

# Bruker Vertex 70 / Very Basic ATR-FTIR Guide

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## System Checkup

1. On the top left corner of the Vertex 70, three status LEDs should show a green light:
  - I. Humidity (contact RP if red).
  - II. Laser (contact RP if red).
  - III. Status (if red, check performance test status from software; see *below*).

## Start Software and Check Performance Test Status

1. Open computer and Opus-software from the desktop.
  - I. Passwords are on the computer.
  - II. Use Operator as the User ID.
  - III. Use default as the Assigned Workspace.
2. If the Status LED shows a red light, check the performance test status.
  - I. Click the small round icon on the bottom right corner of the Opus-software to go to the Instrument Status-menu.
  - II. If performance tests are expired, click the expired status icon.
    - i. If the performance tests are not expired (no expired notification in the Instrument Status) and the instrument's Status LED is red, contact RP.
  - III. Perform the expired performance tests. Check the appropriate tests (PQ and/or OQ) and then press *Run Tests*. Clean the ATR crystal with isopropanol and low-lint wipes when the software prompts to do so.
  - IV. Wait until tests are finished. A PDF opens automatically when finished. The PDF shows a passed status if validation and checked components are ok. If tests are not passed, contact RP. Save the opened PDF to the *Opus OVP* folder on the desktop.

## Measurement Setup

1. Press the green vial icon on the toolbar of the software (rightmost icon) to go to *Measurement*. You can also go to *Measurement* from the *Measure*-menu.
2. Go to the *Advanced*-tab and check that the MIR-ATR experiment is selected. Load the MIR-ATR method if it is not selected. The MIR-ATR experiment has the following measurement parameters as defaults:
  - I. Resolution: 4 cm<sup>-1</sup>
  - II. Number of Scans: 20
  - III. Scan Range: 400 – 4000 cm<sup>-1</sup>
  - IV. Spectral Results: Absorbance
3. You can change the above settings for your own instance of usage, but do not save the MIR-ATR experiment file if you change these settings.
4. Select your own folder as the save location in *Measurement* -> *Advanced* -> *Path*. If you don't have one, create your own folders to the path denoted below:
  - I. C:\Data\Measurements\“Lastname, Firstname”\“Subfolder”

## Perform Measurements

1. Clean the ATR crystal with isopropanol and low-lint wipes.
  - I. You may also clean the tip of the press.
2. Write your sample's filename to *Measurement -> Advanced -> File name*.
3. Measure a background via *Measurement -> Basic -> Background Single Channel*.
  - I. Don't lower the press on the ATR crystal when collecting a background.
4. When background measurement is finished, place your sample on the ATR crystal.
  - I. Use enough sample to cover the whole ATR crystal.
  - II. Use enough sample so that the press can compress the sample *lightly* against the ATR crystal without airgaps. Raise or lower the press from its stand if necessary. Check that the small red circle of the press is within its target circle when compressing the sample. **WARNING! Too much pressure and force can detach or damage the ATR crystal.**
  - III. Liquid samples do not need to be pressed.
5. Measure a spectrum by pressing *Measurement -> Basic -> Sample Single Channel*.
6. When finished, remove your sample from the ATR crystal.
7. Repeat steps 1-6 for other samples.

## Spectral Processing and Data Export

1. Perform spectral processing from the *Manipulate*-menu if necessary. You can also perform the necessary processing with other software after exporting your data. Select the spectrum, then process. Commonly used processing is listed below:
  - I. Atmospheric Compensation to correct for water and CO<sub>2</sub> (if abnormal).
  - II. ATR-correction if you need to compare ATR with transmittance spectra.
  - III. Baseline correction.
  - IV. Normalization.
2. Save your processed spectrum as a separate file from the non-processed spectrum.
  - I. Do not overwrite your original unprocessed spectrum.
3. Export data by saving a spectrum as a data point table.
  - I. Select the spectrum.
  - II. *Menu -> Save File As*.
  - III. Check file name and path.
  - IV. Check *Data Point Table* from the *Mode*-tab.
  - V. Press *Save*.

## Finish Measurements

1. Remove your sample from the ATR crystal.
2. Clean the ATR crystal and the tip of the press with isopropanol.
3. Log your usage to the logbook.
  - I. In the column *Accessory/Signal*, write the accessory you used (ATR) and the MIR signal value read from *Measurement -> Check Signal -> Amplitude*.
4. Do not shut down the Vertex 70, but you can shut down the computer.