# NYU Department of Chemistry
# Thermo Scientific Nicolet-6700 FTIR User Manual

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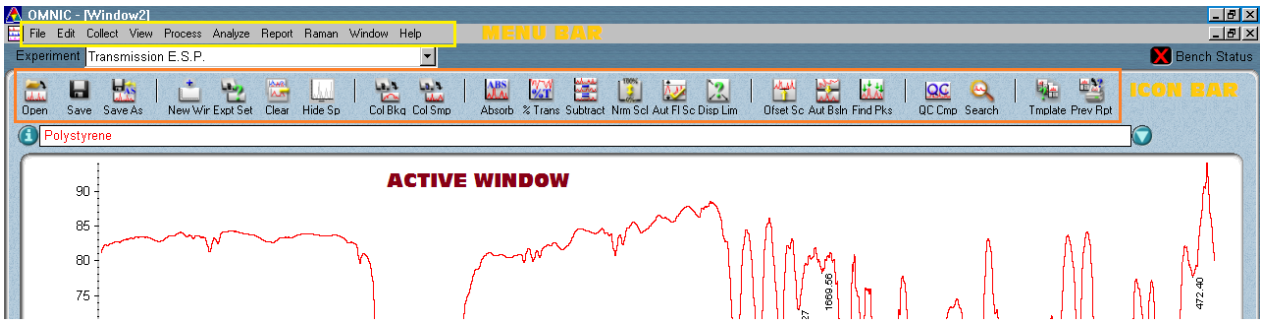
## 1.0 Experiment Setup

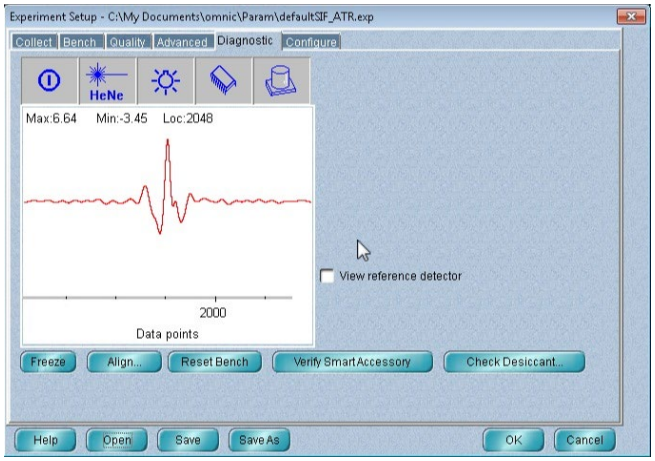
1.1 Click on the OMNIC icon to open the software. 

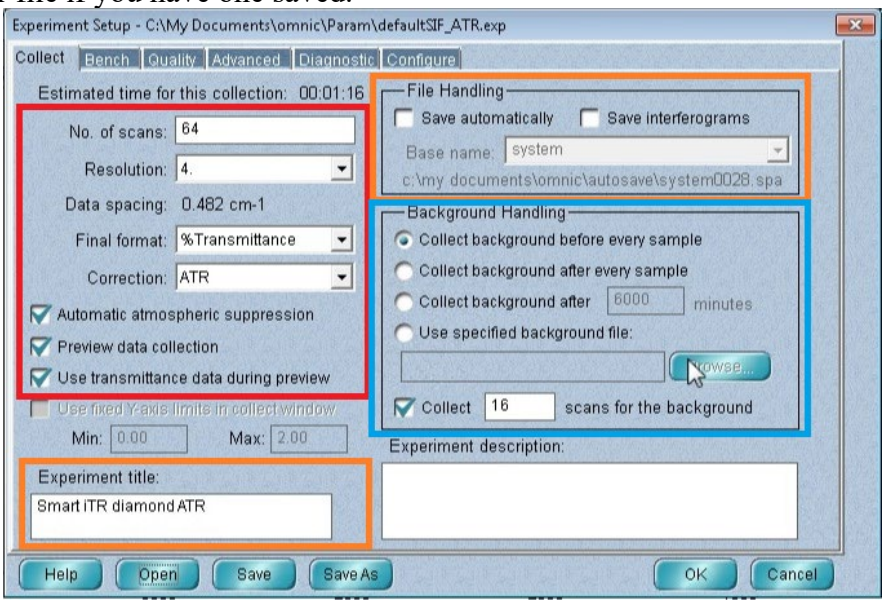

1.2 Using the icon bar, open the "**Experiment Setup**" menu by clicking on 

. Check that a signal is being measured under the "**Diagnostic**" tab. You should see a peak centered in the left window with a max value above 6.5.

1.3 If you have problems seeing a signal, or the signal is low, you can realign the mirrors to obtain an optimum signal. Go into the "**Diagnostic**" tab and click on the "**Align…**" button. This process will take a few minutes. Check the signal strength again.




1.4 Click on the "**Collect**" tab to setup the experiment. Open the default Transmittance experiment setting by pressing on the "**Open…**" button and open C:/My Documents/Omnic/Param/default_ATR.EXP or your parameter file if you have one saved.



i. **No. of scans:** Number of scans to acquire background and spectrum. ***Default is 64.***

ii. **Resolution:** Resolution of the spectrum can be adjusted for course or fine details. Resolution range is between 32 and 0.125. ***Default value is 4.***

iii. **Final Format:** Typically, either % Transmittance or Absorbance scales are used. It can be interchanged post acquisition. ***Default value is % Transmittance***.

iv. **Correction:** Since the ATR is typically used, the correction should always be set to ***ATR*** to adjust for the ATR attachment.

v. **Check Boxes:**

- *Automatic Atmospheric Suppression* is used to remove any common gaseous resonances , e.g. $CO_2$, CO, $N_2$ etc., from the spectrum
- *Preview Data Collection* shows the data before accumulating scans. Will need to hit the collect button on the active window screen to start the acquisition.
- *Use Transmittance Data During Preview* is self-explanatory

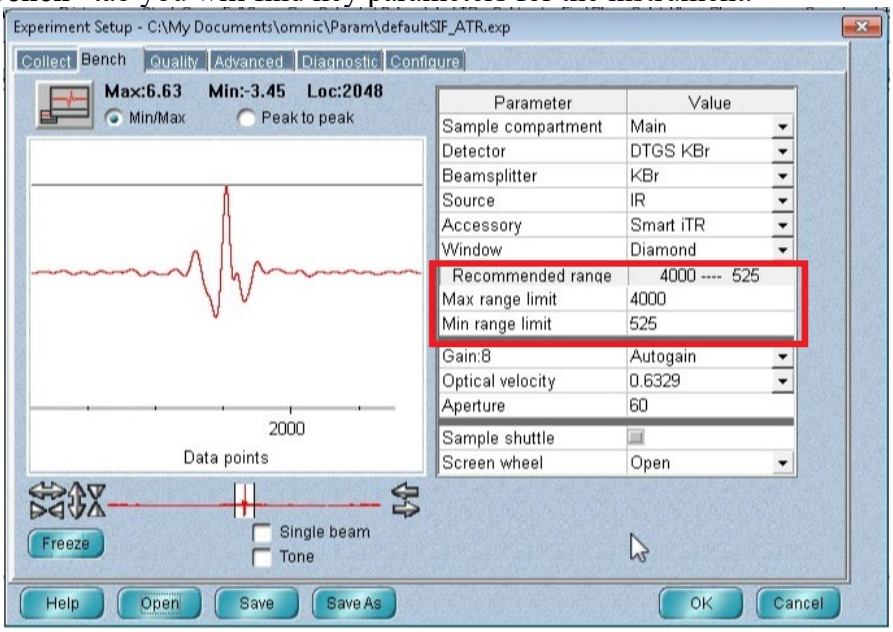
vi. **Experiment Title:** This identifies the type of experiment being performed.

vii. **File Handling:** You can select if you would like to save the data automatically after the acquisition is complete. You will need to define the location where the data is to be saved to. Also, you can decide if you want to save the interferogram as well.

viii. **Background Handling:** There are multiple options when to acquire the background signal. Depending on how many samples you are dealing with, it is recommended to use either of these two options:

- ***Collect background before/after every sample*** - This will prompt the user to collect a background spectrum before or after each sample. Useful when studying only few samples.
- ***Use specified background file*** – Requires the collection of a background spectrum and saved as a file. After it is saved, select "Use specified background file" radio button and browse/open the background file that you recently saved. This is good if you plan on working with numerous samples with the same substrate.
- When collecting a background before or after the sample, the number of scans to be collected for the background could be selected and defined.

1.5 Under the "**Bench**" tab you will find key parameters for the instrument.

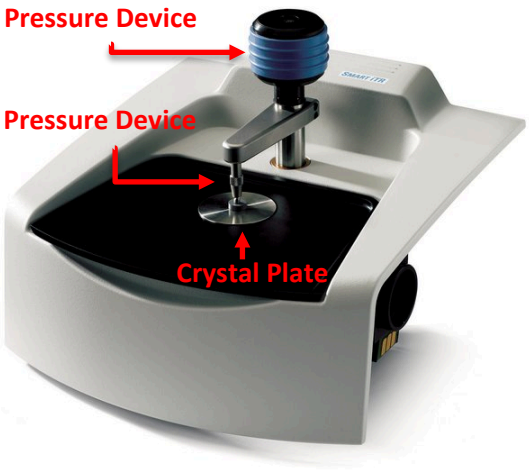


1.6 You can adjust the spectral window here. ***Max range is between 4000 and 525 $cm^{-1}$***. You change to a smaller range if you want to focus on a specific region for better details.

1.7 Click "**OK**" button to exit the Experiment setup.

**NOTE: When acquiring a background spectrum, use the exact same settings (resolution, corrections, suppression options etc.) you will use for your sample.**

## 2.0 Collecting the Background



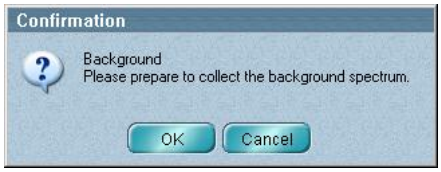

2.1 Clean the iTR, Pressure Device Anvil and Crystal Plate, using a lint-free wipe sprayed with alcohol (isopropanol or ethanol) and let it dry for 30 seconds.

2.2 *For solids* – use a clean blank crystal plate as the background.
*For liquids* - use the solvent that the material is dissolved in as the background.

2.3 *For solids* - Swing the pressure device and lower the anvil onto the plate my turning the Pressure Device Knob. There is a safety setting so that once the desired pressure is applied onto the sample the knob should just slip.
*For liquids* – Place a volatile cap on top of the solvent.

2.4 To start collecting, there are two buttons that can be used:  Collect Background,  Collect Sample. The one you select depends on what was selected in under Background Handling in section 1.0.

- If the option to "Collect background before every sample" is selected, you can just click on collect Sample button. It will automatically prompt you to prepare the sample area for background the background spectrum.
- If you decide to "Use specified background file", you must click on Collect Background to start background acquisition.




2.5 When collecting the background, it will first ask to prepare the sample area for background collection. Once the sample area is clean and dry, press "**OK**".

2.6 If you want to specify the background file later, you must save the background spectrum when the collection is complete. If not, it will then prompt you to prepare to collect the sample spectrum.

## 3.0 Sample Preparation

3.1 Once the background is collected:

- If you are collecting the background before every sample a prompt will ask to prepare your sample right after it finishes collecting.
- If you have collected and saved your background spectrum, go back to the Experiment Setup, and specify to use your new background file in the Collect Tab under the Background Handling section.

3.2 When ready to collect the sample, raise the Pressure Device arm and swing it away from the crystal plate.

3.3 Directly place the solid powder (**never use a large crystal, always grind the sample into a powder**) or liquid sample onto the small crystal embedded in the stainless-steel plate.

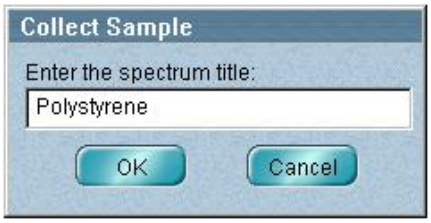
3.4 For solids: Swing arm/anvil over the sample and turn the knob to apply pressure.

3.5 For liquids: Place cap on top to prevent evaporation of volatile solutions. **DO NOT COMPRESS THE ARM ON TOP OF THE CAP**.

Anvil Tips Volatile Cap

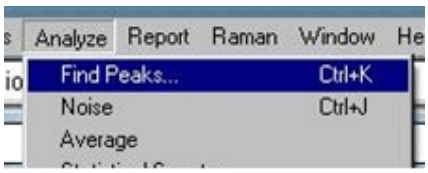
## 4.0 Collecting the Data and Analysis

4.1 Once your sample is ready click the Collect Sample Button  or "**OK**" in the prompt. A new prompt will ask you to enter a title for your spectrum. Enter title or description and click "**OK**" when ready to collect.

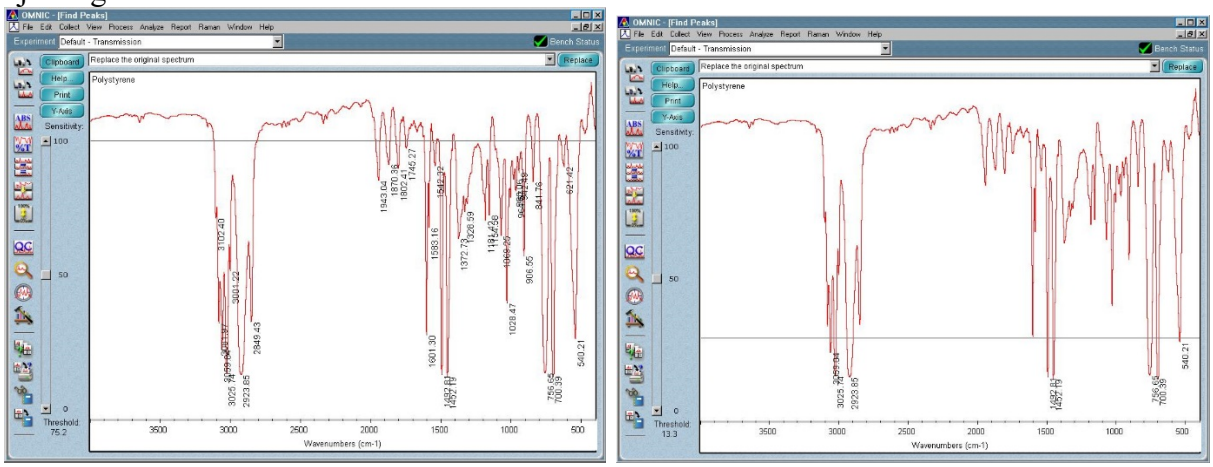



4.2 During acquisition, you can select which window to add the spectrum to when completed. If you want to put them in separate windows, select "Add to new window" in the drop-down menu above the spectrum.

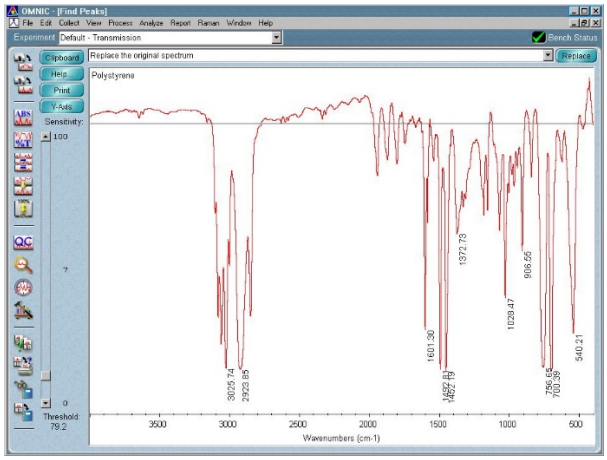

4.3 Once acquisition is complete, peak positions can be determined through the "**Analyze**" menu and "**Find Peaks…**" option or clicking the  icon.

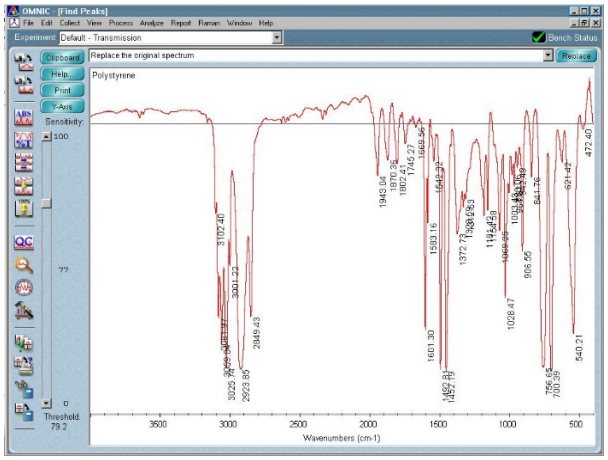



4.4 In the spectrum window you can adjust the peak picking threshold by clicking on the spectrum and adjusting the location of the horizontal line.



The sensitivity of the peak picking can be adjusted by the siding bar on the left of the spectrum.




4.5 Once peaks are selected you can choose to replace the original spectrum, or add it to a different window. To avoid confusion, select "**Replace the original spectrum**" and click on "**Replace**" button.


4.6 You can save your data in your mapped SIF data directory. The file can be saved under different formats:

**Spectra (*.spa)** – Standard OMNIC spectra file format.

**CSV Text (*.csv)** – Comma-separated values, text file containing data points to be read in by a spreadsheet program (e.g. Excel, Origin). Does not save peak labels.

**Windows Metafile (*.WMF) / TIFF (*.TIF)** – image file format. Saves what is seen in the active window.