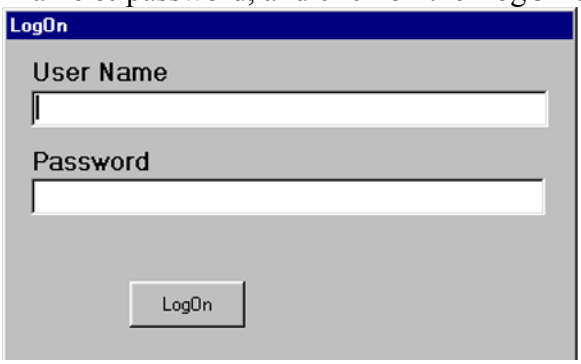
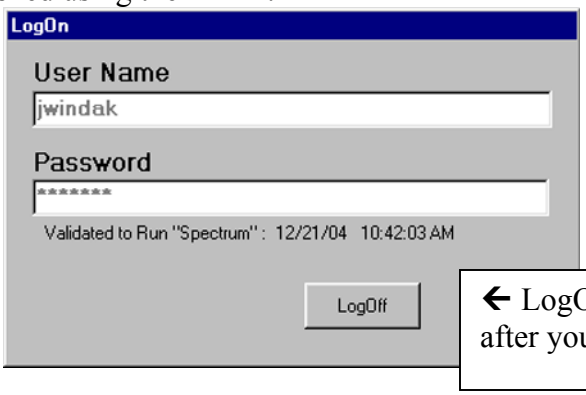
Spectrum BX FT-IR User's Booklet

1) Login with your user name & password, and click on the LogOn button.



After you have clicked on the LogOn button, it will change to a LogOff button, which you will use to log off when you are finished using the FT-IR.



← LogOn changes to LogOff after you have logged in.

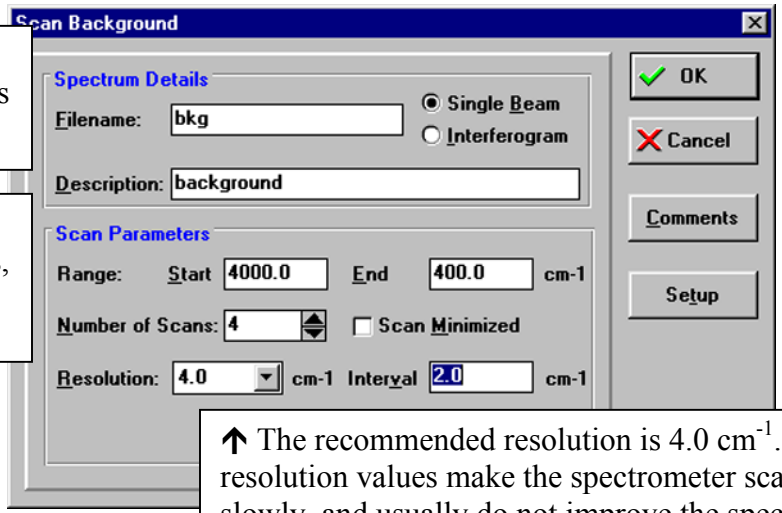
2) Double-click the Spectrum icon 

on the desktop.

3) After the Spectrum program finishes loading, click on the Instrument menu, and click on Scan Background. The following box will come up:

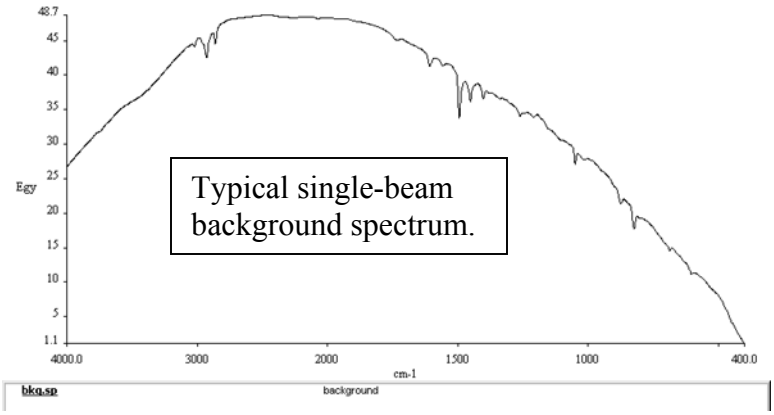
Type in a filename, such as "bkg" here →

For strongly absorbing samples, 4 scans is enough →



↑ The recommended resolution is 4.0 cm^{-1}. Better resolution values make the spectrometer scan much more slowly, and usually do not improve the spectrum quality.

4) After you enter your background parameters and click on OK, the instrument will acquire a single-beam background spectrum.

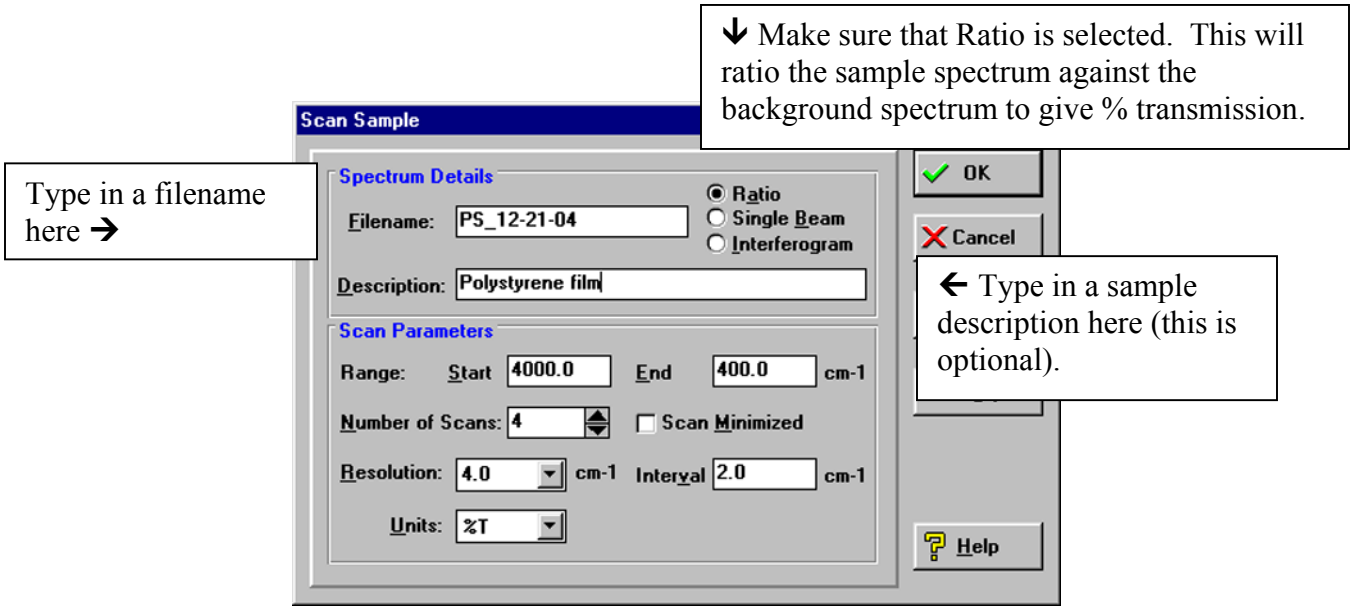


5) Insert your sample into the sample compartment.

6) Click on the New icon 

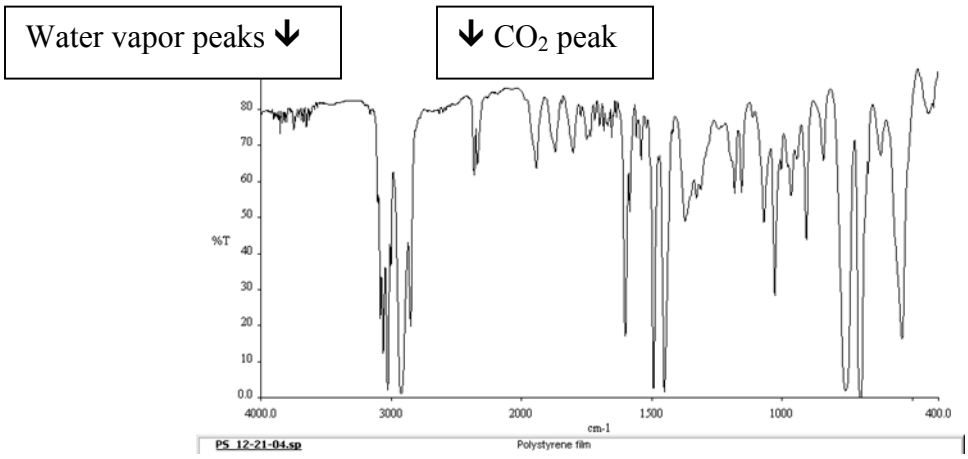
on the toolbar to open a new spectral window.

7) Click on the Instrument menu, and Scan Sample. The following box will appear:



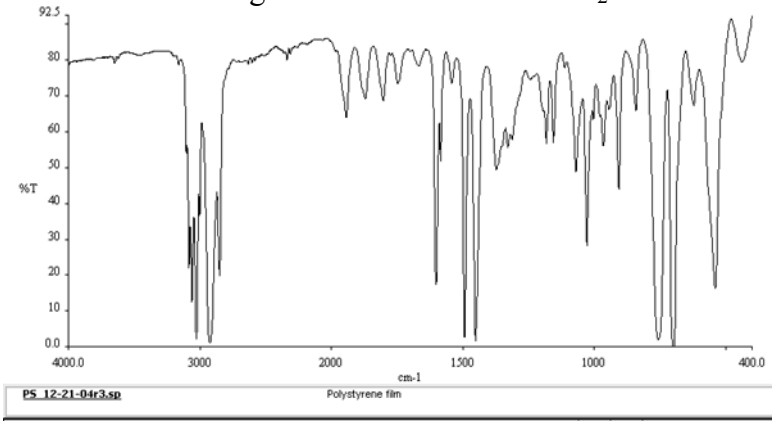
When you click on OK, the instrument will scan your sample spectrum.

Here is a typical sample spectrum.
Notice that CO_2 and water vapor peaks appear in this spectrum. They come from the room air that entered the sample compartment when the lid was raised.

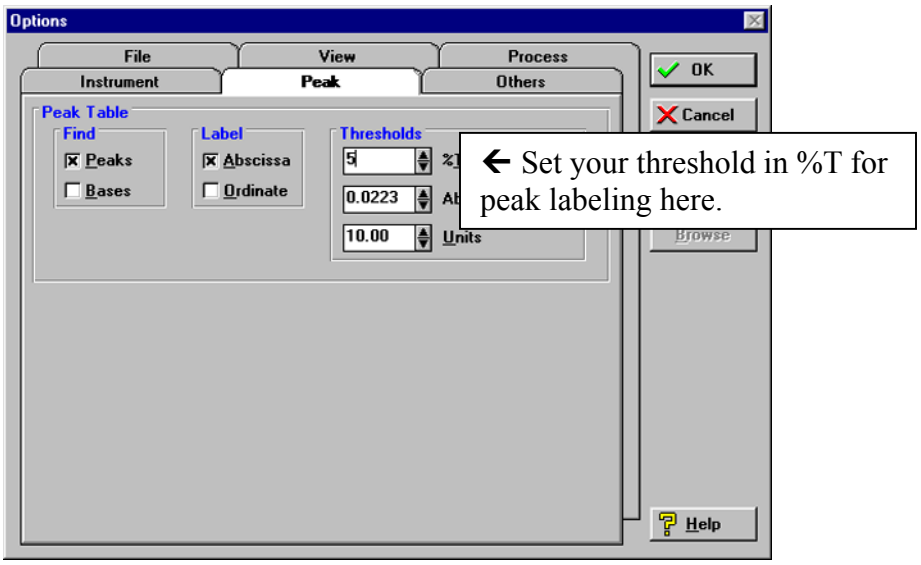


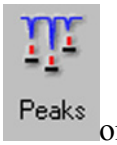
To obtain a spectrum without CO_2 and water vapor peaks, simply wait a few minutes after closing the sample compartment lid. This will allow the nitrogen purge gas to remove traces of CO_2 and water vapor from the atmosphere inside of the sample compartment.

Sample spectrum obtained after waiting a few minutes for the CO_2 and water vapor to purge away:



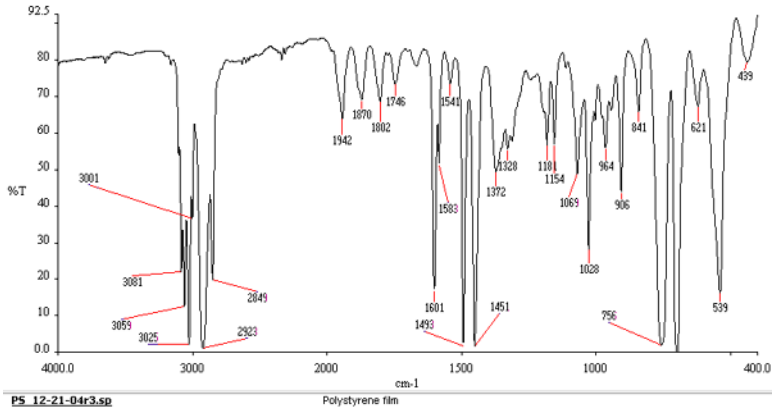
8) To label peak frequencies, first check the threshold for peak labeling. Click on the Setup menu, and click on Options, and then click on the Peak tab. Set the threshold for peak labeling in %T, and then click on OK.



Next, click on the Peaks icon 

on the toolbar. The peaks on the spectrum greater than the threshold will be labeled.

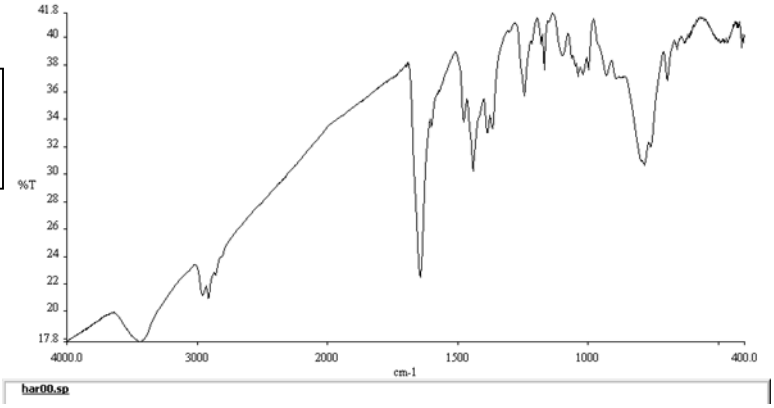
Please note: You can click and drag any peak label to a new position, in order to make it easier to read.



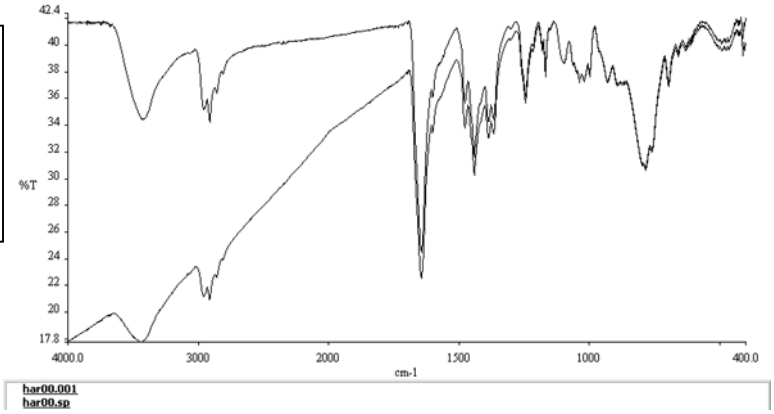
9) How to do baseline correction, if necessary:
Sometimes, a KBr pellet sample will exhibit a slanting baseline, due to wavelength-dependant light scattering. You can alter the baseline of such a spectrum, in order to improve its appearance. Note that this will not change the frequency values of the absorbance bands.

To do this, click on the Process menu, and then click on Baseline Correction. Then click on either Automatic, or Interactive. The Automatic correction usually does a good job. However, there may be times when the Interactive correction works better. The interactive correction allows you to choose points on the spectrum baseline that you want to have aligned horizontally.

Spectrum with a bad baseline.

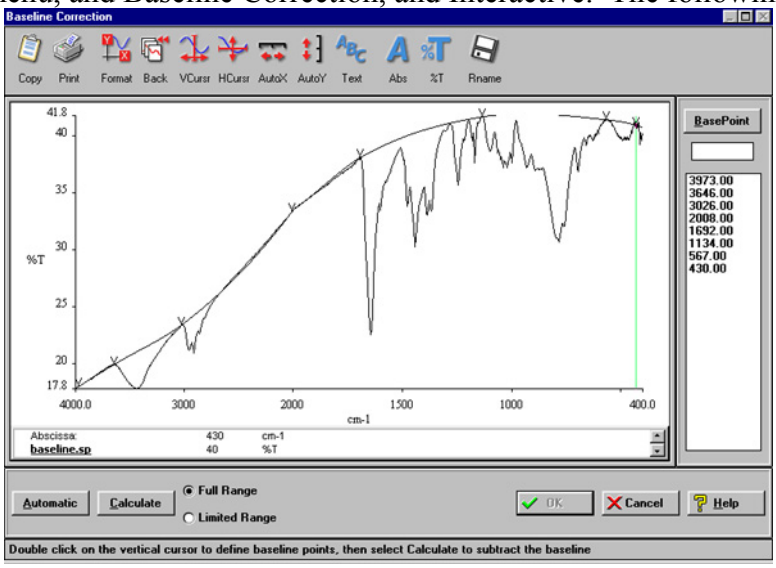


The original spectrum overlaid with the Automatic baseline corrected spectrum.

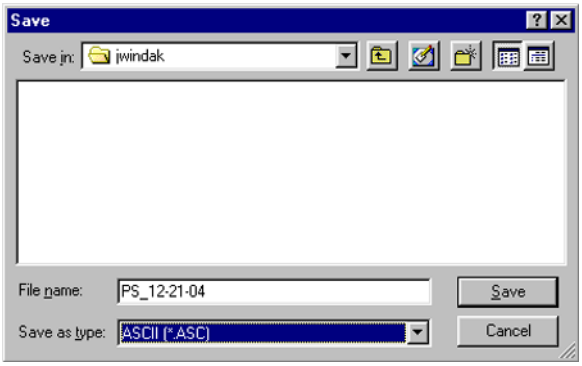


If, instead, you want to manually correct the baseline using the Interactive correction, click on the Process menu, and Baseline Correction, and Interactive. The following box comes up:

Drag the green line to points on the spectrum you want to select, and then double-click on the green line. After you have selected all of the points you want on the spectrum, click on Calculate, and the baseline will be redrawn so that these selected points fall on a horizontal line.

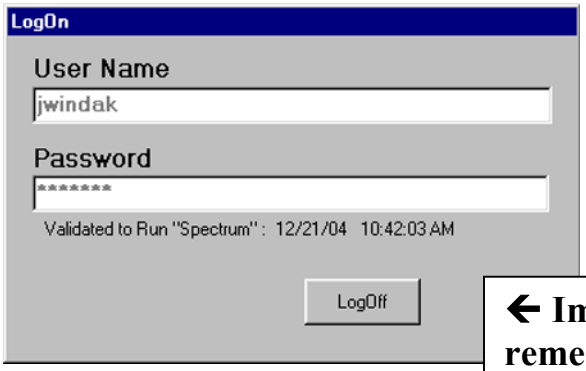


10) How to save a spectrum in ASCII format:
Click on the File menu, and click on Save As.
When the dialog box comes up, you can navigate to the folder where you want to store the data.
Click on the drop-down menu for the "Save As Type", and choose ASCII.
Type in a File name, and click on Save.



11) When you are finished, remove any samples from the sample compartment, and then exit from the Spectrum program.

12) Finally, please remember to click on the LogOff button to log out. If you forget to do this, your account will keep accumulating time, which you will be billed for.



← Important! Please remember to click on the LogOff button when you are finished.