that you have hands-on experience

in Mid-IR transmission measurements.

The default setting of the spectrometer is for Mid-IR. You have to swap the beam-splitter and the detector for visible spectroscopy measurement. For visible spectroscopy, select the quartz-halogen source (25,000~2,000 $\text{cm}^{-1}$ ), quartz beam-splitter (25,000~2,800 $\text{cm}^{-1}$ ), and Si detector (25,000~8,600 $\text{cm}^{-1}$ ). **After you have finished your experiments, please return the “KBr” beam-splitter and the “MCT/A” detector to the spectrometer.**

- 1) Install the black “C-series” screen into the optical port on the right side of the sample compartment. You can also select other screens such as “B-series” or “D-series”.
- 2) Plug out the detector from the location marked as “MCT”. Plug the Si detector into the spectrometer. **Handle detectors with care. Avoid any collision.**
- 3) Swap the beam-splitter to “Quartz”. And store the “KBr” beam-splitter at the spare lot **inside the spectrometer. Handle beam-splitters with care. Avoid any collision or scratch.**
- 4) Start the " OMNIC" software. Select the experimental file of "VIS-NIR-Quartz-Si" from the drop-down list box of Experiment: Transmission E.S.P.
- 5) Under the "collect" menu, open the "experiment set-up" window. Set up the experimental parameters as follows:

In the “Collect” page:

Number of scans: 32, or 64

Resolution: 8 $\text{cm}^{-1}$  or 4 $\text{cm}^{-1}$

Final Format: Absorbance

Correction: None

File handling: save interferogram

Background handling: collect background after 0 minutes.

In the “Bench” page:

Gain: gain 1


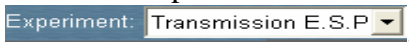

Sample compartment: Main

Detector: Si

Source: white light


Spectral range: 25,000~9,000 $\text{cm}^{-1}$

- 6) Open the "experiment set-up" window under the "collect" menu. In the “diagnostic” page, click the “Align...” button. It is important that the sample compartment is clear of all accessories when this task is performed.
- 7) Watch the live display of interferogram in the “bench” page. Adjust “aperture” or “gain” to optimize the maximum voltage (2.5~8.8).
- 8) Click the “collect background” button to collect the background.


- 9) Load your sample into the sample stage, and then click the “collect sample” button  for data collection.
- 10) If you want to change the X-axis unit to “nanometer” from “ $\text{cm}^{-1}$ ”, firstly click the desired spectrum curve to make it active, and then click “**other conversions**” under the “**process**” menu, subsequently select “**nanometer**”.
- 11) Option: A red square optical filter can be used to cut off the optical signal with the wavenumber  $>16000\text{cm}^{-1}$ .
- 12) After you have finished your visible spectroscopy experiments, please do the following:
  - a) Swap the detector to “**MCT/A**”
  - b) Swap the beam-splitter to “**KBr**”. Store the “**Quartz**” beam-splitter at the spare lot **inside the spectrometer**.
  - c) Remove the black screen from the optical port on the right side of the sample compartment.
  - d) Select the experimental file of “**Transmission E.S.P**” from the drop-down list box of .
  - e) Open the “**experiment set-up**” window under the “**collect**” menu. In the “**diagnostic**” page, click the “**Align...**” button. It is important that the sample compartment is clear of all accessories when this task is performed. After this task is done, click the “**OK**” button.
  - f) Exit the “**OMNIC**” software 
  - g) Return all the stuff to the original location.

## IX. Data analysis

### 1) Function of some buttons:


Click the  button to review the collection and processing information of your spectrum data

Click  to convert the spectrum to %transmittance units.

Click  to convert the spectrum to absorbance units.

Click  to normalize the Y scale.

Click  to zoom in the spectrum.


Click  to zoom out the spectrum.

Click  or  to shift the spectrum

### 2) Automatic Baseline Correct

“**Automatic Baseline Correct**” in the “**Process**” menu lets you automatically correct the tilted baselines of the selected spectra (see the example below), with the baseline points selected by the software.

If the baseline is severely tilted, this means that a KBr pellet was made with coarsely ground KBr powder, or the KBr pellet was improperly pressed. Make the pellet again using adequately fine powder.

- 3) Click the annotation tool  to label a peak. When the annotation tool is selected, you can label a peak by clicking above.

To modify an existing label, click it and then type a new label and press ENTER.


To delete an existing label, click it and then press the DELETE key.

4) Automatically label peaks

- In the "**Analyze**" menu, select "**find peaks**". Then a new window will pop up. The peaks above the threshold will be automatically label. The threshold is represented by a horizontal line passing through the pane in the window. To change the threshold, click a point above or below the threshold line. The line moves to the level you clicked, and the new threshold value appears in the threshold box.
- Use the scroll bar near the left side of the "Find Peaks" window to set the sensitivity. The sensitivity determines how readily "Find Peaks" finds shoulders on peaks and small peaks in the baseline. Sensitivity takes into account the relative size of adjacent spectral features.
- Click the "**Clipboard**" button on the left side of the "Find Peaks" window to past the peak information (peak position and peak intensity) to other software such as Microsoft EXCEL or Word.

5) Blank a peak

Use this function to delete the data points (a peck) in the selected spectral region.

- Choose the  (region tool) button on the lower left of the window and click the mouse button at a desired place, and then two arrows will display on the spectrum, move the arrows to select the spectral region.
- Choose "**Straight Line**" from the "**Process**" menu. A straight line is drawn between the two data points at the limits of the selected spectral region.
- Immediately after you blank a spectral region, you can restore it by using "**Undo**" in the "**Edit**" menu.

6) Unit conversion


If you want to change the X-axis unit to "nanometer" from " $\text{cm}^{-1}$ ", firstly click the desired spectrum curve to make it active, and then click "**other conversions**" under the "**process**" menu, subsequently select "**nanometer**".

7) ATR correction

In the ATR technique, the depth of penetration (*i.e.*, the effective pathlength) of the IR beam depends upon the wavelength of light: The shorter wavenumbers penetrate the sample more deeply than do the longer wavenumbers. As a result, the peaks at shorter wavenumbers are much stronger than those at longer wavenumbers. This skewing of peak intensities causes problems when you search a sample spectrum against a library of normalized spectra collected using standard transmission techniques, since the peaks have a different appearance. Before searching an ATR spectrum against a library of normalized transmission spectra or a library of corrected ATR spectra, correct the spectrum.


In the "**process**" menu, click "**other correction**". Then a small window will pop up. Select "**ATR**" in the drop-down menu, and subsequently click the "**OK**" button.

8) Library search: This helps you to identify the chemical composition of your sample.

- Select the spectrum by clicking it (The spectrum will become red after you have selected it).
- Choose "**library Setup**" from the "**analyze**" menu, a "**library set up**" window will pop up. In the **Search Libraries** page, highlight the preferred library such as "Aldrich condensed phase library" and "Nicolet standard collection of FT-IR spectra", and then click **Add >>** to add the directory to the list. Finally click "**OK**".
- Click the search button  to search for a matching spectrum from the library database. After finishing search, a matching spectrum appears on the bottom of the collected spectrum. If you click **View Match List**, you can see a list of matching spectra.

Note: The "search library" function is used for identifying an unknown compound. The "QC library" is used for comparing known compound rather than for identifying an unknown compound




9) Search the standard spectrum of a compound

In the "**Analyze**" menu, select "**library manager**". Then a new page will pop up. In the "**library names**" page, select "**search libraries**". Then go to "**search for text**" page, and make "**all libraries**" selected (  All libraries ). Type the compound name into the column of "**text in selected item**". Click the "**Search**" button, and a matching list will appear.

10) Choose "**IR spectrum interpretation**" from the "**analyze**" menu to help you with identifying the peaks.

11) Quality control (QC) library:

You can verify the composition of your sample by comparing the collected spectrum with that in a QC library.



- Choose "**library setup**" from the "**analyze**" menu, a "**library set up**" window will pop up. In the  page, available QC libraries will appear. Then highlight the QC libraries, and click  to add the directory to the list
- Click  to begin a comparison. When the comparison is finished, the QC compare window appears.

#### 12) Subtraction:

Select two spectra as active (Hold down the **Ctrl** key while clicking with the mouse on the second spectrum). Display them as absorption spectra.

Choose "**subtraction**" from the "**process**" menu. You will get a new OMNIC window entitled "subtract" and a display with three panes of spectra: the two originals and their difference.

#### 13) Create report:

- Creating a report: Choose "**template**" from the "**report**" menu. Select a template file from the list, a preview image of the template appears at the right. Then click the  button. Subsequently choose "**preview/print**" from the "**report**" menu, and then you can see a desired experimental report.
- Copying and pasting a report: Choose "**preview/print**" from the "**report**" menu. Then click the "**copy**" button. You can paste the report to other software such as Microsoft EXCEL or Word.
- Printing a report: Choose "**preview/print**" from the "**report**" menu. Then click the  button.

#### 14) Export data

Select the spectrum by clicking it (The spectrum will become red after you have selected it). Choose "**save as**" under the "**file**" menu, then save as your file to the "**.CSV**" format, which can be opened by Microsoft EXCEL or ORIGIN 7. If you save as your file to the "**.tif**" format, you can export the spectrum as an image.

#### 15) How to place several spectra into one window


Go to "**window**" menu and select "**new window**" to open a new window.

Copy the spectra from other windows to the new window.

You can drag any spectrum up and down using the left mouse button

Select at least two spectra as active (hold the **Ctrl** key while clicking the mouse on the second spectra), then select "**save group**" in the file menu to save all the spectra into one file.

## X. Ending experiments

- 1) Exit the "OMNIC" software.
- 2) Take you sample out of the sample compartment.
- 3) Clean up the Qwik Handi-Press kit if you have used it.
- 4) Strictly follow the required procedure to clean up the ATR crystal or other IR windows using the proper cleaning solvents if you have used them.
- 5) Put all the stuff to the original location.

**Note:** Don't shut down the power of the spectrometer.