USING iS5 ATR WITH OMNIC

Note: If the iD5 ATR accessory is not installed, get help from the lab manager. If you do have to install it yourself, please select "iD5 ATR-ZnSe iD5_ATR_ZnSe.exp" in the "Smart Accessory Change" window.

- 1. Turn on the computer.
- 2. Open the software "OMNIC" by clicking the icon from the desktop.
- 3. In the "Smart Accessory Change" window choose an appropriate program (e.g., Orgo-iD5 ATR-ZnSe... iD5_ATR_ZnSe.exp) to run and then click "OK". The crystal of the ATR is ZnSe.



- 4. In the "File" pulldown menu, click "Open Configuration", choose "EZ OMNIC.CON", and then click "Open". A method for common usage of iS5 IR is loaded: 8 scans, 600-4000 cm⁻¹, resolution of 4, collect background every 400 min, and "%Tansmittance" for "Final format". If an experiment calls for a different setup, click "Expt Set" and change the appropriate parameters.
- 5. Remove the dust cover from the crystal and move the pressure tip 90° to the side.
- 6. Click "Col Bkg" to collect a background when you're asked to. A spectrum of the background will appear after a couple of scans but **WAIT** for the acquisition to finish. It is not necessary nor advised to add the background spectrum to the window.
- 7. Apply the sample so that it completely covers the crystal. For liquid samples, use a pipet; for solids, use a spatula. Avoid touching the crystal with the pipet or spatula directly.
- 8. Move the pressure tip 90° back to the top of the crystal.
- 9. Screw down the pressure tower until the pressure tip touches the sample. To get the correct amount of pressure, turn the knob clockwise until you hear it click. The knob has a clutch and is designed to prevent from applying too much pressure to the crystal.
- 10. Click "Col Smp"→enter the spectrum title if you want to save the data. Otherwise ignore the box→click "OK" to collect the sample spectrum→When finished collecting, add the spectrum to the window. Sometimes the spectrum is displayed as absorbance. If % transmission is preferred, click on "Process" and select "% Transmittance".
- 11. Under "Process" pull-down menu, select "Automatic Baseline Correct" to correct baseline.

- 12. To correct for unequal absorption at high and low frequencies, under "Process" pull-down menu select "Advanced ATR Correction", which will make the spectrum look more like a classic transmission IR spectrum to compare with known spectra (you may have to switch to % transmission, to view the spectrum in that mode).
- 13. After each correction (e.g., baseline and unequal absorption), a new spectrum is created. It's good to delete the previous spectra by clicking on the previous spectra to highlight it and then click "Clear" icon. The spectra can be hidden by selecting "Hide Spectrum" under "View" pull-down menu.
- 14. At the bottom of the Omnic window, click "T" to annotate your spectrum—click and hold on a peak of interest and move mouse to position the wavelength. Click "T" again to get out of peak label mode. If the annotations run off the bottom of the window, click "Nrm Scl" to normalize scale.



- 15. To delete an annotation, click "T", move the cursor to the annotation to highlight the annotation, and then press "Delete" on the keyboard. The annotation will be deleted.
- 16. Click "Print" to print.
- 17. Using a cotton applicator (or facial tissue) and methanol to clean up your sample. If necessary, use the compressed air to blow your sample off the crystal plate.
- 18. Turn off the computer if you're the last one using the instrument. NEVER turn off the instrument unless absolutely needed. Extended period of power-off may subject electronics in IR to moisture which shortens the instrument life.