



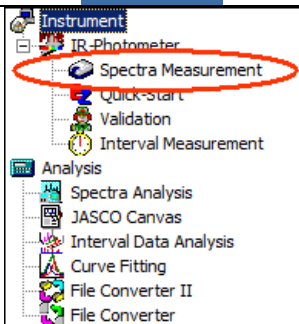
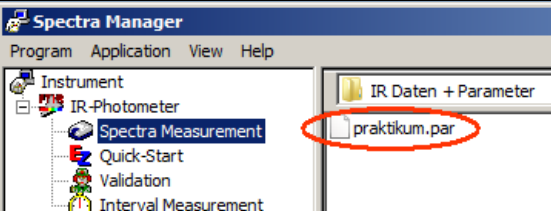

Manual for Jasco-IR-spectrometer

- Do not record spectra of hazardous volatile liquids!
- Do not record spectra of corrosive compounds!
- Do not record spectra of hard and sharp edged material (sand, broken glass etc)!
You will crack the diamond!

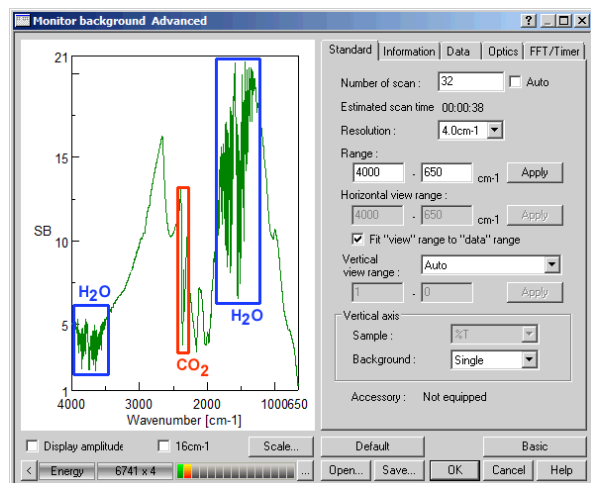
Content:

- Getting started
- Background
- Sample recording
- Data processing
- Data saving and printing
- Cleaning and shut down

Getting started

	<p>„Power on“ the spectrometer. When you hear 3 beeps the instrument is ready.</p>
	<p>Double-click this icon to start the software</p>
	<p>When the application software is started you will see a menu on the left side. Choose</p> <p>Spectra measurement</p>
	<p>It is a good idea now to start data recording by a double-click on “<i>praktikum.par</i>”. This ensures, that all parameters are set as saved in “<i>praktikum.par</i>”. The data recording will also start by a double click on “Spectra measurement”, but then the parameters of the last session are used and mostly you have no idea of the parameters having been used in that session.</p>
	<p>If “<i>Spectra management</i>” has been started there are 4 options found in the menu bar:</p> <ul style="list-style-type: none"> • “B Monitor”: Preview of background • “S Monitor”: Preview of sample • “Bkg”: Data Recording the background • “Sample”: Data recording of the sample

Background



It is not necessary to see first a preview of the background and you may just start recording the background instead.

THE BACKGROUND IS RECORDED WITH A CLEAN AND EMPTY DIAMOND! NEVER EVER PRESS A BLANK TIP ONTO THE DIAMOND!

In the preview window you will not only see the background in the left part of the window but also the parameters for data recording in the right part of the window.

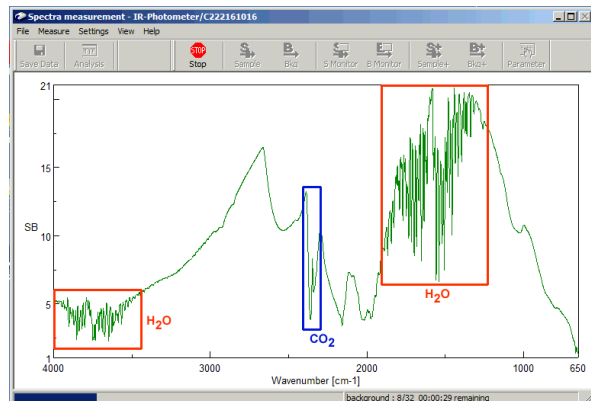
Lab course students should never change the parameters. Other folk may do so but you should **KNOW** what you are doing!

NEVER EVER SAVE ANY CRAZY PARAMETERS TO THE DEFAULT CONFURATION FILE "praktikum.par"!

When you click "OK" you will automatically proceed with the data recording of the background.

It is also possible to skip the background recording but you should only do so if **YOU** are recording several spectra back to back! Do not rely on any other background found - or on "old" backgrounds. In case of doubt record it once more!

Once you clicked "Bkg" at the menu bar or "OK" in the background preview window you are prompted to label the background spectrum. It is not necessary to fill out all the lines but only the first one. A good idea is the actual time.



The background is affected by several facts:

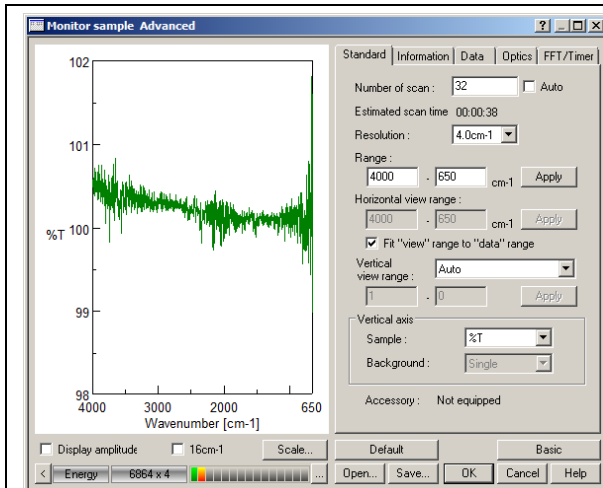
- Absorption by atmospheric carbon dioxide
- Absorption by atmospheric water
- Absorption by the ZnSe-optics
- Absorption by the diamond

Because of the last fact it does not make any sense to record data below 650 cm^{-1} .

Remember the absorption bands of water and carbon dioxide! If you find them in your sample data probably the constitution of the air has changed during data recording – mostly because of your breathing. In this case it is best to record the data once more. Second best is to do a correction of the data (see below).

On data recording you will see a progress bar. In the default settings found in "praktikum.par" 32 scans are accumulated.

Sample recording



If data recording of the background is finished you are ready to measure your sample.

NOW IT IS ABSOLUTELY NECESSARY TO SEE THE PREVIEW OF THE SAMPLE (S-Monitor) FIRST!

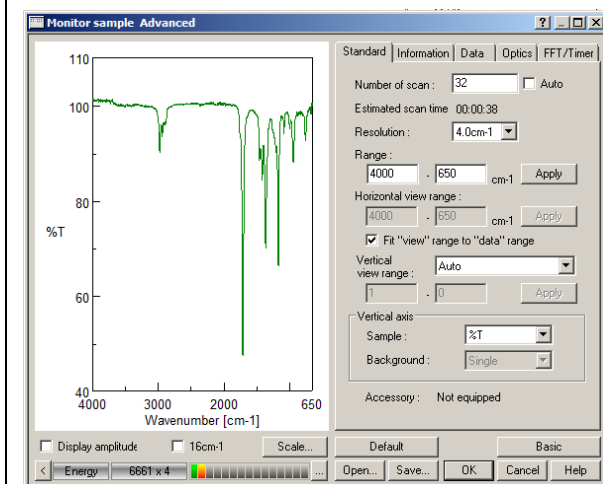
Note:

Again you see the parameters at the right site of the window.

DO NOT USE OTHER PARAMETERS THAN USED IN THE BACKGROUND!

As long as you do not put any compound onto the diamond you will see a baseline "spectrum" close to 100 % transmission.

Compare the amount of noise with the areas of low energy found in the background spectrum!



Apply your sample onto the diamond:

Oily liquids: Put simply a drop onto the surface of the diamond using a pipette.

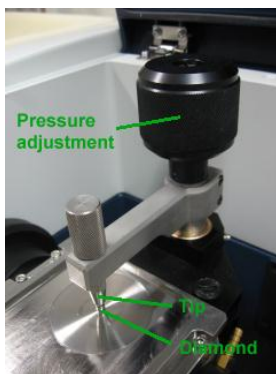
Volatile liquids: Move the tip closely to the diamond so that there is only a very small gap to place the sample.

Powders: Apply onto the diamond. Lower the tip until it has slight contact with the diamond. Be sure that the diamond will be completely covered with the sample, when you start to apply pressure. Grab the knob for pressure adjustment with your left hand and **look at the sample preview!** Apply a little pressure and **look at the sample preview** what is happening. Wait until the next scan is recorded. With an appropriate pressure you should see a spectrum. Enhance the pressure in small steps and after each step **look at the sample preview** to see how the spectrum changes. Once the spectrum is not enlarged any more but only moves down instead, applying of more pressure is only foolish and is nothing but stressing the diamond.

To prevent the diamond from being cracked there is a torque control for the pressure adjustment. If you feel a chattering on turning the pressure adjustment knob you have applied the maximum of acceptable pressure.

Only apply the minimum pressure needed!

KEEP IN MIND THAT YOU MUST NOT RECORD SPECTRA OF HAZARDOUS OR CORROSIVE OR HARD COMPOUNDS!

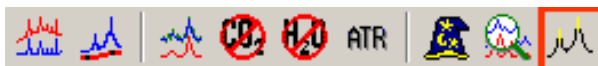


Data processing

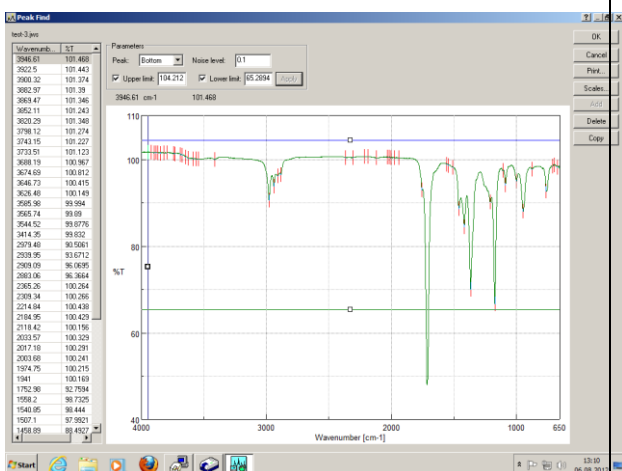


Once you clicked "OK" in the sample preview window you are again prompted to label the sample spectrum. You should label with the name of the sample. Data recording of the sample is completely the same as for the background.

Once recording of sample data is finished both background and sample spectrum are automatically transferred to the "spectra analysis"-application. Open this application by clicking on the new icon found on the windows task bar (See left).



In the "spectra analysis"-Window you will see again the spectrum just having been recorded. The most noticeable change is a new menu bar (see left). There are several options for data correction (for example unwanted carbon dioxide absorption bands) and comparison of data. In most cases you might want to label the bands. This is done by clicking the right icon which in the image found left is highlighted with a red rectangle. This action opens the "peak-find"-window

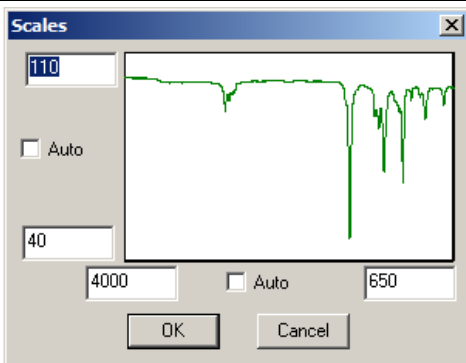


In the "peak find"-window you will see the following options:

There are two horizontal lines, the upper one blue and the lower one green. Only bands with their maximum absorption in the space between the two lines are labeled. You may grab the lines with the mouse and shift them to a different position to proper adjust the range to be labeled. Note that the cursor changes to a pair of tweezers when the mouse is ready to take up the lines.

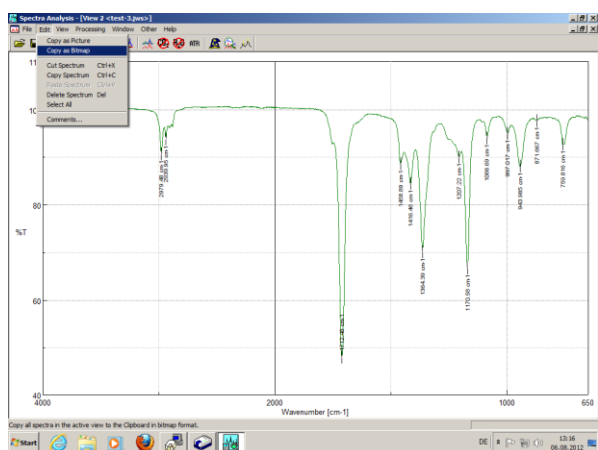
All absorption bands which will be labeled are marked at the moment with a short vertical red line. You may adjust the sensitivity by changing the entry for the "noise level". Lower the "noise level" to get more bands labeled and vice versa. Be sure to use a decimal point and not a "komma".

Fine tuning can be done by hand: Grab the vertical line found at the most left label. If you put it exactly over a label (fine tuning is best with the arrow keys) you may delete the labelling. (See "delete"-button found right hand.) On the other hand you may insert a new label when the vertical line is anywhere else and you use the "Add-button".



To get an exact labeling you may want to temporarily enlarge the range of the absorption band to be labeled. Click the "Scales..."-Button, perform appropriate adjustments and click "OK". If you click "Auto" in the Scales-Window you will retrieve the full-size spectrum.

Data saving and printing



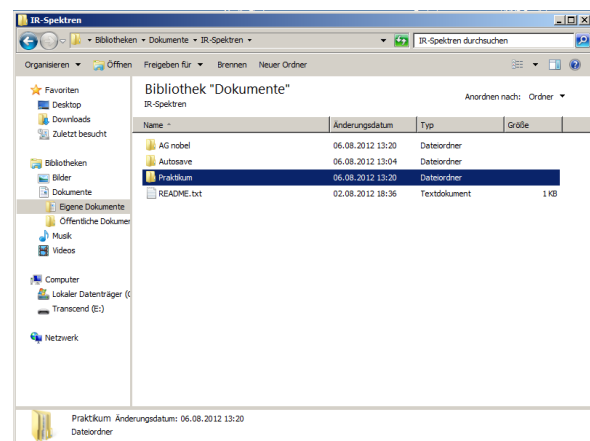
When the peak picking is done the spectrum should look like in the left image. The spectrum is ready to save or to print.

Note:

To copy the spectrum into your report there are two options:

If you like to have only the pure spectrum select “*copy as Bitmap*” as seen on the left image. Paste the Bitmap to the drawing application “*Windows Paint*”! Store the picture of the spectrum in an appropriate format (“*gif*” is a good idea because it is a common and space saving format which is well “known” by text applications.)

More accurate is an output together with the parameters. This is achieved by printing out as a pdf-file. Look for “*Print-Setup*” or “*Print Preview*”. Choose one of the pdf-printer drivers. Once you have clicked “OK” to print the spectrum out you are prompted to state the directory where the pdf-file should be saved.



Spectra should only be stored in folders designed for that purpose. This is:

For lab course students:

Use the folder “*Praktikum*”. Path is:

C:\Users\orggp\Eigene Dateien\Dokumente\IR-Spektren\Praktikum

Within this folder create a subfolder labelled with your own name. No fancy name please! Store **YOUR** data only in **YOUR** folder!

Other staff:

If no folder of your group exists, create a folder „AG+anything” in the path

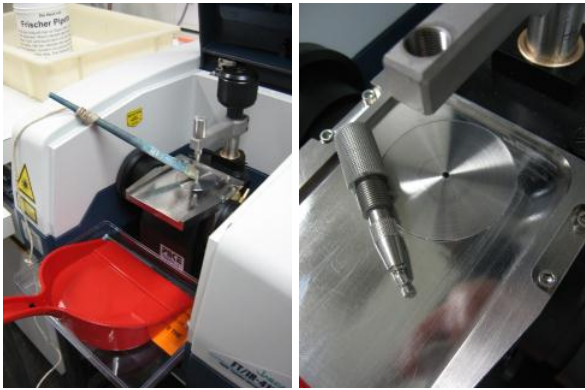
C:\Users\orggp\Eigene Dateien\Dokumente\IR-Spektren\

Within this folder create a subfolder labelled with your own name. No fancy name please! Store **YOUR** data only in **YOUR** folder!

BE SURE THAT I WILL DELETE ALL DATA GARBAGE FOUND ANYWHERE ELSE WITHOUT ANY CALL BACK!

DO NOT STORE ANY DATA “FOREVER”. DATA IN THIS COMPUTER ARE DELETED AFTER A HALF YEAR AUTOMATICALLY!

Cleaning and shut down



CLEAN THE INSTRUMENT!

With solids it is best to use brush and dustpan first. Finish by wiping with a sheet of cellulose moistened with a little ethanol or acetone. To clean the tip it may be unscrewed as seen on the image. Make sure to reassemble the tip immediately.

I WILL BAN PEOPLE FROM USING THIS INSTRUMENT WHO DO NOT CLEAN IT!



If the instrument is not immediately used to record other spectra „Power off“ the spectrometer.

Note that “Power off” is only a stand-by-mode. It is OK and necessary that the “Resume”-lamp is still on. In the stand-by-mode some consumables like the laser are shut off. So “Power off” does not only save electric energy but also preserves the instrument.

NEVER DISCONNECT THE SPECTROMETER COMPLETELY FROM THE ELECTRIC POWER SUPPLY!



If you think you might have been the last user for this workday it is a good idea to move the pressure unit to the park position (turn the rotary arm of the tip completely to the left or to the right and then completely screw down the tip) as seen in the left image and then close the cover.