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Experiment Setup

Experimental parameters should be carefully selected to achieve IR spectra of satisfactory quality within a reasonable amount of time for each application.

Experiment Setup

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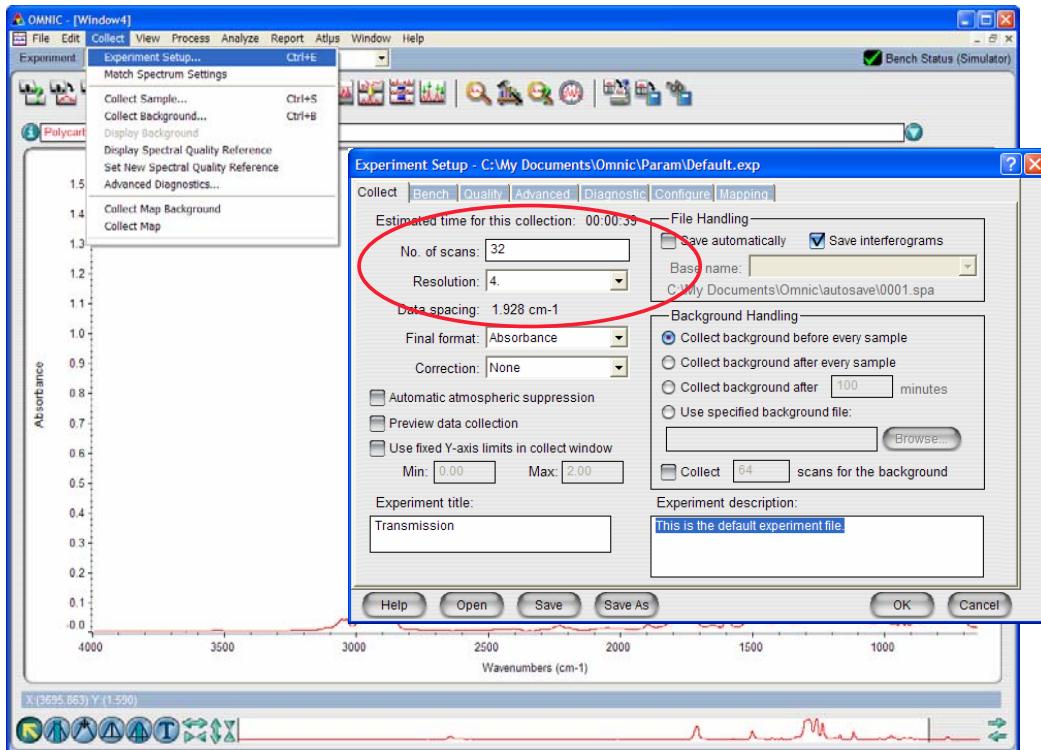
Diagnostics Tab

Align and Reset

100% Transmission Line Noise Test



Collect Tab – Setting Number of Scans and Resolution



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Experimental parameters are selected in the Experimental Setup dialog box under the Collect drop down menu.

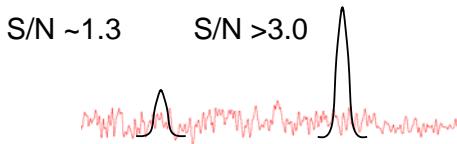
Collect | Experiment Setup | Collect tab

Setting a sufficient number of scans and appropriate resolution is critical for obtaining an acceptable spectral quality for each application. There is no one set parameters that works for all applications.

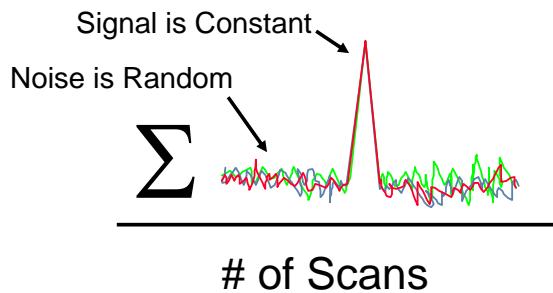
Setting Number of Scans

S/N = Signal to Noise Ratio

Instrumental Noise: extraneous and random fluctuation in measured intensity.



Signal Averaging



$$\frac{S}{N} = \frac{nS_n}{\sqrt{n}N_n} = \sqrt{n} \frac{S_n}{N_n}$$

S: Signal, N: Noise, n: number of scans

D. A. Skoog and J. J. Leary, *Principles of Instrumental Analysis 4th ed.* Fort Worth: Saunders College Publishing, 1992.



Number of scans affects signal to noise ratio (S/N). A higher S/N ration leads to a better quality spectrum. For the final spectrum, spectra are coadded and averaged by the number of scans. Increasing the number of scans increases the S/N to a point, because signal intensity accumulates linearly whereas noise intensity accumulates square root of number of scans.

Types Instrumental Noise - Thermal, Shot, Flicker, and environmental Noise

Thermal Noise (Johnson Noise): noise caused by agitation of charge carriers in resistors and capacitors in an instrument.

Shot Noise: related to statistical fluctuations for random and quantized transfer event of charged particles through junctions.

Flicker Noise (1/f): Noise with magnitude inversely proportional to frequency; hence the name “1/f noise”.

Environmental Noise: Noise created from sources other than the instrument, but environment.

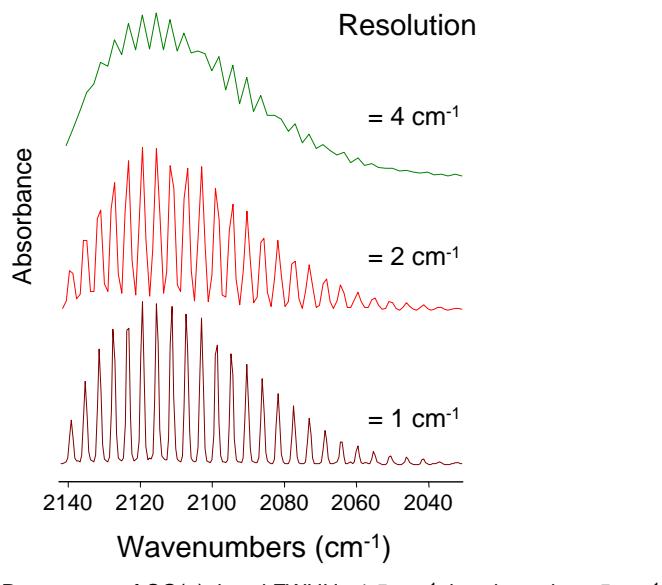
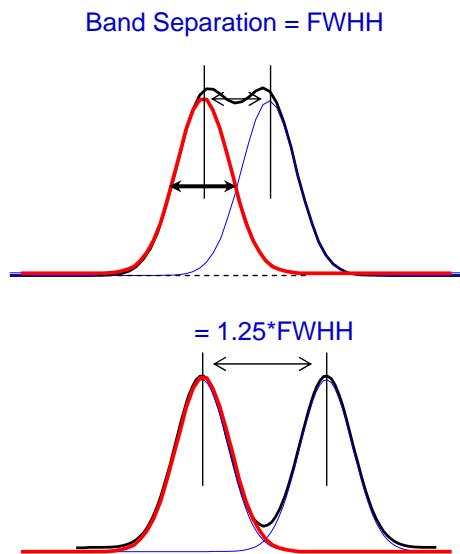
Types of Noise Measurements*

Peak-to-peak noise is the difference between the highest and lowest noise peaks in the selected spectral region. Before measuring the noise, the software corrects any baseline tilt using a least-squares correction method.

Root mean square (rms) noise measurement is a statistical analysis of the noise variation. The rms noise level is equal to the square root of the average of the squares of the data points in the selected spectral region.

Resolution

- The ability to separate two closely spaced bands.
- Bands with Full Width at Half-Height (FWHH) broader than the resolution setting are distinguished.



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Resolution is the ability to distinguish two closely spaced bands. According to the FWHH criterion, two bands with identical intensity and FWHH are considered resolved when the spacing between the lines is greater than the FWHH.*

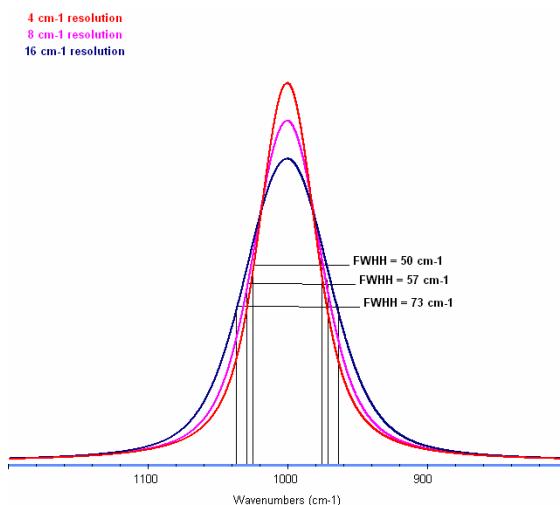
*Griffiths, P. R. and De Haseth, J. A., eds. *Fourier Transform Infrared Spectroscopy*, Wiley: New York 1986.

To distinguish between closely spaced bands, the resolution setting must be less than or equal to the separation of the bands.

In solids and liquids, many features are naturally overlapping and improving the resolution of the analysis will not separate these features.

Resolution (cont.)

- The ability to accurately depict the band shape
 - Band width and height can be distorted if system resolution is not set correctly, affecting quantitative determinations
 - The loss of intensity will effect the low level detection limit of a feature
 - Sensitivity to small variations in band intensity are diminished
 - Qualitative determinations can be affected
 - Search library resolutions should match sample resolutions
 - Visual interpretation relies on recognition of band positions and band shapes



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A band is detected if the resolution (in cm^{-1}) is less than or equal to the band FWHH. Therefore, if the resolution were setting for 4 cm^{-1} , a band with a FWHH of 2 cm^{-1} would not be resolved and identified.

Beyond simple detection, the true shape of the band is accurately depicted if the resolution setting is less than 1/7 to 1/10 of the band FWHH.

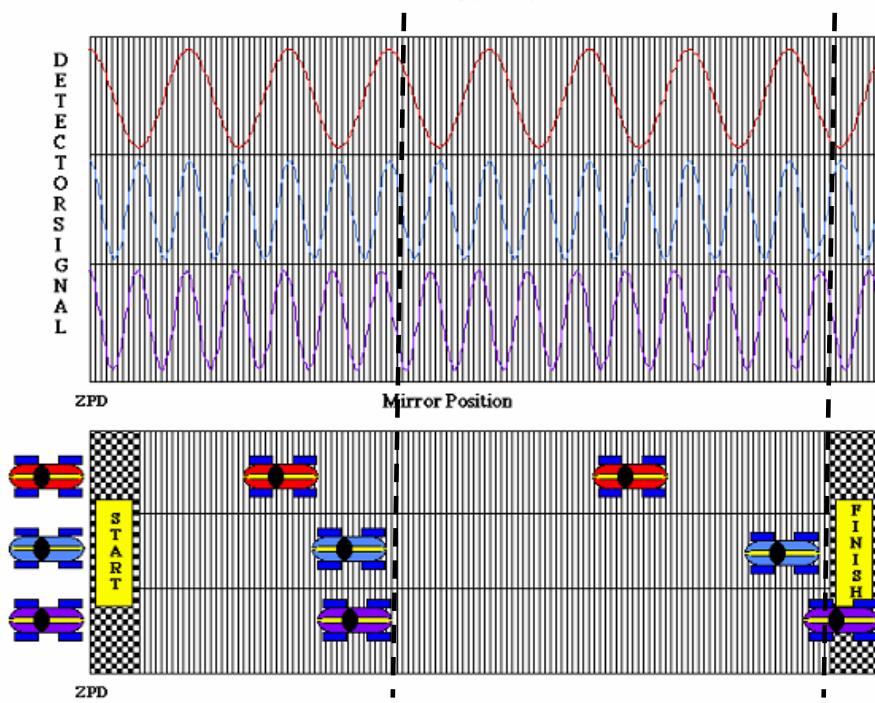
System resolutions less than this criteria will cause the bands to become broader and less intense.

The FWHH of a band is a feature of the band in much the same way the position is.

Using better resolution than necessary does not enhance the peak shape further, instead results in an increase of noise, degrading the quality of the spectrum.

In solids and liquids, resolution better than 4 cm^{-1} is rarely needed. Gas samples require higher resolution due to the narrower bands.

Resolution and Moving Mirror Travel



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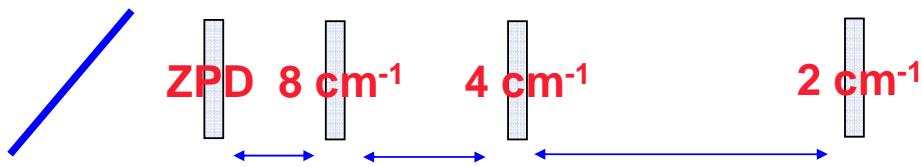
When a higher resolution is selected, (lower number), the mirror must move farther. This idea is demonstrated in this example.

Three racing cars that are traveling at three different speeds represent signal with different frequencies. The red car at the top is traveling at the lowest speed. Two cars at the bottom are traveling at similar faster speed, but one at the very bottom is slightly faster. If the mirror were moved only to the distance of the first marker, separation would occur between the lowest frequency signal and higher frequency signals. But higher velocities still have not separated. By running the race farther, it is possible to see that eventually cars with the middle and highest velocities can be separated. This is because the small, undetectable difference at the first marker is enhanced as the mirror moves further.

Resolution and Moving Mirror Travel

Increase in Resolution

- Increases **Distance** mirror moves
- Increases **Time** required for data acquisition
- Increases Instrumental **Noise**
- Decreases **Throughput** due to aperturing of the beam for collimation



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An increase in the distance the mirror moves increases the time of the experiment, increases electronic noise and decreases overall intensity throughput because the beam must be collimated using an aperture.

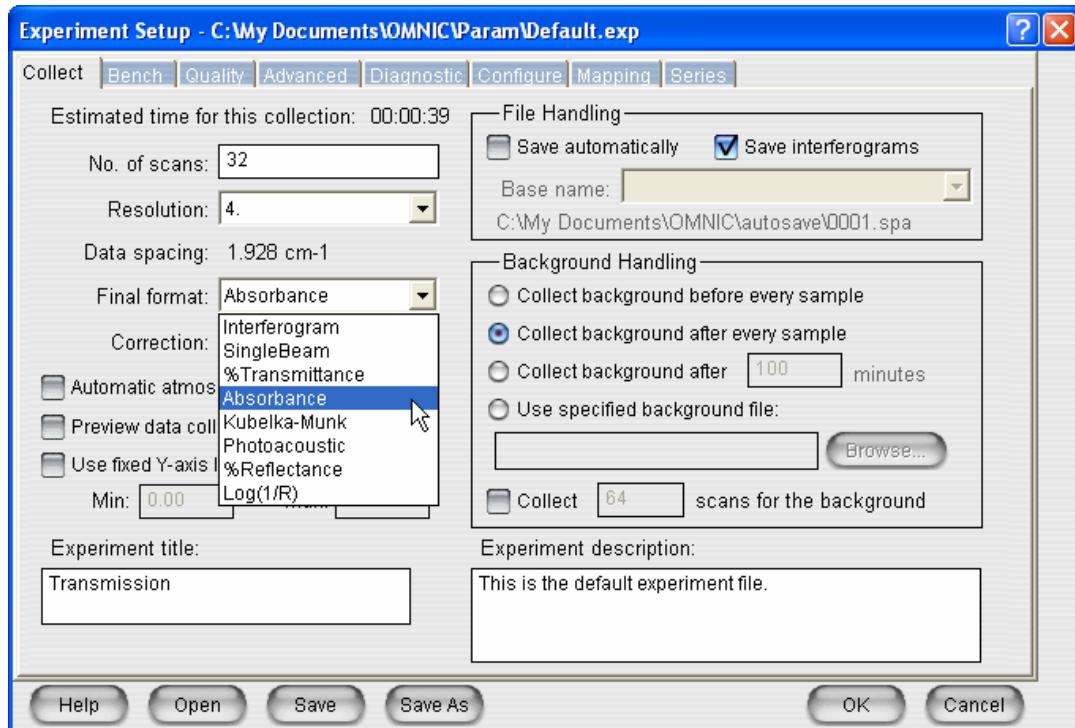
The relationship between mirror distance from ZPD and resolution is

$$\text{Resolution} = (2 * \text{Mirror distance})^{-1}$$

Resolution can be reduced but can not be increased at post-collection. Select a resolution that produces acceptable spectra without overly increasing data acquisition time. Higher resolution can provide invaluable information in certain applications.

Most commercial libraries have a resolution of 16 or 8 cm^{-1} . There are newer commercial libraries with a resolution of 4 cm^{-1} . For most applications, 4 or 8 cm^{-1} is typically used.

Final Format



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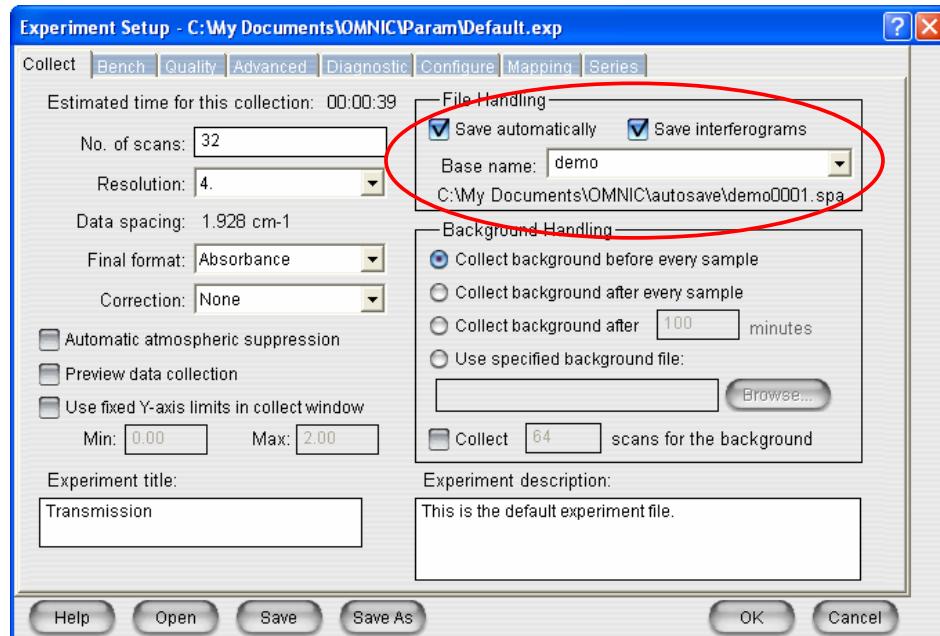
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Final Format on the Collect tab in the Experiment Setup dialog box determines the units used for the collected data. The following table shows the available final format settings and the units used by each format:

Final Format	X-Axis Unit	Y-Axis Unit
Interferogram	data point	volt
Single Beam	wavenumbers	Single Beam
%Transmittance	wavenumbers	%Transmittance
Absorbance	wavenumbers	Absorbance

File Handling Options



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To save files automatically enable Save Automatically. You may choose to enter a 4 character alpha-numeric base file name. Note the location of the “autosave” subdirectory. Recall that using Edit | Options | File Tab and setting intial autosave subdirectory will allow you to change the destination subdirectory. Automatically saved files will increment up. In this example, demo0001.spa, demo0002.spa, demo0003.spa etc. OMNIC always looks for the highest number to increment, even if you have deleted files from the subdirectory with lower numbers.

Turn on Save Interferograms if you want to include the associated reference and sample interferograms when a spectrum is saved. The interferograms will be saved in the same file as the spectrum. The interferograms will be included whether you are saving spectra automatically or saving them by using Save in the File menu.

Saving interferogram data lets you reprocess a spectrum in case you want to restore the original data.

When you reprocess the spectrum, you can use a different reference or change some of the parameter settings used for the transformation. With the abundant storage space available in current computer's, it is a good idea to always save interferogram data so that full reprocessing can occur. An interferogram is raw data that can be processed.

Background Handling Options

Collect Before Every Sample	Most commonly Used
Collect After Every Sample	Microscope date collection when aperture size limits energy
Collect After Specified amount of time (0 = infinity)	Well purged environments when fast data collection is paramount
Collect using specific named background on hard drive	Not recommended but useful if background is well defined

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Remember first to match experimental conditions between background collection and sample collection. Choose appropriate background handling option for each experiment.

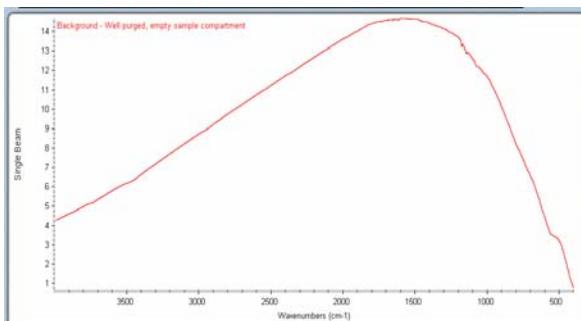
Collect background before each sample: This more closely pairs the energy of the background and environmental contamination to the sample data collection.

Collect background after each sample: This allows some adjustment to be made between sample and background collection. In the example of the microscope, the aperture is set based on the sample size and the stage moved to background material to collect background.

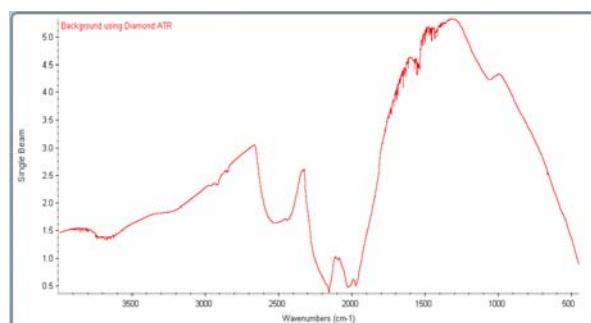
Collect background after __ minutes: (setting this to 0 means a new background is only needed when experimental parameters change or OMNIC is closed). This allows the user to determine when and if a new background is required. Setting it to a time value reminds the user to collect a new background periodically.

Use selected background file: If you have collected a background and saved it to your hard drive as a file with .spa extension you may select this option. However, this can be a dangerous practice if not changed periodically!

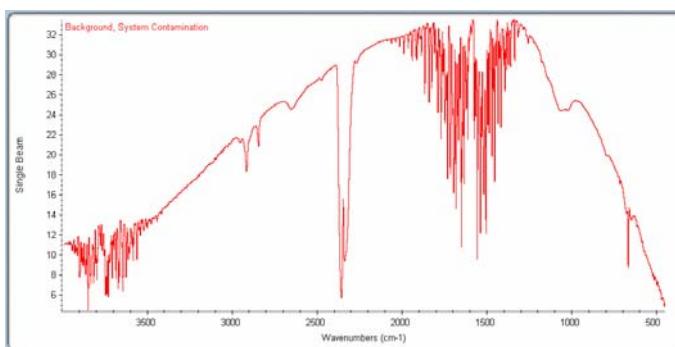
What does a background represent?



Background- Purged with nothing in Sample Compartment



Background - Diamond ATR



Background - Nothing in Sample Compartment, Purge Line Contamination



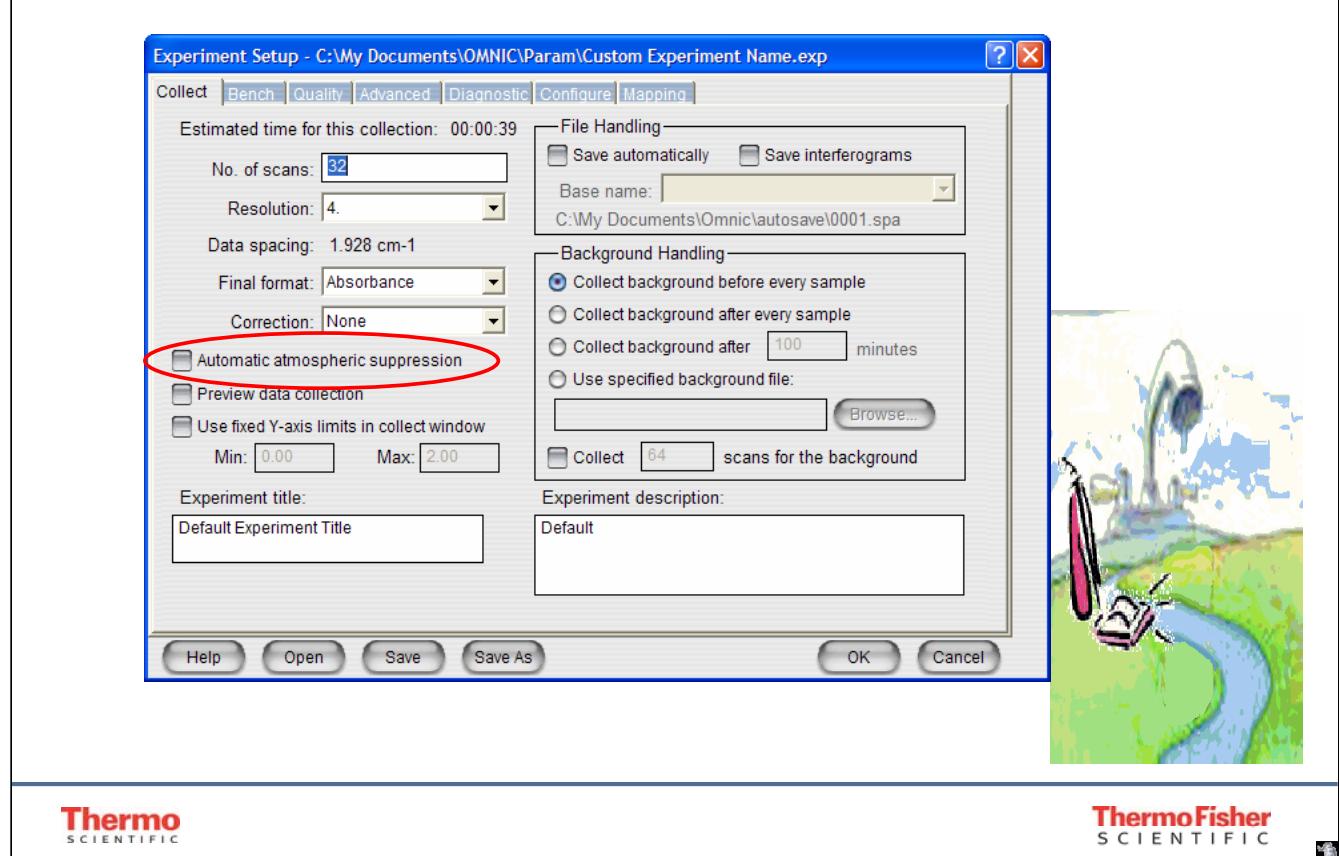
The single beam of a background is used to ratio against the single beam of a sample to produce a spectrum (either in transmission or absorbance). It represents a measurement of the maximum throughput available at each and every wavelength that might be absorbed by a sample. Because of this, it is important that the background collection represent the experimental conditions used for sample data collection.

For example, when analyzing a sample with an ATR accessory, you would first clean the ATR crystal and, with NOTHING on the ATR crystal analyze the background. This will produce a single beam of the background which represents the maximum energy available using your ATR crystal. When a sample is placed on the ATR crystal, some of the energy is absorbed by the sample and is never detected. We know which frequencies and how much of each were absorbed by the sample by knowing the original amount of energy available (the background).

The background can be thought of as the spectrum of the instrument (and accessory) and needs to be removed from the instrument plus sample spectrum to see the unique sample spectrum.

It is tempting to think that the background is subtracted from the sample. This is not the case. It is ratioed.

Atmospheric Suppression



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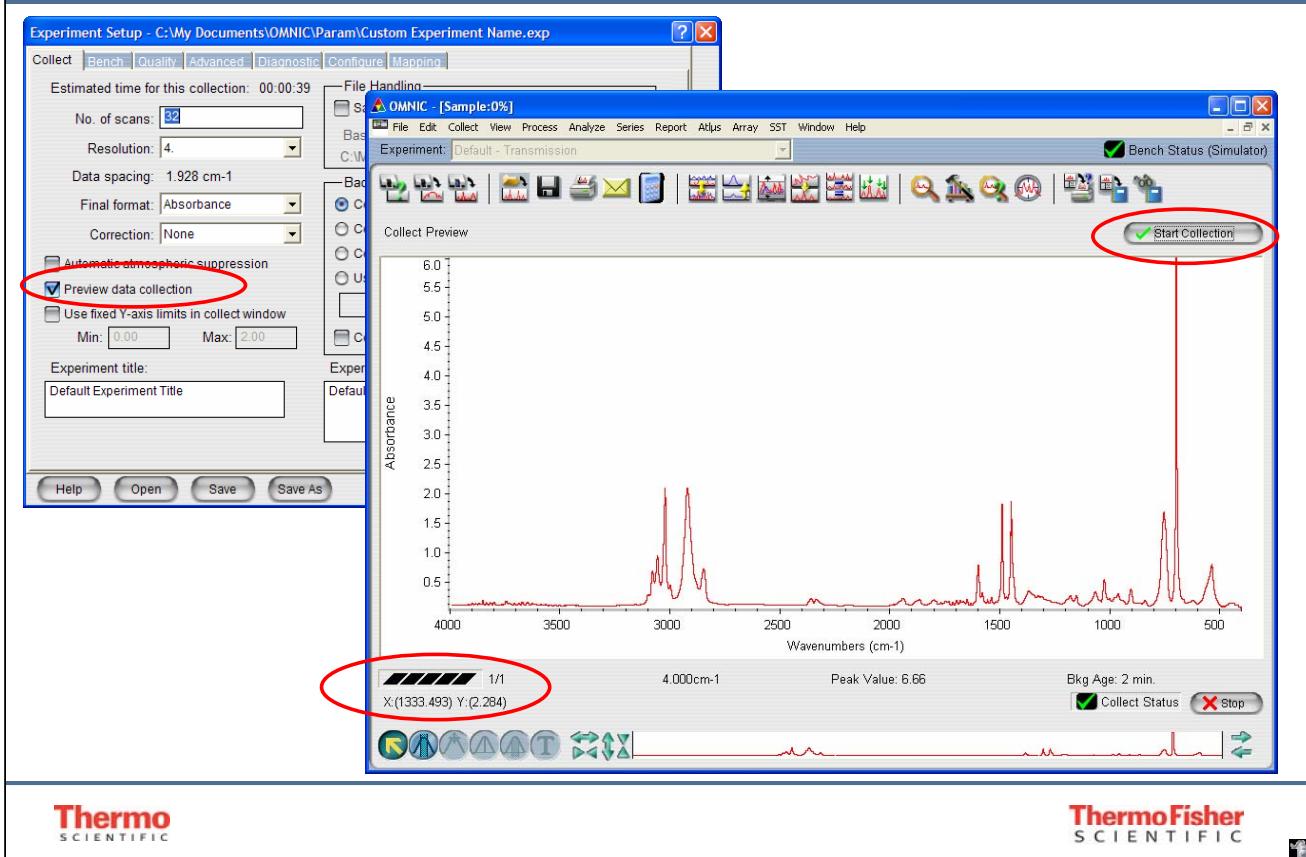
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Atmospheric Suppression is designed to remove the presence of water and CO₂ vapor *while* you are collecting data, as opposed to subtracting it from final data. To use this feature you must load and unzip all the associated quant files that came with OMNIC. Then enable this feature.

This is considered as a collection parameter and cannot be performed in post-processing as a correction. To post-collection process the spectrum and remove the water vapor and carbon dioxide contributions, the H₂O and CO₂ correction should be used in the Process | Other Corrections Menu.

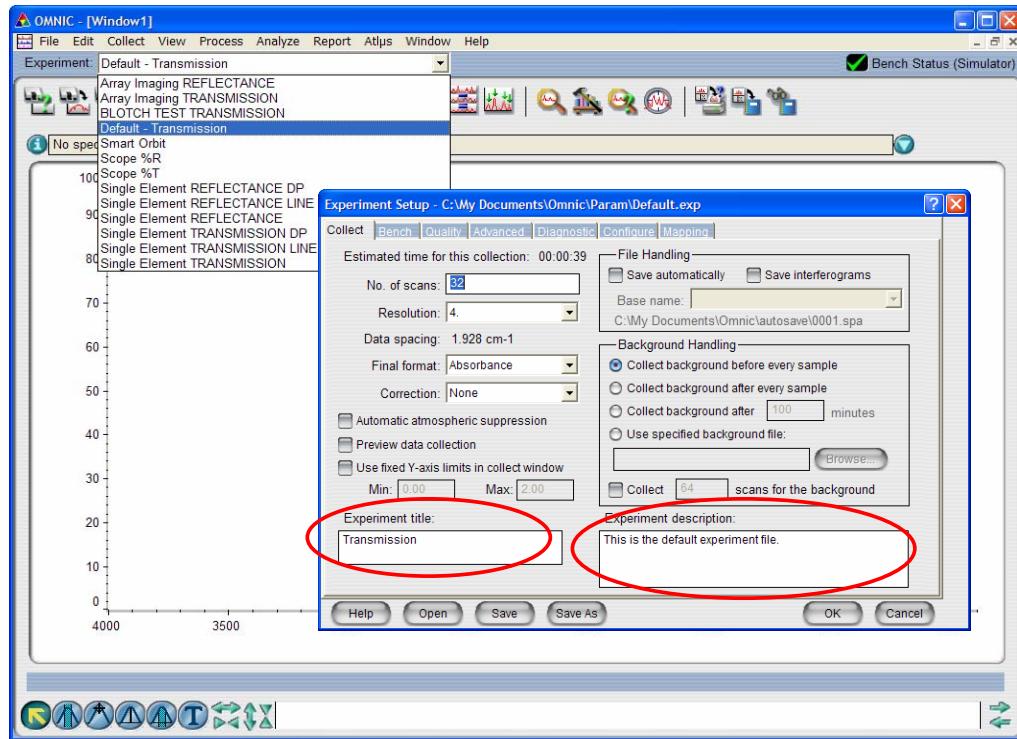
When performing quantitative analysis it is probably best not to enable automatic atmospheric suppression as it will add one additional variable to your method.

Preview Data Collection



Use preview data collection function if you would like to spend some time repositioning the sample prior to collection (nice for ATR and Microscope samples). If you use it, be sure to set an appropriate Background Handling technique (after a fixed amount of time) so that you see "ratioed" data. Also, do NOT forget to hit the Start Collection Button in the upper right hand corner of the screen when you are ready for data collection.

Experiment Description and Title



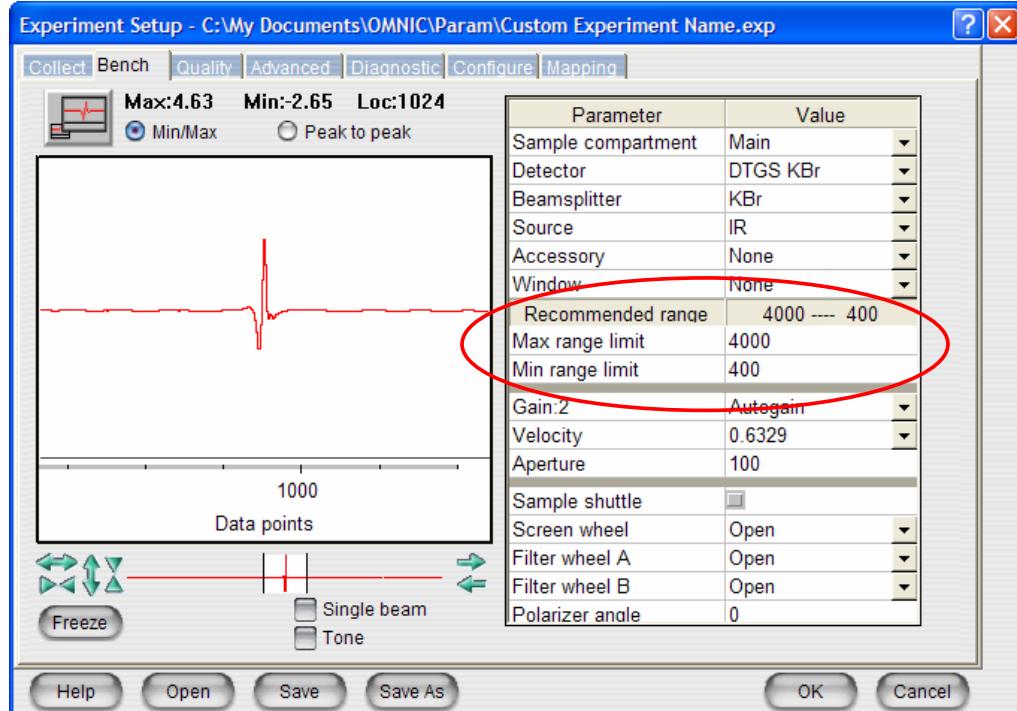
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The experiment title will appear on the experiment title drop down menu in OMNIC. It is good practice to make the title and the description meaningful before saving.

Multiple experiments may be saved and added to the Experiment drop down list. The only way to permanently remove an experiment from the list is to *delete* the experiment file from your computer hard drive.

Bench Tab - Setting Spectral Range



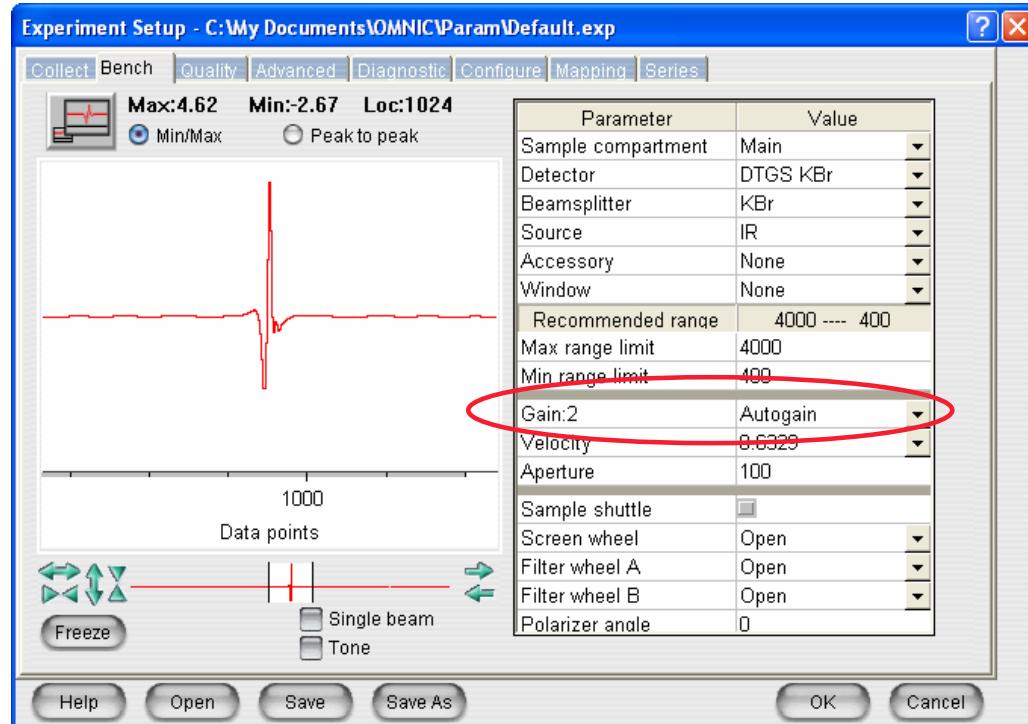
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Use the Bench Tab of Experiment Setup to set Spectral Range. Setting the appropriate spectral range for your experiment is important for things like improving the quality of a commercial library search, or, more important, developing your own spectral library.

Note: When the Smart™ Accessory is inserted into the sample compartment an experiment file is automatically loaded changing all the collection parameters. You should review these settings to be sure they meet the needs of your sample.

Gain



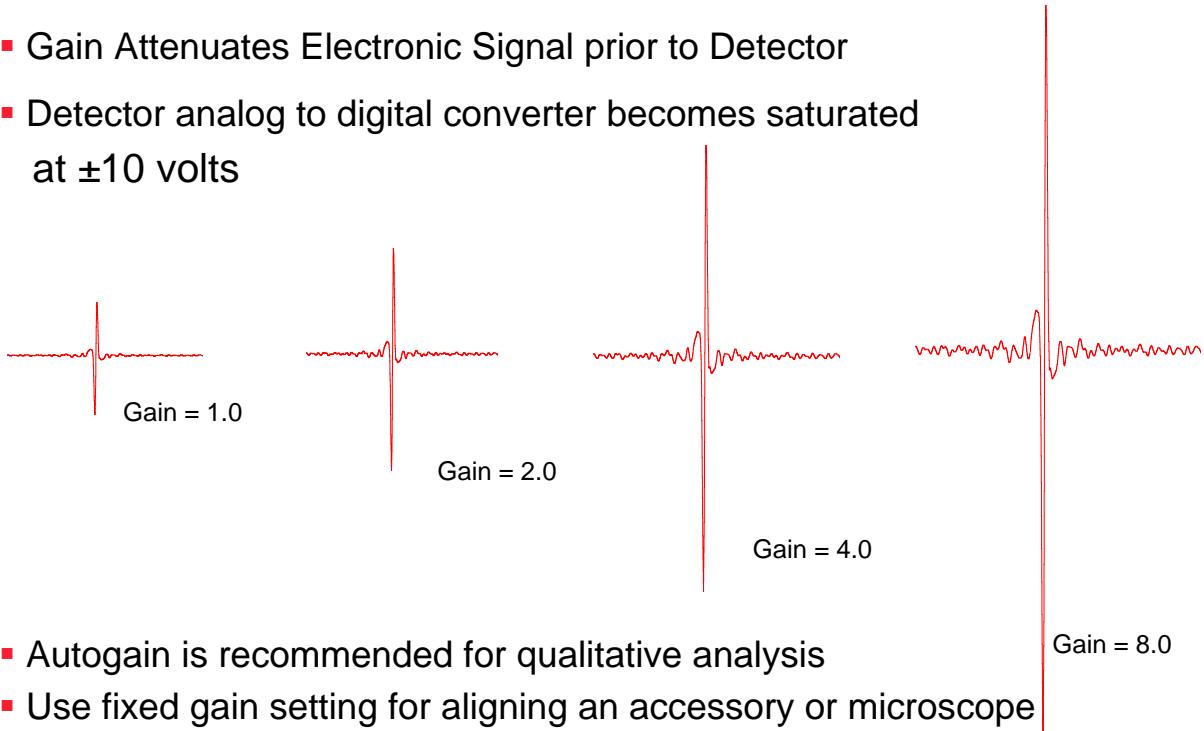
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The Gain parameter on the Bench tab in the Experiment Setup dialog box determines how much the detector signal is amplified electronically. You can set Gain to 1, 2, 4, 8, or Autogain. The Autogain setting allows the system to optimize the gain automatically. Use a gain setting that results in a signal intensity of less than 20 volts peak-to-peak +/- 10 volts min/max. Select the desired setting from the drop-down list box.

Setting Gain

- Gain Attenuates Electronic Signal prior to Detector
- Detector analog to digital converter becomes saturated at ± 10 volts



- Autogain is recommended for qualitative analysis
- Use fixed gain setting for aligning an accessory or microscope

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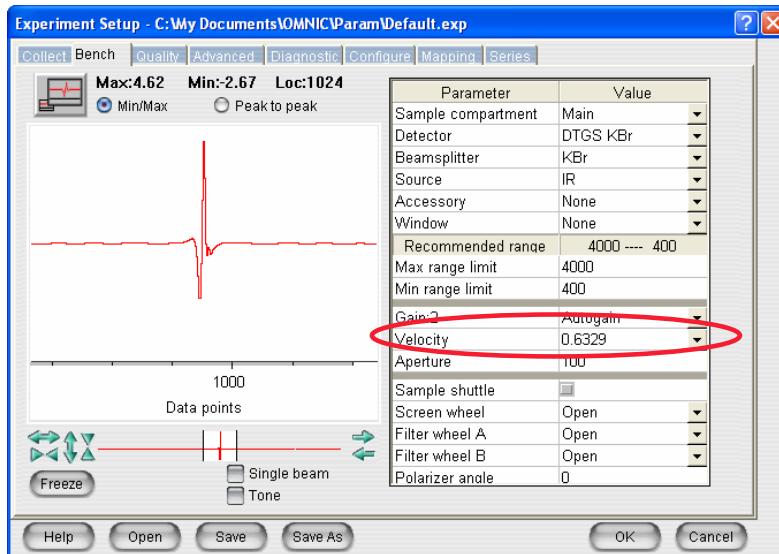
Increasing gain increases the signal from the detector. When the gain is improperly set the detector electronics can saturate. This occurs when the interferogram measurement is $+$ / $- 10$ volts (see the Max and Min measurement on the top of Bench Tab).

For qualitative analysis the gain should be set to Autogain. This allows the electronics to select the most appropriate gain for the experiment. When you are doing sensitive quantitative analysis you should determine the best gain for your experiment and run using a fixed gain value.

Because the interferogram display is “live”, it may be used as a tool to monitor energy throughput while aligning an accessory or a microscope. You should select a fixed gain value to prevent the interferogram from jumping between gain values during alignment.

Velocity

- Velocity controls the speed of the moving mirror (cm/s)
- Setting is dependant on type of detector
 - For DTGS (room temp), slower (~0.6 cm/s)
 - For MCT-B, MCT-A, and MCT-A* (liquid N₂ cooled), faster (~1.8 cm/s)



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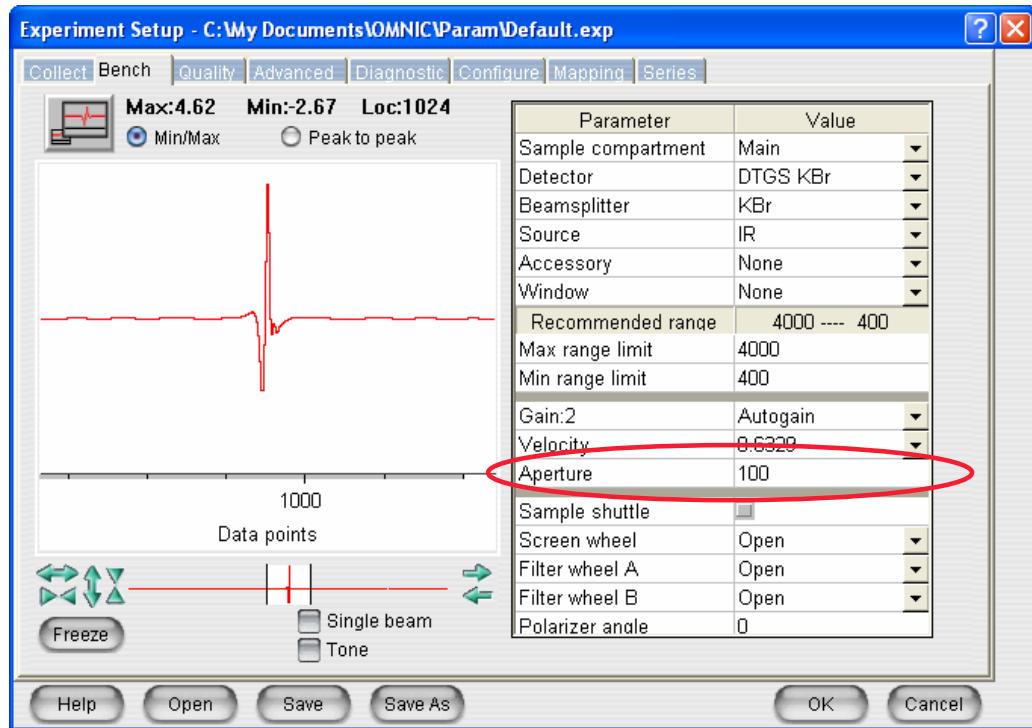
The Velocity parameter in the Bench tab determines the velocity of the moving mirror in the interferometer. The default value is determined by the detector type and is set when you select a detector using the Detector parameter. Select the desired setting from the drop-down list box at the right end of the Velocity row.

Using a faster velocity allows you to collect more scans in a given amount of time; however, using a velocity that is faster than the default setting will produce a smaller signal intensity.

Using a slower velocity increases the time required for an individual scan, but that does not mean the total measurement time needs to be longer. The stronger signal obtained (with some detectors) at the slower velocity can allow you to collect fewer scans, resulting in a shorter measurement time and better quality spectra.

The velocity is the speed with which the moving mirror moves inside the interferometer. It is constant on both the forward and reverse stroke. Slowing the mirror down while using a DTGS detector will improve sensitivity. However, if you are using an MCT detector you may collect with a higher velocity. This is advantageous because very often experiments that use an MCT detector are already “low energy” and the number scans is increased to improve the signal to noise ratio. Increasing the velocity of the moving mirror will decrease the amount of time required to collect data.

Aperture



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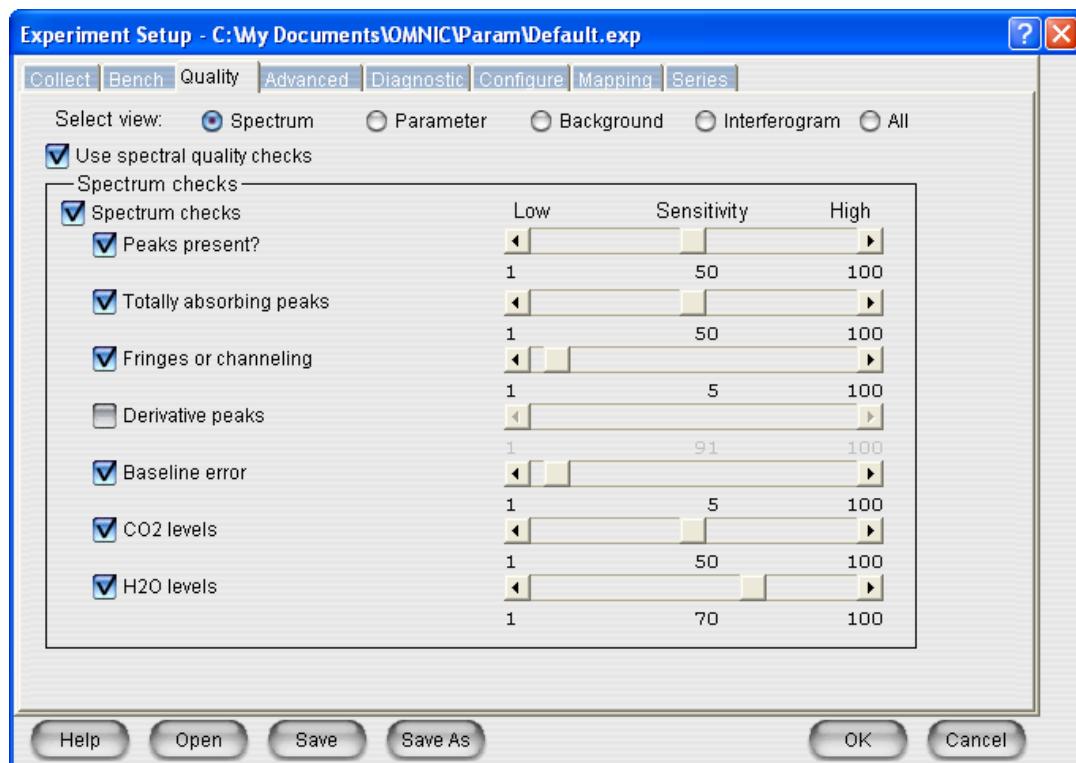
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The Aperture parameter on the Bench tab in the Experiment Setup dialog box allows you to set the size of the optional adjustable aperture to any value from 0, the minimum size, to approximately 150, the maximum size.

To change the setting, double-click the table cell to the right of Aperture. Then type a value or click the up and down arrow buttons to the right of the value.

The Aperture parameter is dimmed if the aperture is not installed.

Quality Tab



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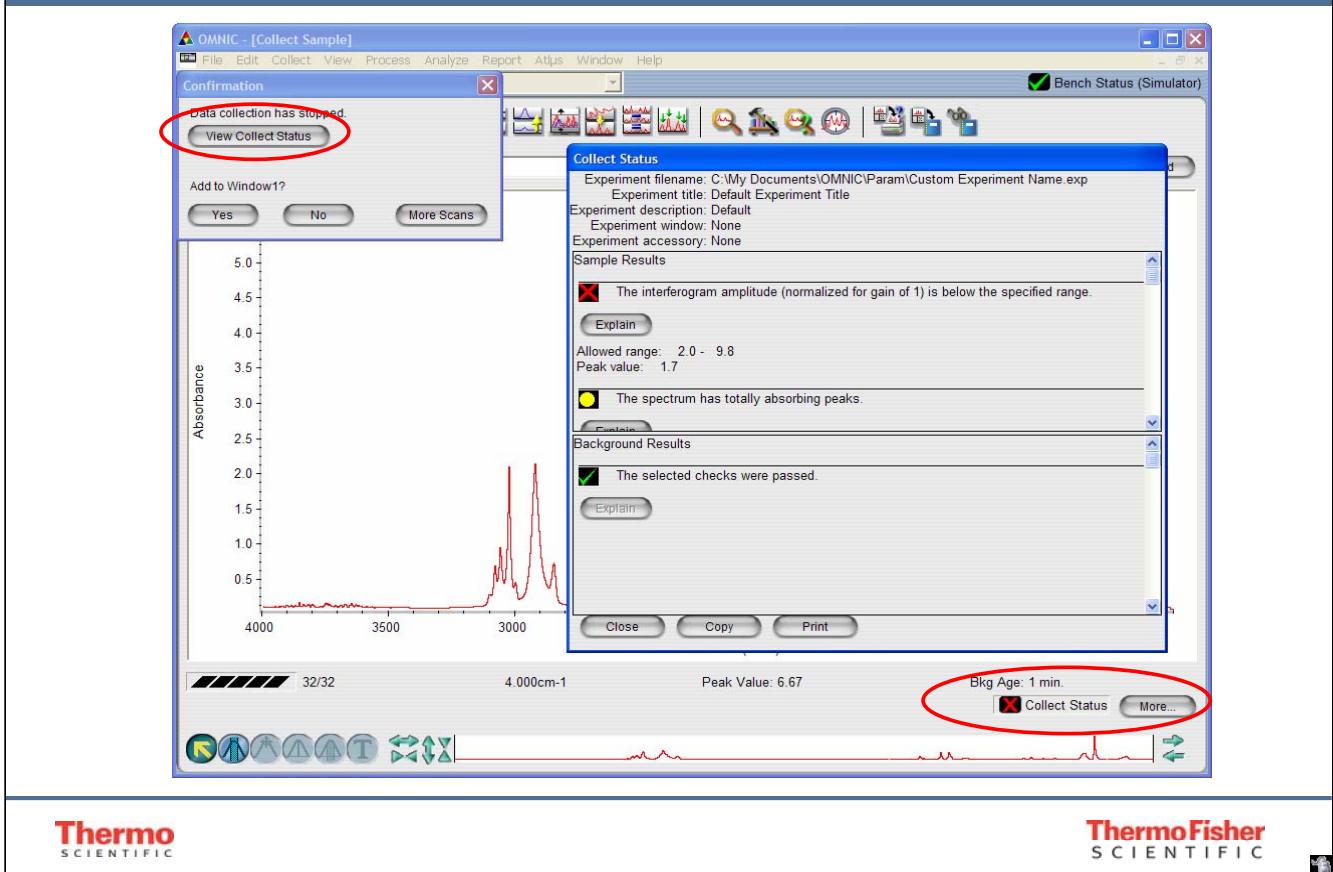
To display a category of checks or all the checks on the Quality tab, select the appropriate option to the right of Select View.

If you want any of the spectral quality checks to be performed when you collect spectra using the current experiment, turn on Use Spectral Quality Checks near the top of the dialog box. This makes the various checks available for you to select. If you don't want any checks to be performed, turn off the check box.

Spectral Quality checks are designed to look for conditions which exist during data collection and test for the selected feature/error. If the test fails (or nears failing) the Collect Status indicator (lower right hand corner of the OMNIC Collect window) will turn from a green check mark to yellow flashing or to red "x". This indicates that one or more of the quality parameters is outside limits.

If you choose to use Quality checks you *must* first set each parameter with the appropriate sensitivity level. For example, if you want to check for the presence of CO₂ vapor, first set the sensitivity to 100. Collect data. Using View Confirmation Status you can determine the level at which CO₂ as a vapor was recorded. If, in fact, there was an acceptable amount of CO₂ in your environment then you must set the sensitivity setting just below this number. In this way, the collect will "pass" (a green check mark appears at the Collection Status at the lower right hand corner).

Spectral Quality Collection - “Collect Status errors”



When OMNIC performs a check and detects a problem, the Collect Status indicator is displayed in yellow or red. You can click the indicator (or click the View Collect Status button at the end of data collection) to see a summary of data collection problems encountered during the collection and other information about the collection.

In this example there were totally absorbing peaks present, as well as partially absorbing. This is not a surprise when analyzing polystyrene. The sensitivity values should be reset to lower numbers for the Collect Status to “pass”.

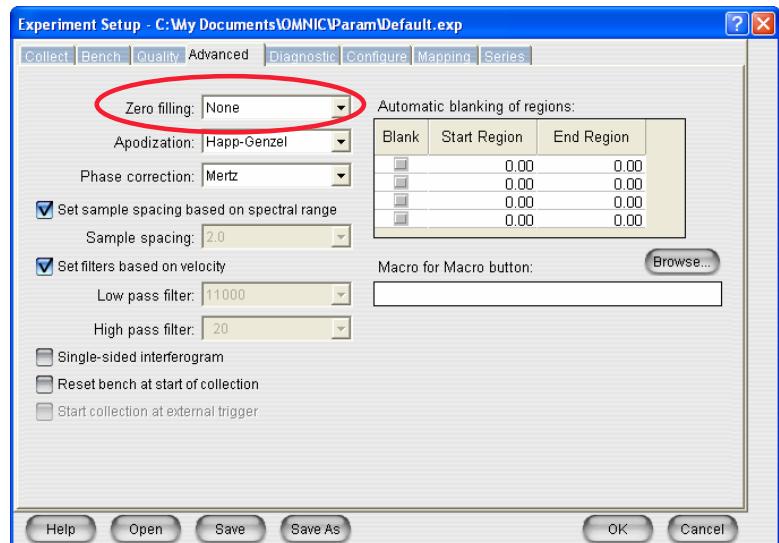
Advanced Options – Zero Filling

Artificially improves resolution of spectrum by adding additional data points as zeros prior to Fourier Transformation

$$I(\delta) = \int_{-\infty}^{\infty} \beta(\bar{v}) \cos 2\pi \bar{v} \delta d\bar{v}$$



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Advanced options should only be changed if you are confident in your choices. Remember that a simple right click and choosing discussion on the window that pops up will bring a detailed explanation of everything related to the window.

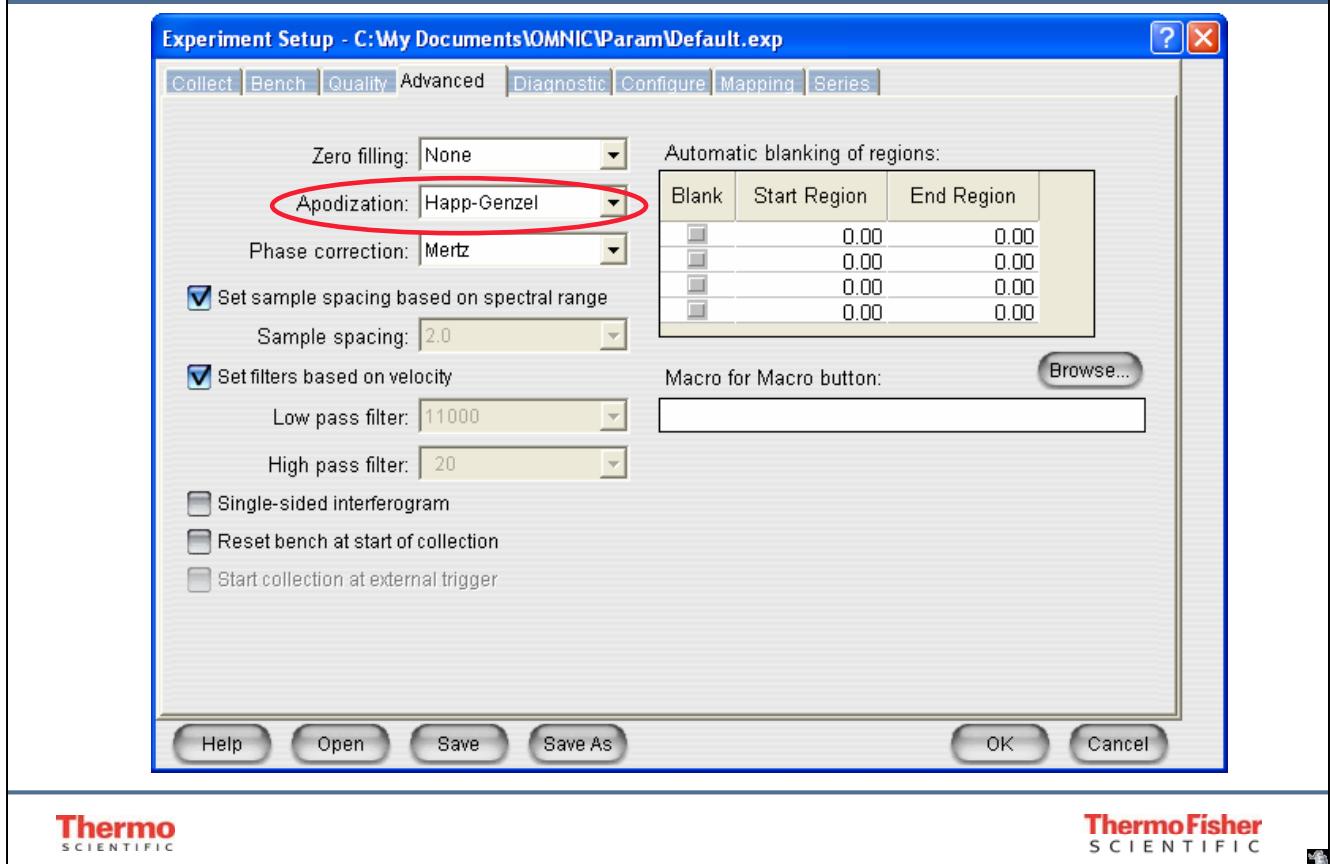
The two options changed most frequently in this tab are the Apodization and Phase Correction. To mathematically improve the data spacing frequency based data, zeros may be added to the Fourier Transform. One level of Zero Fill adds a number of data points to the end of the interferogram and sets them to zero. This is then transformed and the results is to add an interpolated data point in between every real data point in the spectrum.

This is useful in enhancing the peak shapes in the resulting spectrum, allowing for better interpretation of the information. The spectrum data is not changed by adding zeros and this should not be used as a substitute for increasing the resolution to meet the needs of the sample analysis.

A second level zero fill adds a second set of data points to the end of the interferogram. This will have the effect of inserting 3 interpolated data points in between each real data point in the frequency spectrum after the Fourier transform, further enhancing the peak shapes.

If you need to collect higher resolution data, it is better to experimentally improve resolution than artificially.

Apodization



Apodization removes peak side lobes that can occur because the interferogram is not an infinite set of data. The apodization types described in the following table are available. Collect your sample and reference spectra using the same apodization type.

The two most commonly used apodization functions are Happ-Genzel and Triangular. Triangular apodization is used during the 100% line noise test with infrared microscopes.

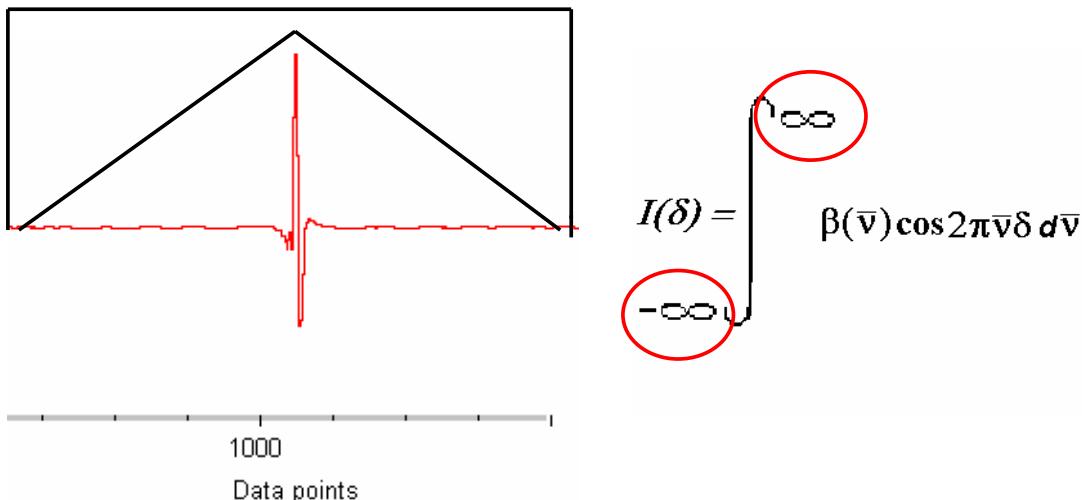
Happ-Genzel: This setting is the best choice for most applications. It suppresses side lobes more effectively than the triangular apodization but with more reduction in resolution than the triangular and boxcar type apodizations. If you are measuring condensed-phase samples, use Happ-Genzel apodization.

Triangular: Mathematically weights interferogram data to reduce ringing effects (side lobes), resulting in lower resolution than that obtained with the boxcar type apodization but higher than that obtained with the Happ-Genzel apodization.

The other apodization types available are described in the help file accessed by right clicking on the item of interest.

Apodization

Mathematically applies limits of integration to Fourier Transform because we are not collecting data from +/- infinity



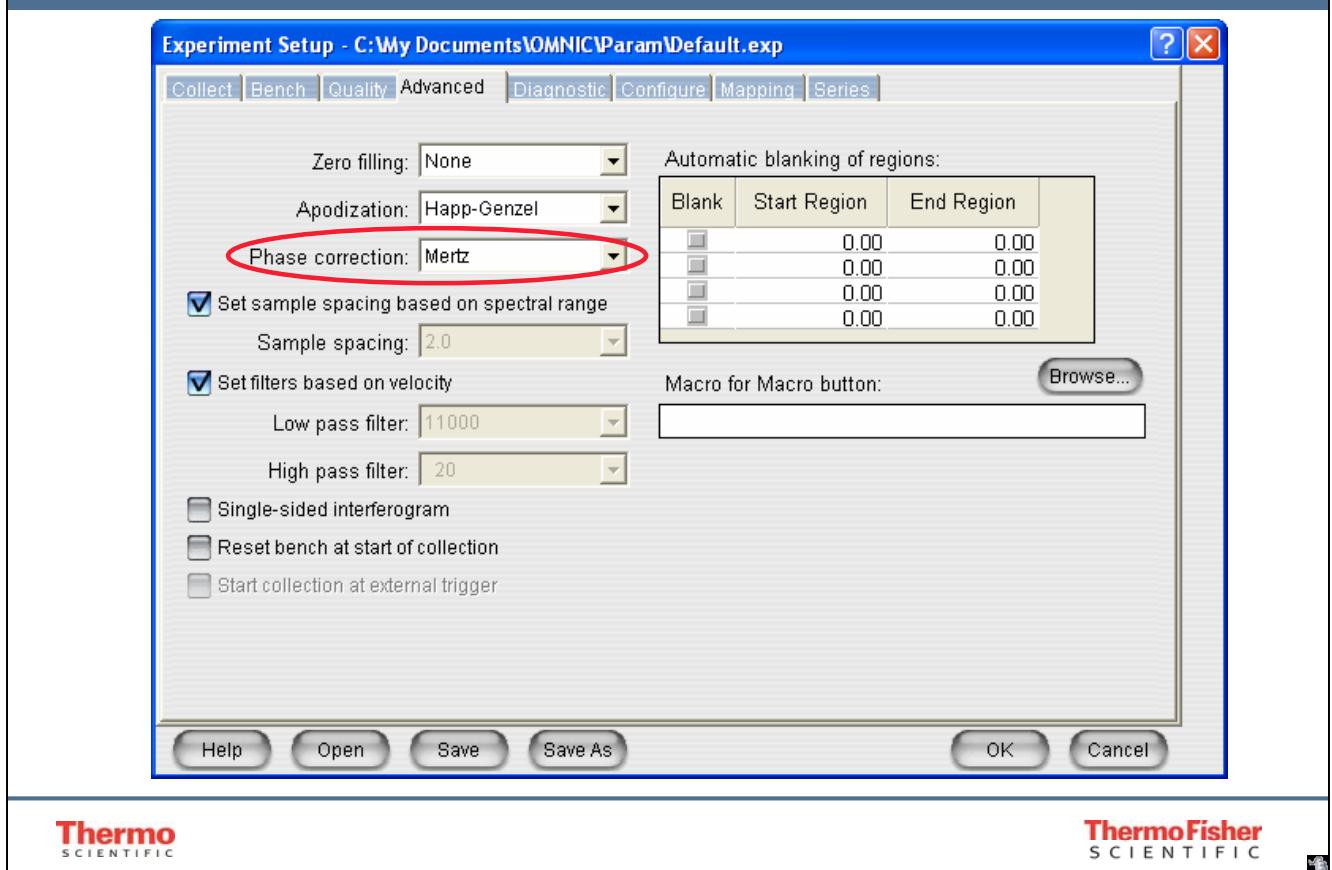
Prior to the Fourier Transform, limits of integration must be identified (because we are not collecting data from negative to positive infinity). The limits are found by applying an Apodization function to the data. Each apodization function is the description of a mathematical calculation performed on the interferogram prior to the Fast Fourier Transform. (ex. Boxcar or Triangular all describe mathematical formulas).

These functions serve to smooth the transitions at the ends of the interferograms and eliminate the artifacts that could be introduced due to the abrupt discontinuation of the real data in the interferogram.

From the above picture, it can be seen that more attenuation is applied to regions that are far from the center burst. These regions have also been shown to contain the higher resolution information in the data. The application of an apodization function then has the effect of lowering the resolution slightly in the final spectrum.

Happ-Genzel is recommended for ordinary data collections. Triangular may be better for noisy, low energy experiments (like working with a microscope). Whichever you choose, be consistent. Apodization function impart their own unique peak shapes to the final data. This can cause problem in analysis and may result in misleading interpretations or quantitative determinations.

Advanced Options



Power Spectrum: Always produces a spectrum that is positive. In this correction the power equals the square root of the sum of the squares of the real and imaginary parts of the Fourier transform. This is the normal setting for Raman data.

Mertz: Uses the Mertz algorithm to calculate the phase-corrected spectrum.

For more information on the Mertz and Power Spectrum corrections, read

Transformations in Optics by L. Mertz, published by John Wiley and Sons, New York, 1965.

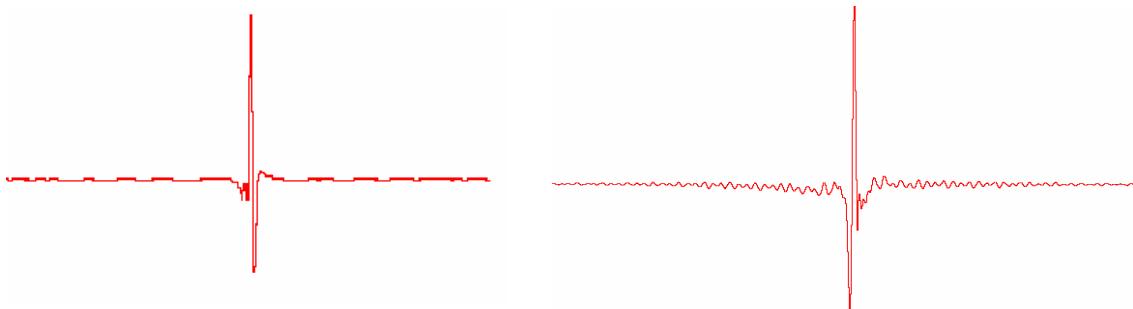
de Haseth: Phase corrects vibrational circular dichroism (VCD) spectra. These spectra can have both negative and positive peaks, so the correction is designed to accommodate negative spectral features. For more information, see the article titled "Phase Correction of Vibrational Circular Dichroic Features" by Colleen A. McCoy and James A. de Haseth in the *Journal Applied Spectroscopy*, Volume 42, Number 2, 1988.

Phase Correction

Corrects the phase angle term of the Fourier Transform where distortions to the interferogram occur as a result of noise or laser sampling effects.

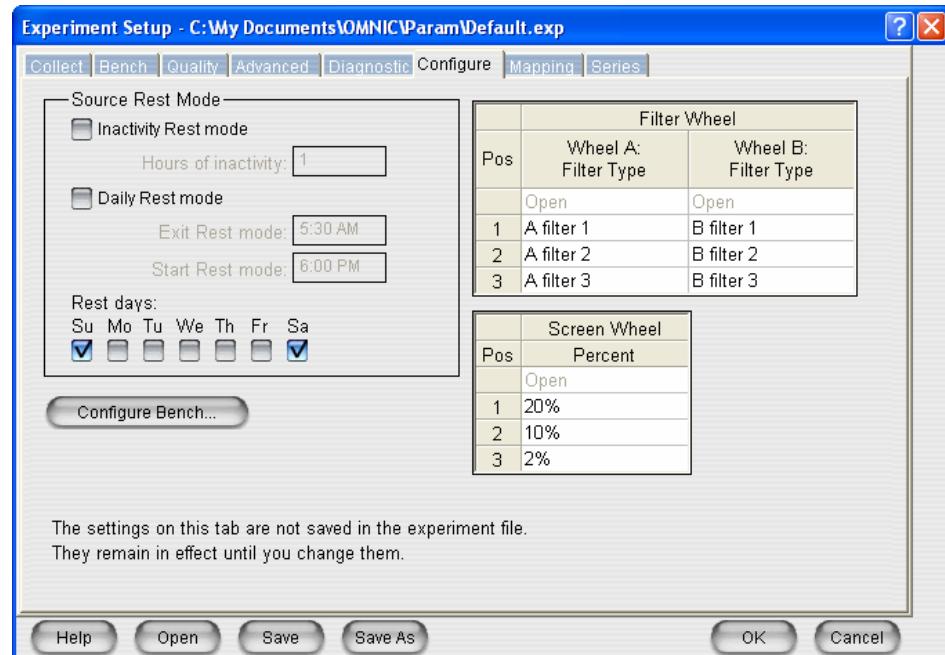
Makes the interferogram symmetric around ZPD

-Use Mertz Correction-



Phase correction corrects for any distortions around the centerburst (ZPD) caused by noise or other sampling effects. It is possible that "imaginary" ($-1^{0.5}$ or i) data is introduced into the mathematical calculations and this correction removes this effect. The result is that it makes the interferogram more "symmetric" about the centerburst. Mertz is always recommended for FTIR data.

Configure Tab

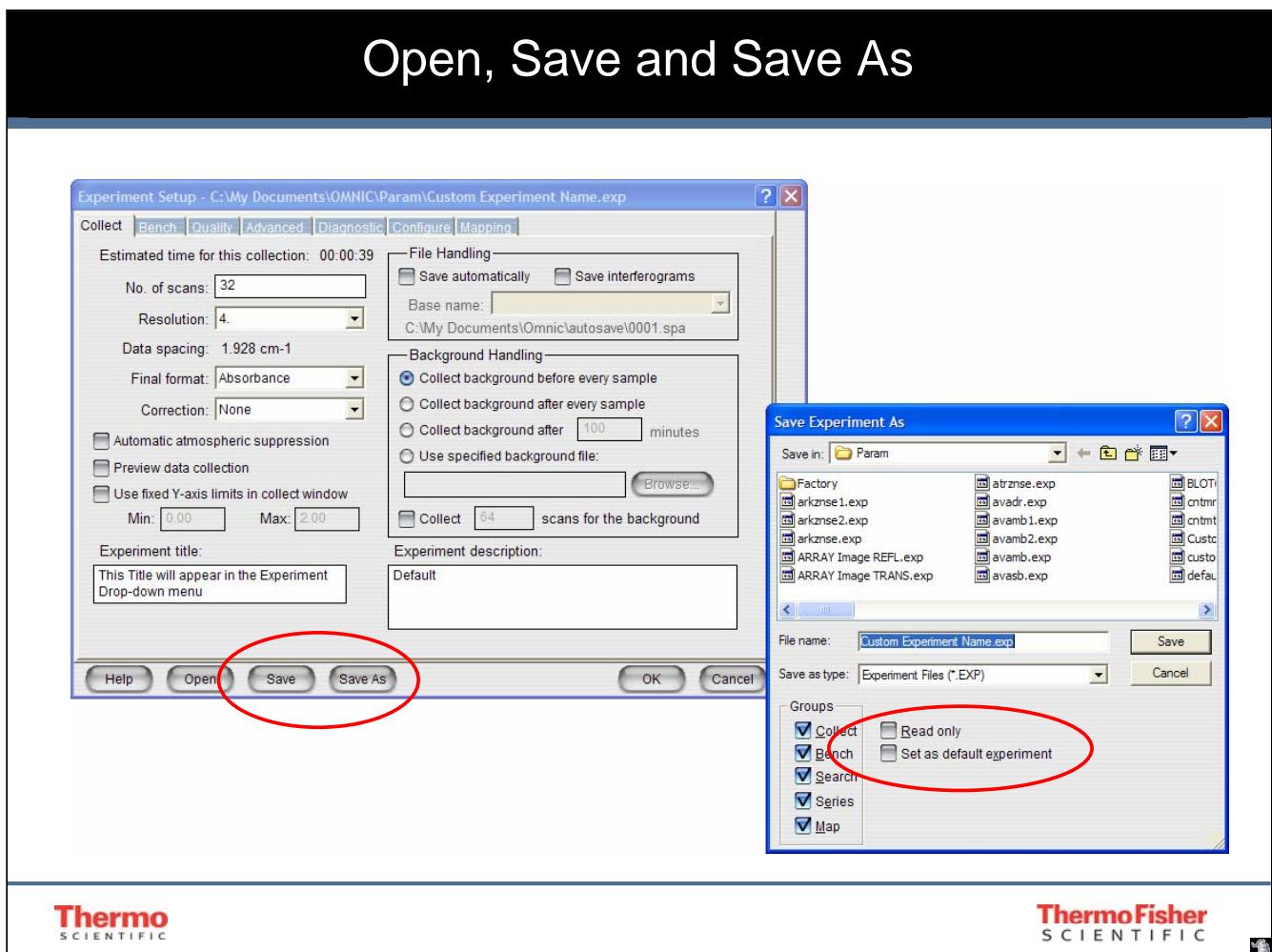


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Configuration tab contains Source Rest Mode, Bench, and Filter Wheel configuration options. The source can be set to rest (not turned off, but set at lower power) at scheduled times.

Open, Save and Save As



Experiment files have the .exp extension. Several pre-existing experiments are loaded with your software. They are located in the OMNIC\Params subdirectory. If you use a pre-existing experiment be sure to check all settings to ensure they are appropriate for your data collection.

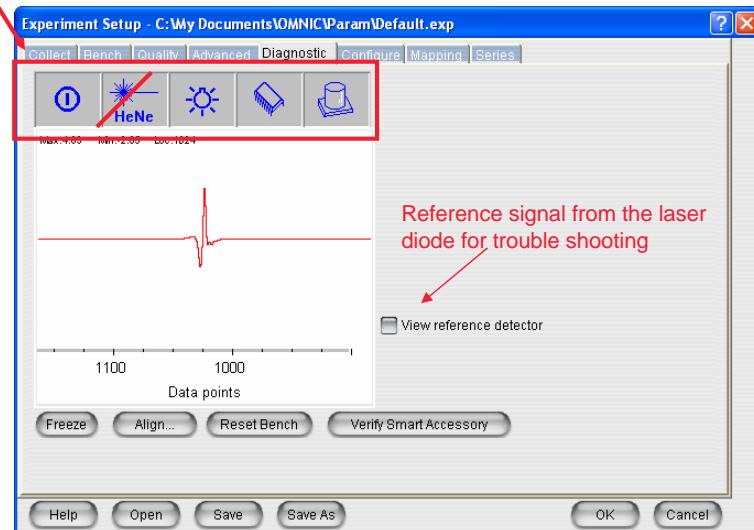
When saving an experiment it may be set as default. This is the experiment which is automatically loaded when OMNIC is launched (assuming that OMNIC log in feature is *not* enabled). You may also write protect experiment files so that they can not be overwritten by selecting Read Only.

On the lower left side of the Save As Dialog box there are several check boxes. These tie various collection parameters together as part of your experiment file. Selections made in Quality, Advanced, and Configuration tabs (discussed later) are also saved with experiment file.

Note: If the Search checkbox is selected, selected library setup with your experiment is saved as a part of the experiment file. This function is covered again in the Library Setup section of this course.

Diagnostic Tab

Performance Indicator for Power Supply, HeNe Laser, Source, Electronics, and Detector.
Red line across the figure indicates a problem.



Freeze: Freezes the interferogram in the live display

Align: Aligns the interferometer to maximize the throughput

Reset Bench: Repositions the ZPD

Verify Smart Accessory: Displays which Smart™ accessory is installed



Above the live display are several icons that can be selected to check the status of the following spectrometer components: Power, HeNe laser, White Light, Electronics, and Detector. If an indicator is continuously marked with a red diagonal line for at least one minute, there may be a problem with the corresponding component in the spectrometer.

You can use the Align button to perform an automatic alignment of the interferometer.

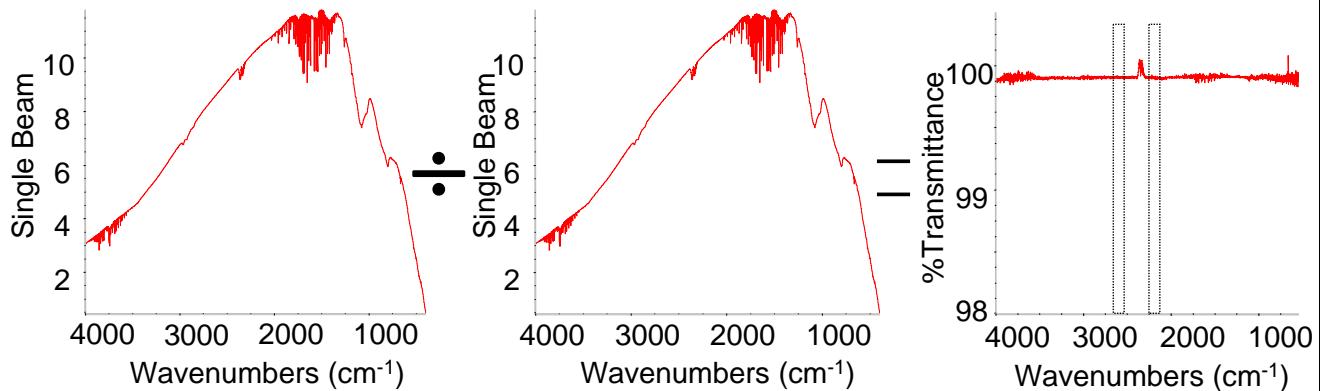
If the interferogram peak has drifted from its normal location, you can click the Reset Bench button to reposition the peak. If you find that the interferogram peak in the live display tends to drift from its normal location, turn on Reset Bench At Start Of Collection on the Advanced tab in the Experiment Setup dialog box. This repositions the peak before data collection starts.

Periodically you should Align your instrument. When you select this button the hardware will automatically perform this task. It is important that the sample compartment be clear of all accessories when this task is performed. By adjusting the position of the beam splitter the amplitude of the interferogram can be maximized.

Reset Bench will flush the electronics of the instrument. This may be used in establishing communication with the instrument.

100 % Transmission Line Noise Test

A transmission spectrum of the bench with nothing in the beam path is taken to evaluate noise; therefore, the performance of spectrometer.



$$\frac{\text{Blank}}{\text{Blank}} = \text{Noise}$$

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The 100% Transmission Line spectrum is used to evaluate instrument noise. It is the ratio of two single beam spectra, with nothing in the sample compartment. This, theoretically, should produce a straight line. Any instrumental noise may then be calculated using this data.

100% Transmission Line Collection Parameters

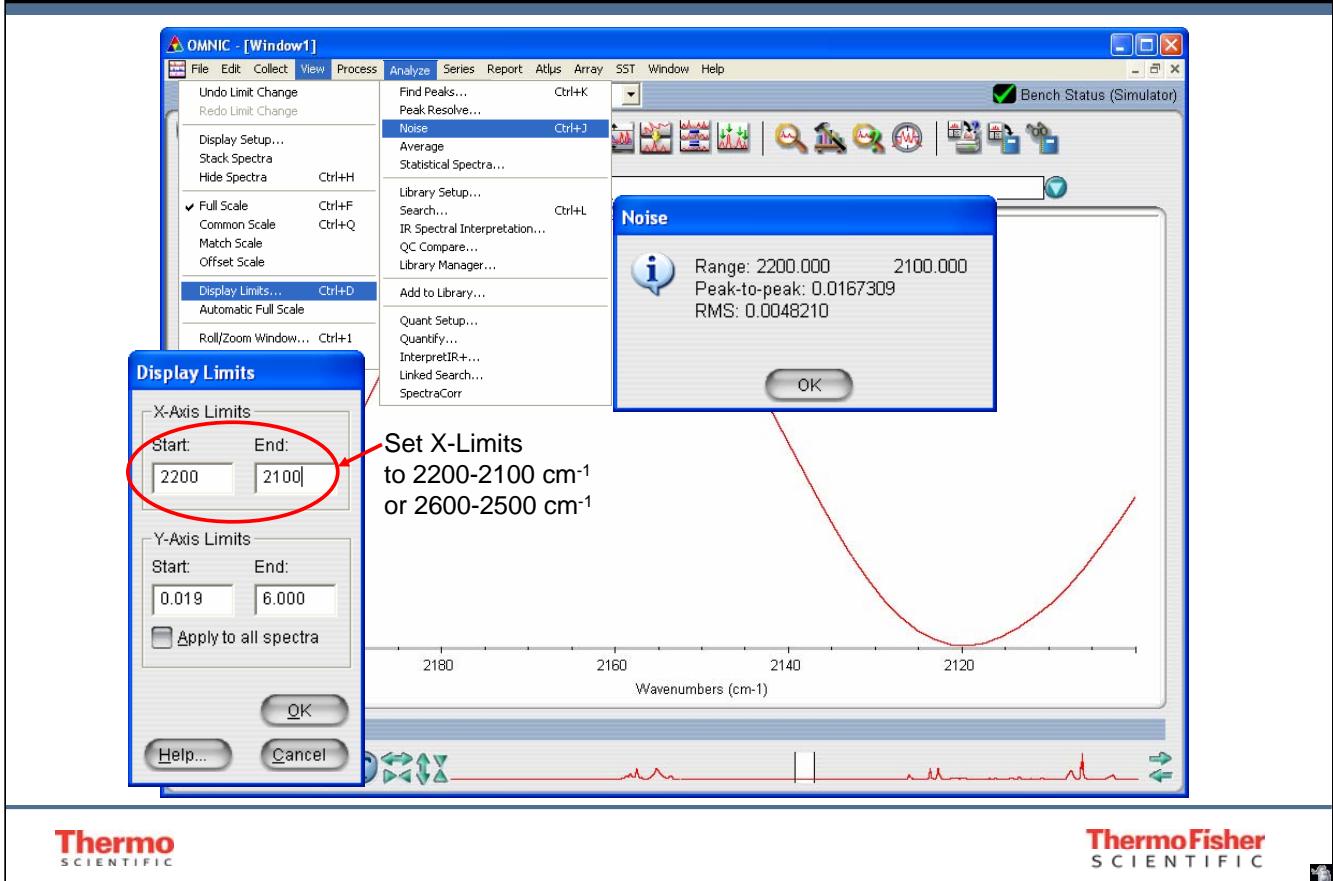
	Main Bench	Microscope
Scans	64	200
Resolution (cm ⁻¹)	4	4
Apodization	Happ-Genzel	Triangular
Final Format	% Transmission	% Transmission
Correction	None	None
Spectral Range (cm ⁻¹)	2200-2100	2600-2500

Whichever parameters you choose, always be consistent!



Thermo Fisher Scientific recommends parameters listed above to evaluate the performance of your instrument over time. Unless you have developed a test for an accessory, be sure to always clear the sample compartment of any accessories. Whichever collection parameters you choose, be consistent so that all results obtained can be compared. Final format can be changed later in OMNIC. Different apodization function can be applied post-collection if interferograms are saved.

100% Transmission Display Limits and Noise Result



Select a display limit range either 2200 to 2100 or 2600 to 2500 cm⁻¹ to ensure that water and CO₂ vapor does not interfere with the noise test.

View | Display Limits

Noise is easily calculated in OMNIC by selecting

Analyze | Noise

The published specification on peak-to-peak (p-p) noise values vary between spectrometer models. A value less than 0.1 should be expected. Thermo does not recommend the use of a root mean squared (rms) noise value for this evaluation. You may track p-p noise in your lab notebooks and watch for trends. If the p-p noise begins to drift up significantly, this may indicate a problem with the bench. Be sure to align the bench periodically. If a problem occurs, align the bench and then run this test again.

Experiment Setup - Review

Collect Tab

Setting Number of Scans and Resolution

Final Format

Saving Files and Interferograms

Background Handling Options

Atmospheric Suppression

Preview Data Collection

Experiment Descriptions and Titles

Bench Tab

Setting Spectral Range, Gain, and Velocity

Quality Tab

Advanced Tab

Zero Filling, Apodization, and Phase Correction

Configure Tab

Diagnostics Tab

Align and Reset

100% Transmission Line Noise Test

