

IR Users Guide

This guide is only a guide on how to use the IR. Not all steps may be required or additional steps may be needed for your experiment.

If the computer is off, you will need to log onto the computer. The password is either chemistry or chemistry!

1) Determine in what mode you want to take your spectra. Your choices are using the Universal ATR Sampling Accessory (hereafter the ATR) or using the chamber.

2) If you are using the chamber, you will need salt plates which are located in the dessicator. Salt plates are not needed if you are using the ATR. Using the chamber may be required in certain situations.

3) Start the IR software called Spectrum. A username and password is required. Your choices for username are *user1* and *user2*. *User1* has everything available to the user. *User2* has only scan, background scan and print available. *The password for user1 is user1* while the password for *user2* is *user2*. If you are the first person to start the software it asks you to take a background, suitability check or cancel. Hit the background button.

Background: The first person using the software will be required to take a background. The background will remove the gases in air (CO₂, N₂) from your spectrum. You are welcome to take a new background if you think it is necessary. Name the background **bkgground.sp**. It will ask you to overwrite the current spectra. Click overwrite and ok. If you do not take a background, go to the next step.

4) **QUICK SCAN:** This can only be used for liquids.

Put your sample on the ATR and click scan. The number of scans is set to 4. Click print to print out the spectra (although you can't change to landscape. **NAME YOUR SCAN**. The usual method for naming is the semester followed by your initials followed by the experiment number. For example, if I was running an IR for a sample from experiment 10, I would name it fall2010ddexp10.

5) **NORMAL SCAN:** This can be used for both solids and liquids. The procedure that follows is for a liquid.

Liquid Sample: Click on Instrument followed by Scan and this brings up the Spectrum One Scan and Instrument Setup. It consists of four different tabs which are Sample, Scan, Instrument and Accessory. For the Sample tab, **name your scan**. The next tab is Scan. You control the range, the options and the duration from this window. The range should be from 4000 cm⁻¹ to 650 cm⁻¹. **ADD YOUR SAMPLE TO THE ATR BY PUTTING A DROP OF LIQUID AT THE CENTER OF THE DISK**. Click on scan on the right part of the window. Wait until the scan completes. The Instrument tab sets the resolution and should be 4 cm⁻¹. The Accessory tab should not be changed.

When you are scanning, a box pops up with scan, accessory and display. The display shows what the spectrum looks like. The window then goes away and shows the spectra full screen.

Once the spectrum is displayed, add text to the scan. Click on View and then Add/Edit Text. A text label pops up and type in whatever you want to show up on your scan. Click on OK and the text is added to your scan. Clicking on the text opens a box that can be put wherever you want it to be. Click on View and then Label peaks and this will add the labels as to where the peaks are located.

Finally, print out your spectra. Click on File, Print and the Print Graph window appears. Click on Layout and change the Page Orientation to Landscape. Click OK.

6) When you are finished, clean off the ATR with a little methanol. **SIGN THE LOGBOOK. Turning in an IR spectrum but failing to sign the logbook will result in your lab not being counted.**

7) NORMAL SCAN:
This is for a solid sample:

CHANGE FROM A Liquid Sample:

DO NOT CLICK SCAN WHILE YOU ARE CHANGING THE FORCE. AN INCORRECT SPECTRA WILL BE PRODUCED.

REPEATING: DO NOT CLICK SCAN WHILE YOU ARE CHANGING THE FORCE. AN INCORRECT SPECTRA WILL BE PRODUCED.

Put your solid sample on the ATR. Click on Instrument and then Scan to get the setup window again. The scan type should be on sample. Click on the Monitor window on the top left part of the window. It looks like an RPM gauge from your car. The Energy Maximum and Current are displayed. You are most interested in the Force Gauge at the bottom. Move the arm over the sample and turn the weight on top of your sample. **STAY IN THE GREEN ON THE FORCE GAUGE.** If you turn it too much, it will turn RED. Once the force gauge is where you want it, click stop which returns you to the setup window. Click on Scan and the instrument will scan the solid.

Remove the arm and weight carefully from the ATR. *The arm costs \$1200 to replace and you will be charged if you break it.*

Clean the solid sample using a little methanol. Workup the spectra as before by adding text, saving the spectra, and printing the spectra off.

The software has LOTS of options available to it. Explore the possibilities if you have time.