Essential FTIR®
Data collection for Mattson Instruments Spectrometers

Essential FTIR can collect data from Mattson FTIR spectrometers. The models that can be used are all Galaxy, Genesis, Research Series and Infinity spectrometers.

Installation

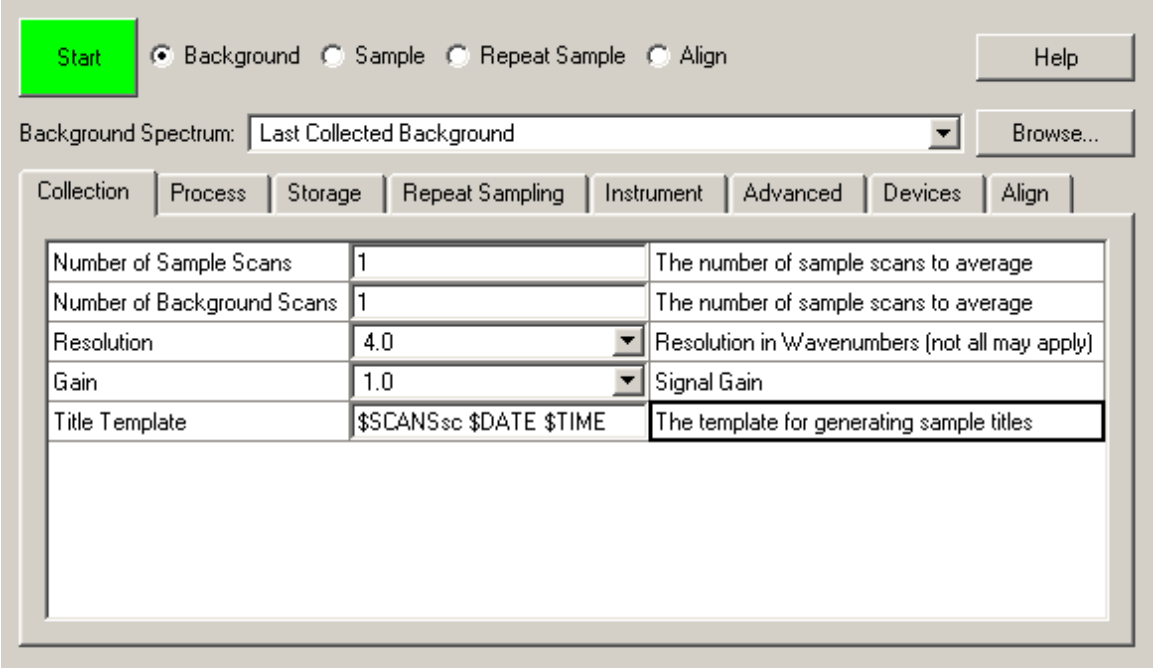
First install Essential FTIR. The Essential FTIR setup program can be downloaded from http://www.essentialftir.com/download.html. After installing Essential FTIR, install the separate Mattson Data Collection Tool, which can be obtained by sending a request to support@essentialFTIR.com.

After installing the software, you will need to configure some settings. Go first to the 'Instrument' tab on the 'Mattson Data Collection' tool (documented below) and choose the type of instrument, the serial communications port, and the baud rate for the instrument. To verify that communications is working, go to the 'Advanced' tab and click on the 'Get Setup' button. If the instrument settings are correct and everything is working, the current setup of the instrument will be displayed in a text window in the Essential FTIR workspace.

Computers today rarely have a physical serial port. You will need a USB to Serial adapter to communicate with the instrument. There are many such available, but one we have had good experience with is the Sabrent USB 2.0 TO SERIAL DB9 MALE (9 PIN) RS232 CABLE ADAPTER 1 ft. Prolific Chipset (CB-RS232).

The Mattson Data Collection Tool

After installing the software, you will find the Mattson Data Collection tool in the 'Instruments' category. It looks like this:



At the top left is a green 'Start' button, which naturally enough starts data collection. To the right of this Start button are four radio buttons, which control what data is acquired and how it is handled.

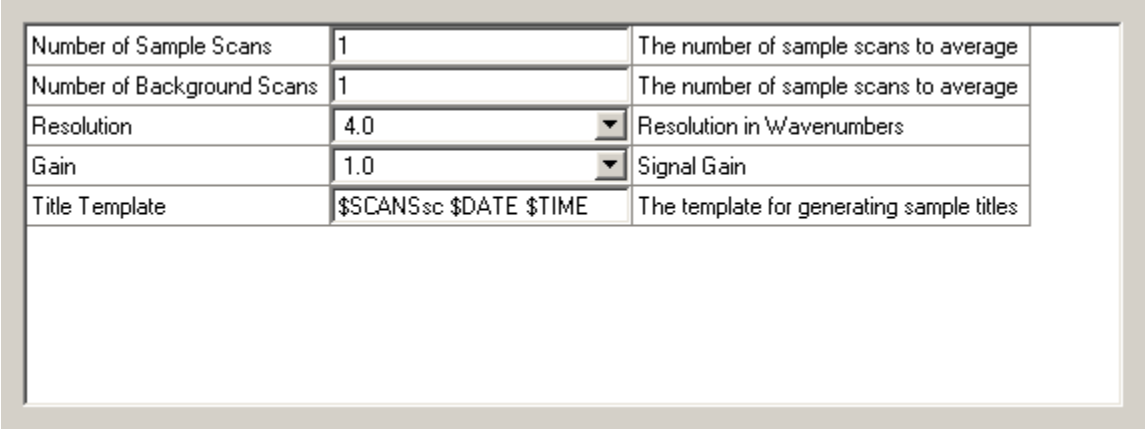
Background	Collect a new background spectrum
Sample	Collect a sample spectrum
Repeat Sample	Collect multiple spectra
Align	Collect data repeatedly for the purpose of aligning, or tuning, the instrument

Below these radio buttons is a drop-down list box labeled 'Background Spectrum'. All singlebeam spectra loaded into Essential FTIR will be listed in the dropdown list. The Browse button allows you to select a stored background file from disk for use in processing sample data.

Below the Background Spectrum list box is a row of tabs. Each of these tabs contains a table of settings that control aspects of the instrument interface, collection parameters, data processing and storage, and other related functions and settings.

Collection Settings

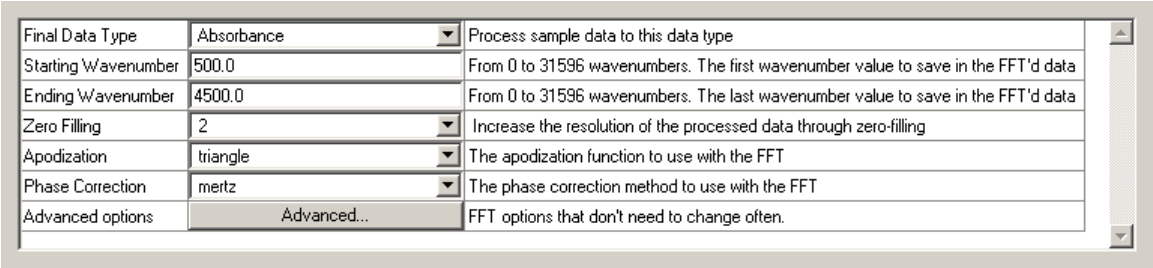
These settings are the ones that are commonly changed the most.



1. ***Scans***: Sets the number of scans to be co-added during the collection of a spectrum
2. ***Background Scans***: Sets the number of background scans to be co-added during the collection of a background spectrum
3. ***Resolution***: Sets the optical resolution for data collected from an instrument. The resolution is changed via a drop down menu and may take values of $0.5cm^{-1}$ –$32cm^{-1}$.
4. ***Gain Multiple:*** Sets the gain for the data acquisition.
5. ***Title Template:*** Sets the information to be recorded into the spectrum file. In the example given in figure 4.23 the number of scans, gain, resolution, date and time are entered in the template. A template does not have to be used, or can be used together with any other text that is needed.

Process Settings

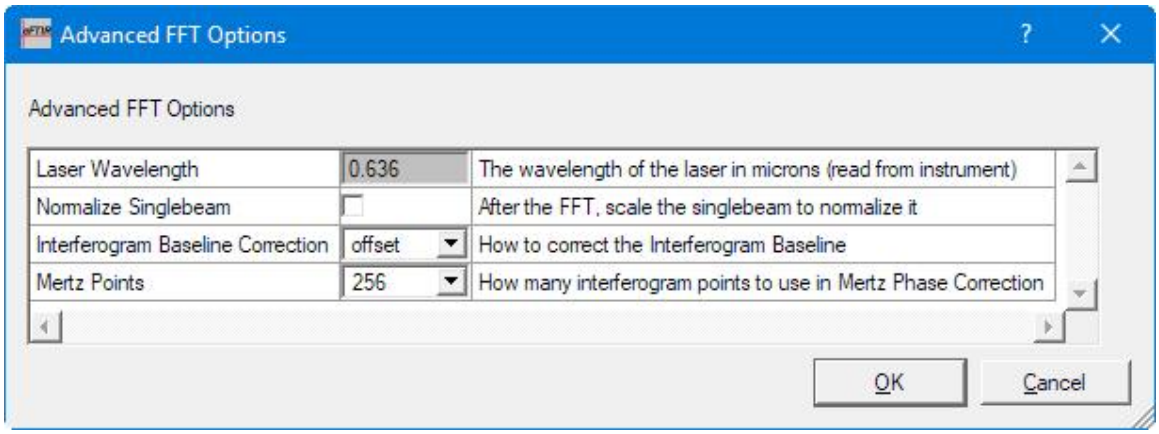
These settings control how the raw interferogram data is handled after it is acquired from the spectrometer. The



1) ***Final Data Type***: Sets the level of processing of the data. The data type is selected from a drop down menu, in a hierarchy of increasing processing from ***Interferogram***, ***Single Beam***, ***Transmittance*** or ***Absorbance***.
2) ***Starting Wavenumber***: Sets the lower limit of the wavenumber range to be computed in the fast Fourier transform.
3) ***Ending Wavenumber***: Sets the upper limit of the wavenumber range to be computed in the fast Fourier transform.
4) ***Zero Filling***: Sets the interpolation factor via a drop down menu for smoothing of acquired data. The interpolation factor may take the values 1, 2, 4, 8, or 16. Zero filling increases the resolution of the data by Fourier interpolation.
5) ***Apodization*** sets the type of apodization function to use in the fast Fourier transform to remove truncation artifacts. ***Triangle, Boxcar, Beer-Norton Med, Beer-Norton Weak, Beer-Norton Strong, Happ-Genzel, Bessel, Cosine, Blackman-Harris 3 Term and Blackman-Harris 4 Term*** are selectable via a drop down menu.
6) ***Phase Correction:*** Sets the type of phase correction function to be used. ***Mertz*** and ***Magnitude*** are selectable via drop down menus.
7) ***Advanced Options.*** Click the 'Advanced…' button to bring the screen which is discussed in the 'Advanced Process Settings' section, below.

Advanced Process Settings

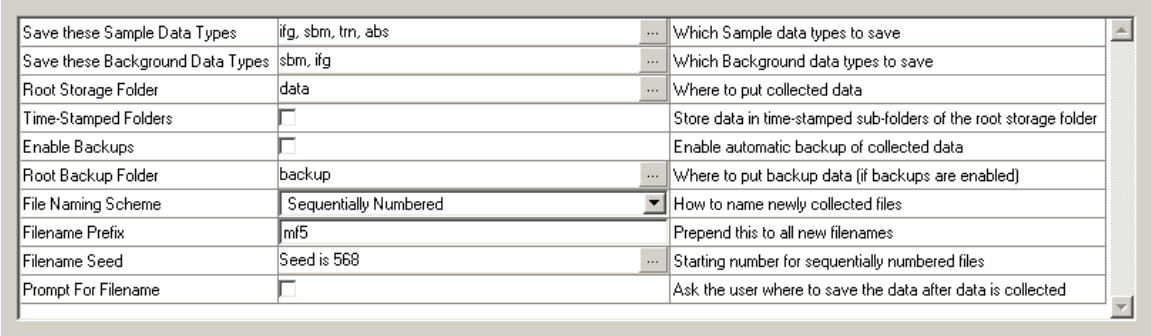
Clicking on the 'Advanced' button brings up the Advanced Process Parameters. These are options that are seldom changed, and should probably be left as is.



1. ***Laser Frequency:*** Used to define the nominal frequency of the HeNe laser used as a clock in a Fourier transform infrared spectrometer. The actual laser wavelength will remain unaffected by any changes to the ***Laser Frequency parameter*** – historically this number was manipulated to correct for shifts in the *x*-axis..
2. ***Normalize Singlebeam:*** After the data is FFT'd, some software will scale the data by the inverse of the number of FFT points. This setting is here so the you can produce data compatible with data from other software.
3. ***Interferogram Baseline Correction:*** The choices are 'offset' and 'linear'. Any offset or slope in the interferogram must be removed before the FFT. If set to 'offset', the average value of the interferogram is subtracted. If 'linear', a straight line fit to the interferogram is subtracted.
4. ***Mertz Points:*** determines how many points, centered around the ZPD, are used in computing the phase correction.

Storage Settings

These settings control what data is saved to disk, and how the files are named.



1) ***Save these Sample Data Types***: Offers the choice of saving any of four kinds of data. On the right of the row, notice the edit button labeled with three periods (**…**). Clicking this button summons a dialog containing four check boxes. These are labeled ***Absorbance***, ***Transmittance***, ***Single Beam*** and ***Interferogram***. Checking ***Interferogram***, while leaving the other options unchecked, will save only the raw interferogram to disk. Adding the ***Single Beam*** option will additionally save the Fourier transform of the interferogram to disk. Checking the ***Transmittance*** box will enable saving of the ratio of the single beam against the current or selected background. Finally, and as is recommended, if all boxes are checked the ***Absorbance*** spectrum (negative logarithm of the transmittance spectrum) will also be saved.
2) ***Save these Background Data Types***: When recording background spectra, two options are available for data storage. These are Interferogram and Single Beam. Again, it is recommended that all data types be saved to disk.
3) ***Root Storage Directory***: Defines the default directory to which data is saved. Clicking the edit button (…) summons a dialog allowing you to specify or create a folder for data collection.
4) ***Enable Backups***: Toggles on or off automated backing up of data – see line 6. If backups are enabled, new data is automatically copied to the backup directory as it is generated.
5) ***Root Backup Directory***: Enables you to set the directory for backups of collected data. This may be on a different drive from the original data, thus providing insurance against disk failure.
6) ***File Naming Scheme***: A drop down menu allows specification of the system for naming consecutively collected files. Three options are available – ***Time Stamped***, where files are named according to the time of acquisition (on the computer clock), ***Sequentially Numbered***, where each file is named with an number which is incremented each time a spectrum is acquired, and ***Sequentially Numbered in 8.3 Format***., where the incremental numbering is observed in accordance with the old DOS format. This results in eight-character filenames (padded with leading zeros) and three character file extensions, hence the term 8.3.

7) ***Filename Prefix***:: The editable text box in row 8 accepts a string, which is used as a prefix for file names, unless the File Naming Scheme is set to 'Time-Stamped' For instance, if the filename prefix is 'br' and the filenaming scheme is 'Sequentially Numbered in 8.3 Format', the first filename will be 'br000001', the second 'br000002', and so on.
8) ***Filename Seed***: Provides the starting number for sequentially numbered data files. Note that if the 8.3 format detailed in option 7 is applied, an absorbance file with the seed "1" will become *00000001.abs*
9) ***Prompt for Filename***: Checking this box instructs the program to offer a file naming and saving dialog box after each data file is collected.

The ***Storage*** settings collectively control the names of acquired data files. As an example, consider the results of settings where option ***6*** is set to ***Sequentially Numbered in 8.3 Format***, option ***7*** is set to "test", and option 8 is set to "1"**.** The name of the fourteenth file acquired under this scheme would be: test0014.spc.

Repeat Sampling Settings

Collection of data in repeat sampling mode is controlled by these settings.

Sample Fast	☑	Sample as fast as possible; ignore Sampling Frequency
Sampling Frequency	00:00:00	Start a sample this often (HH:MM:SS); only if 'Sample Fast' is unchecked
How long to sample	Forever	How many repeat samples to collect
Sampling Duration	00:00:00	Collect samples for this long (HH:MM:SS); only if 'How long to sample' is 'Time-limited'
Number of Samples	10	Collect this many samples; only if 'How long to sample' is 'Sample-limited'
Max Spectra	50	The maximum number of spectra in the collection window
Save to a multifile	☐	Save the data into a GRAMS multifile
Start Now	☑	Start collection when 'Start' is clicked, otherwise wait for the Starting Time (below)
Starting Time	00:00:00	Start data collection at this time (HH:MM:SS), in 24-hour time. Only if 'Start Now' is unchecked

1) ***Sample Fast***: Collects spectra immediately upon finishing the previous collection, regardless of other settings specifying wait times.
2) ***Sampling Frequency***: The edit box is used to specify a time interval for sampling. The interval may be input in an HH:MM:SS format, where HH is hours, MM is minutes and SS is seconds. This parameter is ignored if the check box in line 2 is selected.
3) ***How long to sample.*** Instructs This determines when the repeat data collection ends. The choices are 'Forever', meaning the collection must be manually stopped by a user, 'Time-limited', meaning data collection will stop after an elapsed time, and 'Sample-limited', which means the collection will stop after a specified number of spectra are collected.
4) ***Sampling Duration***: An edit box in HH:MM:SS format allows specification of duration for sampling. The instrument will sample continuously according to the ***Sampling Frequency*** parameter until the duration is reached. This parameter is used only if 'Time-limited' is chosen for 'How Long to Sample'.
5) ***Number of Samples***. If 'How long to sample' is set to 'Sample-limited', the data collection will end after this number of spectra have been acquired.
6) ***Max Spectra***.. During Repeat Sampling, every spectrum is displayed. When collecting hundreds, or even tens of thousands of spectra, the program would quickly run out of memory unless the number of spectra held in memory is restricted. This setting determines the maximum number of spectra that will be displayed at one time. In the figure, the setting is 50. After 51 spectra are collected, the 1st spectra will be removed from the display so that the 51st can be displayed. This setting does not have any affect on the saving and storage of data, only on the display of the most recent data.
7) ***Save to a multifile***: If checked, the spectra collected during repeat sampling will be saved to a multifile. A multifile is a single file that contains multiple spectra. Multifiles are useful for organizing related spectra and keeping them together in a collection, and also for batch processing.
8) ***Start Now***: The sample collection can be delayed to start at a particular time of day. If this is not checked, the 'Starting Time' will determine when sampling will start.
9) ***Starting Time***: If 'Start Now' is unchecked, sampling will begin at this time.

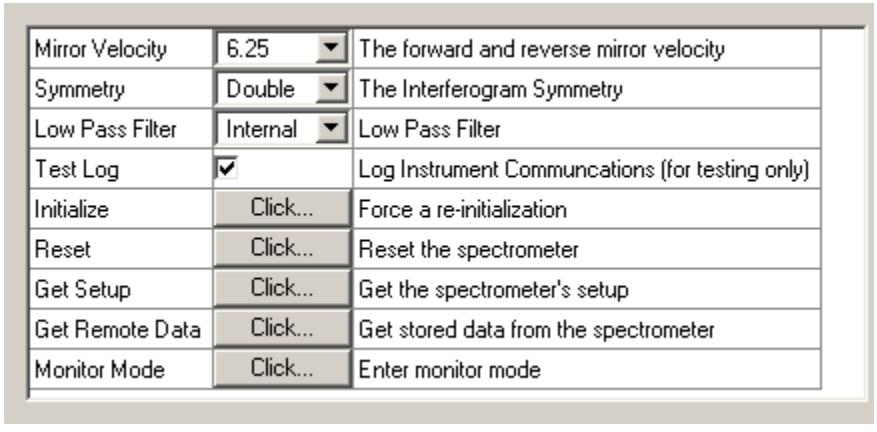
Instrument Settings

Instrument Model	Genesis II	The model of instrument this software is interfaced to
Comm Port	6	The number of the serial port to use
Baud Rate	38400	The baud rate for serial communications
Find Instrument	Click...	Scan all ports for the instrument

1) ***Instrument.*** On this box, choose the model of instrument.
2) ***Comm. Port.*** Select the serial communications port that the instrument is connected to.
3) ***Baud Rate***. Choose the baud rate that the instrument is configured to use. The default is 38400.
4) ***Find Instrument***: Clicking this will scan all the serial ports on the computer to find the Mattson spectrometer.

Advanced Settings

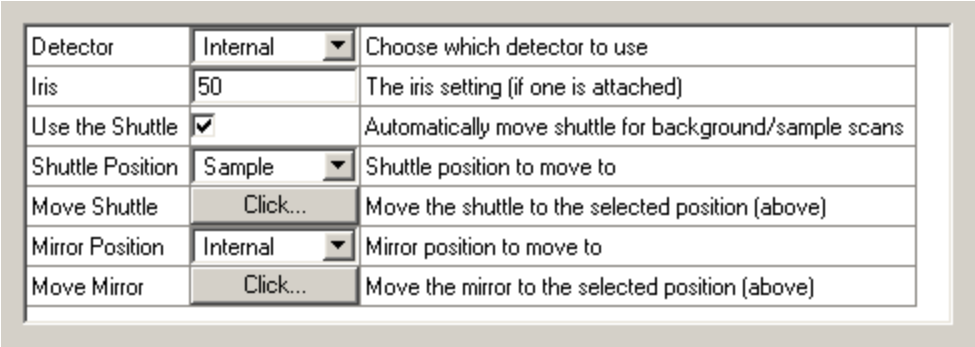
These are settings that don't need to be changed often, if ever. Some diagnostic and maintenance tools are gathered here.



Be careful with these settings. If you don't know what they do, it is best to leave them alone. In particular, 'Monitor mode' is for use by trained service technicians.

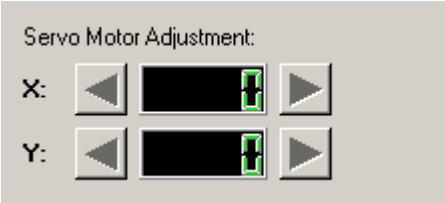
Devices

External devices may be attached to the spectrometer and under the control of the spectrometer's firmware. These settings tell Essential FTIR how to use these peripheral devices, and allow the user to manually move them.

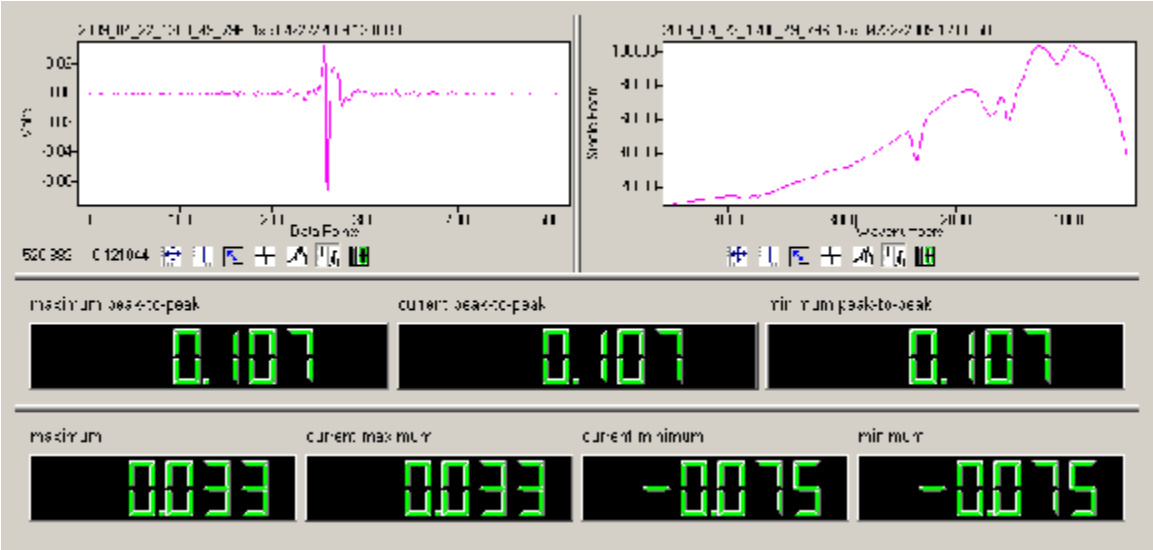


Align

When collecting data in 'Align' mode, the servo motors attached to the beam splitter (on some models) can be moved by the arrow keys.



When collecting data in align mode, the data is displayed on a special screen:



The current peak-to-peak, minimum and maximum signal values of the interferogram are displayed.

The buttons on the data window control how the data is displayed.

	Autoscale the display along the X and Y axes.
	Autoscale the display along the Y axis only.
	Display the data full-screen. Click this button again to return the display to normal.
	Display only the interferogram data.
	Display only the singlebeam data.
	Display only
	Toggle the display of the min/max readouts on and off.

In addition, two splitter bars on the align display allow adjustment of the relative screen area given to the spectra / min-max readouts, and the side-by-side interferogram/singlebeam displays. For instance, but clicking the full screen icon, and moving the horizontal splitter just above the min-max readouts, the readouts can be easily read from across a room.

Trouble Shooting

If you are having trouble with your instrument, Madison Instruments, Inc. has a list of symptoms and their causes for FTIR instruments. It is on the Internet at http://www.madisonir.com/trouble.htm.

If you suspect the problem is due to software, please send a bug report to Operant LLC. In Essential FTIR, choose 'Submit Bug Report' from the Help menu. Fill in all information needed to help us reproduce the problem, and be sure to include your email address so we can respond with a solution.