

Manual for the IFORS software (Iterative Fitting of Raman Spectra)

Installation

Windows

The software was tested under Windows 7 64bit with python 3.6.4 64bit, but it is very likely that it will also work under Windows 8 and 10.

Go to <https://www.python.org/downloads/windows/> and download the current python version (at the time of writing it is version 3.6.4).

Run the python installer and follow the instructions therein. Be sure to select the tick-mark which says “ADD TO PATH”.

IFORS requires the following packages: Numpy, Scipy, Matplotlib, PyQt5. Open a command prompt in Windows and write:

- **pip install numpy** (hit enter)
 - this will install numerical python (<http://www.numpy.org/>)
- **pip install scipy** (hit enter)
 - this will install the Scientific Computing Tools for Python (<http://www.scipy.org/>)
- **pip install matplotlib** (hit enter)
 - this will install the Matplotlib plotting library for Python (<https://matplotlib.org/>)
- **pip install pyqt5** (hit enter)
 - this will install the PyQt5 library for Python (<https://pypi.python.org/pypi/PyQt5>)

All needed files for the IFORS-software are contained in the ‘ifors_win.zip’ (Linux: ‘ifors.tar.gz’) archive. The archive contains three folders with following files:

- docs\
 - ifors_default_config.cfg
 - ifors_manual.pdf
 - reference_series_data.xls
- test_spectra\
 - Almandine.txt
 - KL2-8HS_1_ics.txt
 - KL2-19_2.txt
 - KL16_8B_532_1.txt
- ifors\
 - setup.py
 - ifors\
 - ifors_canvas.py
 - ifors_cli.py
 - ifors_estimate_temperature.py
 - ifors_gui.py

- ifors_ifors.py
- ifors_optimize_python.py
- ifors_readout.py
- ifors_run.py
- ifors_start_curve-fit.py

Extract the 'ifors'-folder in a directory of your choice, for this manual 'C:\Python_scripts\packages' is chosen.

- In the command prompt navigate to 'C:\Python_scripts\packages\ifors'.
 - **cd Python_scripts\packages\ifors**
 - Now the command prompt is active in the chosen director, e.g. 'C:\Python_scripts\packages\ifors'
- To install the ifors-package type in the command prompt:
 - **pip install .** note: the dot (.) and space are part of the command!(Figure 1)
- To uninstall ifors type in the command prompt:
 - **pip uninstall ifors**

```

C:\Windows\system32\cmd.exe - cmd.bat
c:\Python_scripts\packages\ifors>pip install .
Processing c:\python_scripts\packages\ifors
Installing collected packages: ifors
Running setup.py install for ifors ... done
Successfully installed ifors-0.1
c:\Python_scripts\packages\ifors>

```

Figure 1: Install the ifors-package using pip.

NB!

You will have to edit the 'ifors_default_config.cfg' file during usage and you will need a text-editor for this. Notepad++ (<https://notepad-plus-plus.org/>) is suggested for this purpose, but you can use any other text-editor. **When editing the script files, make sure that you set the 'Tab-settings' in your editor to: Tab-size = 4 and replace tab by space. You can do this in Notepad++ in 'Settings → Preferences → Tab Settings'. '.' (dot) is used as decimal separator in the '.fit' files (section 1.3). To interrupt ifors started from the command prompt, type in the command prompt: 'Strg+C'**

OSX (MAC)

Many thanks to Lukas Nibourel (University of Bern) who worked out these detailed instructions for the installation of IFORS on a Mac system.

Instructions:

IFORS (version ifors-0.1.1) was tested using a MacBook Pro (13" Early 2015), OSX El Capitan 10.11.6, Lukas Nibourel, 2017-06-01

Command line entries are marked with a \$, press enter to run a command

step 1 get Xcode:

- Download and install Xcode from your Apple Store. You also need to open Xcode agree to the license and it will install its components.
- Open your Terminal from: Applications/Utilities/Terminal
- To activate the associated command line tools, go to your Terminal command prompt and run:
- **\$ xcode-select --install**

step 2 download and install Homebrew

Homebrew helps you to download, install and manage complex packages such as Python.

- To download and install Homebrew type:
- **\$ ruby -e "\$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/install)"**
- If Homebrew is already installed, to update to the latest version type:
- **\$ brew update**
- After installing/updating Homebrew and as suggested in the command line, to check for any issues with the installation run:
- **\$ brew doctor**

step 3 download and install python3

- Download Python3 with Homebrew (python2 is installed by default on most Macbooks Python2 is installed by default). From your command prompt run:
- **\$ brew install python3**
- This will take a few minutes. Pip (a command that will be used later on) is included the Python3 package when installed with Homebrew.

step 4 create a new virtual environment

The best way to use a specific Python software which requires specific packages (and Python versions) is to use virtual environments. They allow you to have a "virtual" Python installation, that does not interfere with the main system.

- **\$ mkvirtualenv --python=\$(which python3) ifors**
- This will create and enter the virtual environment ifors, indicated by (ifors) in your command prompt
- If you need to leave the virtualenv, type "deactivate". If you need to enter it again, type "workon ifors".
- To verify that python3 is installed on your virtual environment, type:
- **(ifors) \$ python -version**

The '(ifors)' before the \$-sign on your command prompt indicates that the virtual environment 'ifors' is currently activated.

step 5 install prerequisites (into the environment, not the system)

- While in the virtual environment, install the following required packages:

- **(ifors) \$ pip install PyQt5 numpy scipy matplotlib**

step 6 install ifors

- Unpack the attached zip (version ifors-0.1.1), and from that folder (the one with setup.py) run local install:
- **(ifors) \$ pip install .**

With that, ifors_run should be ready to use, by following your detailed explanations (see below).

Additional convenient info:

- To find out which python version is installed on your system and used in default mode (outside your virtual environment)
- **\$ python --version**
- Check if and which version of python3 is installed on your computer
- **\$ python3 --version**
- To find out where python3 is stored on your computer type
- **\$ which python3**

Linux

Install the following packages: PyQt5, Numpy, Scipy, Matplotlib

Python3 should be implemented in most Linux distributions.

Extract the ifors-folder in a directory of your choice, open the console and navigate to the extracted ifors-folder, install the ifors-package with pip install . (super-user rights might be necessary if Python is not installed into a virtual environment)

1. Usage (Windows/Linux)

The usage of the software is command line driven, but only very few commands are needed. In this manual command line input is written in bold **Courier New** font. A [...] in the command line input indicates that the following line break is due to text formatting and that the actual command line input has no line break. Make use of the tabulator-key and the arrow-keys when writing in the command line. Hitting the tabulator-key triggers the auto-completion, i.e. file- or folder-names will be completed. The up and down arrow-keys let you cycle through already submitted commands. This avoids repetitive typing.

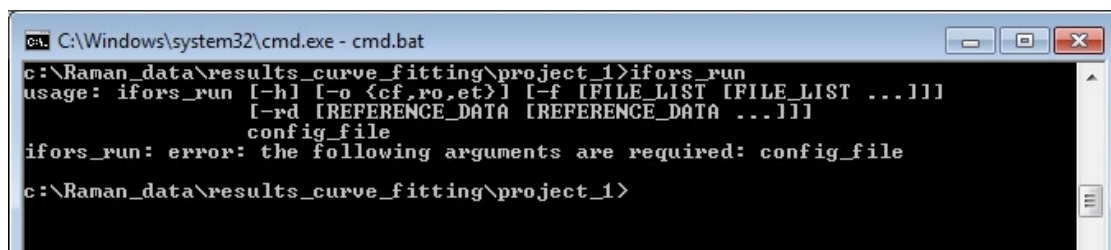
The software works with Raman spectra that have been saved in txt-files. These files are from now on referred to as 'spectrum-files'. A spectrum-file contains two columns and the first column lists the Raman-shift values (relative wavenumbers) and the second column lists the associated intensity.

1.1 Curve-fitting with IFORS:

To start a curve-fit with ifors you have to use the command-prompt. Before you start to evaluate your spectra, it is suggested to keep your folder structure clearly arranged. Therefore, copy or move your spectra into a specific folder or follow the suggestions of this manual (see below):

- In Windows Explorer create a '*Raman_data*' folder with four sub-folders. In this example the following paths are used:

- C:\Raman_data\spectra
 - C:\Raman_data\results_curve-fitting
 - C:\Raman_data\ifors_aux
 - C:\Raman_data\reference_data
- Of course you can use other folders, but it is advised to use a consistent folder structure.
 - From the 'ifors_win.zip'-archive (linux: 'ifors.tar.gz') extract the contents of the 'docs'-folder into the 'ifors_aux'-folder.
 - In the 'ifors_aux'-folder open the 'reference_series_data.xls'-file, follow the instructions in the explanation box. Save the reference data as a tab-delimited txt-file, name it 'reference_series_data_488.txt' or 'reference_series_data_532.txt' depending on the reference data you selected from the xls file and move it into the 'reference_data'-folder. The reference data is needed later for estimating metamorphic temperatures (see section 3).
 - When you start a new project, create a sub-folder in the 'spectra' and 'results_curve-fitting' folders. Here, we will use 'project_1':
 - C:\Raman_data\spectra\project_1
 - C:\Raman_data\results_curve-fitting\project_1
 - Copy your spectrum-files to the 'Raman_data\spectra\project_1' folder (in this example the spectrum-files KL2-8_HS_1_ics.txt and KL2-19_2.txt of the test_spectra folder from the 'ifors_win.zip'-archive)
 - In the command prompt navigate to the folder in which you want to save the results of the curve-fit, in this example C:\Raman_data\results_curve-fitting\project_1. By default, the command prompt is active in e.g. C:\Users\currentUser. To navigate to the results_curve-fitting\project_1 folder type in the command prompt:
 - **cd ..** (hit enter)
 - **cd ..**
 - now the command prompt is active in the root of drive C:
 - **cd Raman_data\results_curve-fitting\project_1**
 - Now the command prompt is active in the chosen directory, e.g. C:\Raman_data\results_curve-fitting\project_1.
 - Now you can start ifors by typing in the command prompt (continuing from the example above):
 - **ifors_run**



```

C:\Windows\system32\cmd.exe - cmd.bat
c:\Raman_data\results_curve_fitting\project_1>ifors_run
usage: ifors_run [-h] [-o {cf,ro,et}] [-f [FILE_LIST [FILE_LIST ...]]]
               [-rd [REFERENCE_DATA [REFERENCE_DATA ...]]]
               config_file
ifors_run: error: the following arguments are required: config_file
c:\Raman_data\results_curve_fitting\project_1>
  
```

Figure 2: Starting ifors with the ifors_run command.

This will provide you with a short help on the ifors_run command and also produces an error, which tells you that you need to specify the config_file (Figure 2). The config_file allows you to control the

behavior of ifors. See below for details on settings, constraints, options, etc. For now, you use the '*ifors_default_config.cfg*'. The short help text tells you that you further need to provide some options to the ifors_run command. Possible options are:

- config_file: this is a positional option and must be provided as the first option. It points to the config_file you want to use with ifors.
- -o: this option takes the value of:
 - 'cf' → to start the curve-fit
 - 'ro' → to readout the data of a finished curve-fit
 - 'et' → to estimate peak metamorphic temperature from data generated with the readout option
- -f: this option is the file list, you have to specify which files you want to work with. Multiple files are possible.
- -rd: this option refers to the reference data, you have to specify which reference_data file you want to use for temperature estimation.

To start a curve-fit, type the following in your command prompt (continuing from the example above):

- `ifors_run c:\Raman_data\ifors_aux\ifors_default_config.cfg -o cf -f [...]`
`c:\Raman_data\spectra\project1\KL2-19_2.txt`
- This command consists of four parts (Figure 3 and 4):
 - The first part '*ifors_run*' initiates ifors
 - The second part '*c:\Raman_data\ifors_aux\ifors_default_config.cfg*' points to the config_file you want to use.
 - The third part '*-o cf*' initiates the option '*curve-fit*'
 - The fourth part '*-f c:\Raman_data\spectra\project1\KL2-19_2.txt*' initiates the option '*file_list*' and points to the spectrum file that you want to evaluate.

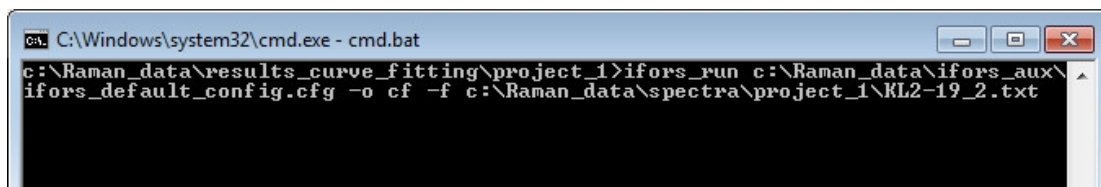


Figure 3: Starting the '*ifors_run*' command with the *cf* option using the command prompt.

Structure of the 'ifors_run' command

```
c:\Raman_data\results_curve_fitting\project_1> ifors_run [...]
```

Path to the folder you want to save your results to

Initiate ifors,
can be done in any folder

```
c:\Raman_data\ifors_aux\ifors_default_config.cfg -o cf [...]
```

positional argument of the 'ifors_run' command,
must follow 'ifors_run', points to the config file you
want to use for curve-fitting

optional argument of the 'ifors_run' command,
can take any position after the positional argument,
-o: option, cf: curve-fit;
controls the operational mode of ifors

```
-f c:\Raman_data\spectra\project_1\KL2-19_2.txt
```

optional argument of the 'ifors_run' command,
can take any position after the positional argument,
-f: file_list, path to files
specifies the files/spectra you want to use with ifors

Figure 4: Structure of the 'ifors_run' command.

- When you hit enter, a new window will open, showing the live progress of curve-fitting, from now on named live-view (Figure 5), and some output about the progress of the curve-fitting is printed in the command prompt (Figure 6).

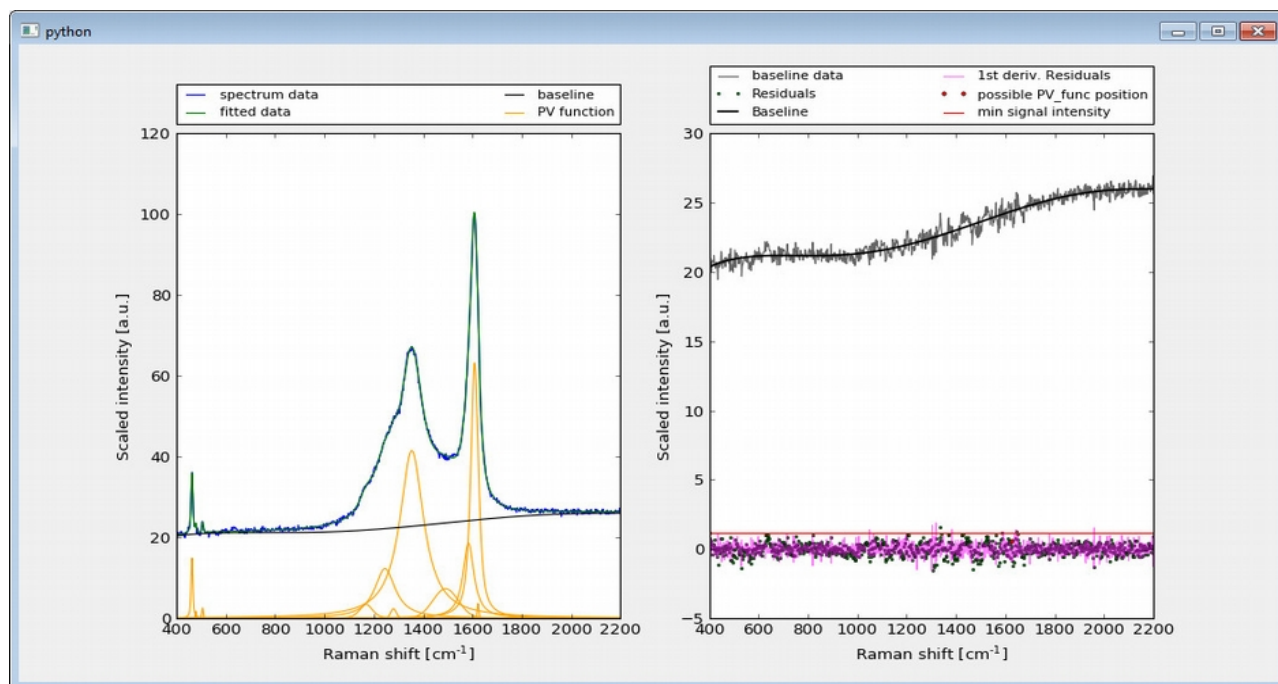


Figure 5: The live-view window showing a curve-fit in progress.

```

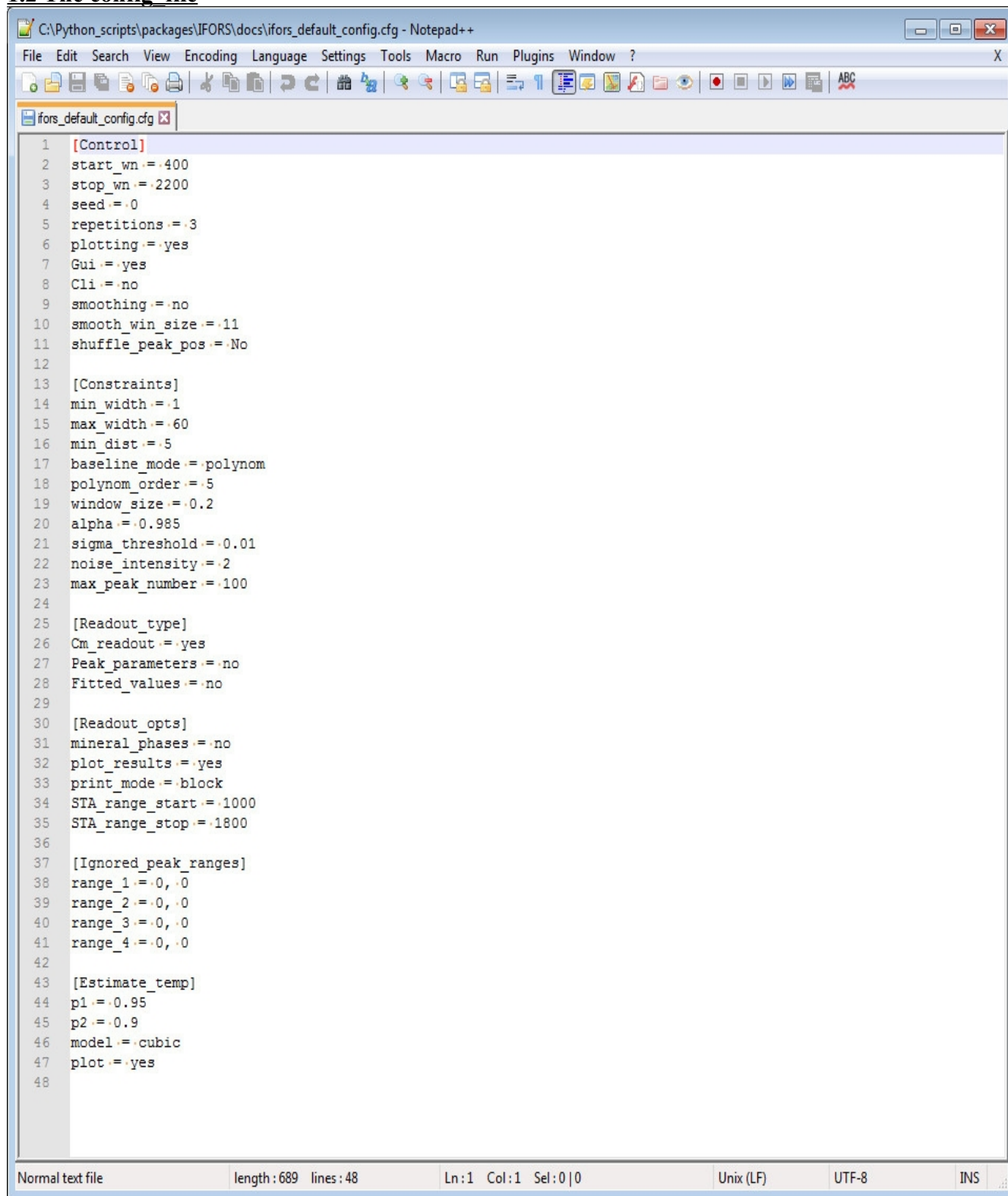
C:\Windows\system32\cmd.exe - cmd.bat - ifors_run c:\Raman_data\ifors_aux\ifors_default_conf...
adding peak 194.342736009
min_signal_intensity 1.17091570494
Testing position: 68.1330472103 best_rating 194.342736009 rating 192.223701274
peak position 68.1330472103
model rating 192.223701274 194.342736009
Improve
rating after improve 175.008829503
## model ##
[[ 6.31841395e+01 -2.80738524e+00 6.71788537e+01 1.03188870e+00]
[ 4.14930829e+01 8.31359724e+02 5.30168415e+01 3.23960866e+00]
[ 1.49392050e+01 1.72261767e+00 3.52201154e+00 2.44146120e-01]
[ 1.22801711e+01 -2.62519769e+02 4.69841140e+01 2.81511726e+00]
[ 7.29979072e+00 1.00345196e-05 6.06305996e+01 3.33332161e+00]
[ 1.85656899e+01 3.15972419e+02 6.57962195e+01 1.49953117e+00]
[ 2.53203748e+00 -5.60093481e-05 5.90875832e+00 1.87657019e-01]
[ 3.44222460e+00 -7.38377656e-01 4.27327051e+01 1.70584593e+00]
[ 2.37686330e+00 -5.60200076e-05 4.89022444e+01 7.29787364e-01]
[ 1.72856453e+00 0.00000000e+00 4.38767002e+00 1.26220889e-01]
[ 3.67293976e+00 1.63482566e-04 6.79462784e+01 2.10936574e-01]]
adding peak 175.008829503
model rating inf 175.008829503
found no improvement
--- duration 387.031250
--- Final Rating --- 175.008829503

```

Figure 6: The command prompt output when the curve-fit is finished. As long as the live-view window is displayed, you can not enter new commands in the command prompt. Close the live-view window to issue new commands.

- The curve-fit will continue until optimization with the current constraints is reached, or if you close the live-view window.

1.2 The config file



```
C:\Python_scripts\packages\IFORS\docs\ifors_default_config.cfg - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?
ifors_default_config.cfg
1 [Control]
2 start_wn.=.400
3 stop_wn.=.2200
4 seed.=.0
5 repetitions.=.3
6 plotting.=.yes
7 Gui.=.yes
8 Cli.=.no
9 smoothing.=.no
10 smooth_win_size.=.11
11 shuffle_peak_pos.=.No
12
13 [Constraints]
14 min_width.=.1
15 max_width.=.60
16 min_dist.=.5
17 baseline_mode.=.polynom
18 polynom_order.=.5
19 window_size.=.0.2
20 alpha.=.0.985
21 sigma_threshold.=.0.01
22 noise_intensity.=.2
23 max_peak_number.=.100
24
25 [Readout_type]
26 Cm_readout.=.yes
27 Peak_parameters.=.no
28 Fitted_values.=.no
29
30 [Readout_opts]
31 mineral_phases.=.no
32 plot_results.=.yes
33 print_mode.=.block
34 STA_range_start.=.1000
35 STA_range_stop.=.1800
36
37 [Ignored_peak_ranges]
38 range_1.=.0,.0
39 range_2.=.0,.0
40 range_3.=.0,.0
41 range_4.=.0,.0
42
43 [Estimate_temp]
44 p1.=.0.95
45 p2.=.0.9
46 model.=.cubic
47 plot.=.yes
48
Normal text file length: 689 lines: 48 Ln: 1 Col: 1 Sel: 0|0 Unix (LF) UTF-8 INS
```

Figure 7: The default configuration of IFORS. The default configuration is designed for carbonaceous matter spectra, but works also for most mineral spectra.

Figure 7 shows the contents of the default configuration file of IFORS. The configuration parameters are arranged in six sections, e.g. Control, Constraints, Readout_type, Readout_opts, Mineral_peaks and Estimate_temp. The default configuration is designed for carbonaceous material Raman spectra.

[Control]:

- *start_wn*: This parameter specifies the start wavenumber (relative, or Raman shift) of the spectrum. If you choose a value less than the minimum wavenumber of the spectrum, *start_wn* is set to the minimum wavenumber. **The value must be an integer. (default: 400)**
- *stop_wn*: This parameter specifies the stop wavenumber (relative, or Raman shift) of the spectrum. If you choose a value greater than the maximum wavenumber of the spectrum, *stop_wn* is set to the maximum wavenumber. **The value must be an integer. (default: 2200)**
- *seed*: This parameter sets the seed-value of the random-number generator for live-view curve-fits. **The value must be an integer. (default: 0)**
- *repetitions*: This parameter sets the number repetitions. It determines how often the spectrum is repeatedly evaluated. It is only used when the 'Cli'-parameter (see below) is used. **The value must be an integer. (default: 3)**
- *plotting*: This parameter applies only if the 'Cli'-parameter is used and determines if plots of the curve-fits are saved as pdf- and png-files. **The value must be a string. Options: 'yes' or 'no' (default: yes)**
- *Gui*: This parameter controls the live-view window. If 'Gui' is set to 'yes' the curve-fit will start in the live-view window (Figure 5). **The value must be a string. Options: 'yes' or 'no' (default: yes)**
- *Cli*: This parameter starts the curve-fit without the live-view window and will save all results when curve-fitting is finished. **The value must be a string. Options: 'yes' or 'no' (default: no)**
- *smoothing*: If set to 'yes', smoothing is enabled and the spectrum will be convoluted with a Hanning-Window filter. **The value must be a string. Options: 'yes' or 'no' (default: no)**
- *smooth_win_size*: This parameter controls the window size of the Hanning-Window used for smoothing. The value refers to the number of datapoints included in the window, e.g. 11 → the window is 11 datapoints wide (not wavenumbers!). **It must be an odd integer (default: 11)**
- *shuffle_peak_pos*: This parameter determines if the list of possible peak positions shall be randomized or not. **The value must be a string. Options: 'yes' or 'no' (default: no)**

[Constraints]:

- *min_width*: This parameter controls the minimum half width at half maximum (HWHM) of the pseudo-Voigt functions during curve-fitting. The value is multiplied with the spectral resolution (e.g. the distance between two data-points). **The value must be an integer. (default: 1)**

- *max_width*: This parameter controls the maximum HWHM of the pseudo-Voigt functions during curve-fitting. The value refers to wavenumbers and **must be an integer. (default: 60)**
- *min_dist*: This parameter controls the minimum distance between two pseudo-Voigt functions during curve-fitting. The value is multiplied with the spectral resolution (e.g. the distance between two data-points). **The value must be an integer. (default: 5)**
- *baseline_mode*: This parameter lets you choose the style of baseline approximation. If set to 'window_filter', the baseline is approximated by a convolution of the baseline-data with a moving Hanning-window. If 'baseline_mode' is set to 'polynom', the baseline is approximated by a polynomial of the order set with the 'polynom_order' parameter. If 'baseline_mode' is set to 'off' no baseline will be used during curve-fitting. **The value must be a string. Options: 'window_filter', 'polynom', 'off'. (default: polynom)**
- *polynom_order*: This parameter sets the order of the polynomial used during baseline approximation. **The value must be an integer. (default: 5)**
- *window_size*: This parameter sets the size of the Hanning-window used during baseline approximation when baseline_mode is set to 'window_filter'. The value of 'window_size' is multiplied with the length (e.g. number of data-points) of the spectrum. If the spectrum is 1024 data-points long the Hanning-window will be of length 205, if 'window_size' is set to 0.2. Large values lead to more linear baselines. **The value must be a float. (default: 0.2)**
- *alpha*: During curve-fitting, this parameter controls the width of the normal distribution from which the value is chosen that is added or subtracted from a randomly chosen pseudo-Voigt function parameter. A 'alpha' close to 1 results in small value and thus, chances are higher to find a valid change in parameters, e.g. the time spent in the mutation-loop increases (see Lünsdorf & Lünsdorf 2016 for details). An 'alpha' close to zero leads to a larger value added or subtracted from a randomly chosen pseudo-Voigt function parameter and thus, the duration in the mutation-loop is shorter. **The value must be a float. (default: 0.985)**
- *sigma_threshold*: This parameter controls the duration of the mutation-loop more directly. Legit values for 'sigma_threshold' are from the interval $2 > \sigma_threshold > 0$. Values close to 2 result in short and values close to 0 in long mutation-loop duration. **The value must be a float. (default: 0.01)**
- *noise_intensity*: This parameter is a multiple of the standard deviation of the estimated noise distribution. **The value must be a float. (default: 2)**
- *max_peak_number*: This parameter sets the maximum number of pseudo-Voigt functions allowed during curve-fitting, e.g. if this number is reached the program stops. **The value must be an integer. (default: 100)**

[Readout_type]

- *Cm_readout*: If set to 'yes' the curve-fit results ('.npz'-files) are interpreted for carbonaceous material, e.g. STA-values according to Lünsdorf & Lünsdorf (2016) among other are computed

and saved to '.fit'-files (see section 1.3). These are needed for later temperature estimation. **The value must be a string. Options: 'yes' or 'no' (default: yes)**

- *Peak_parameters*: If set to 'yes' only the parameters of the fitted pseudo-Voigt functions are saved in the 'ifors_peaks.fit'-file. This mode is used for spectra other than carbonaceous material. **The value must be a string. Options: 'yes' or 'no' (default: no)**
- *Fitted_values*: If set to 'yes' all pseudo-Voigt function, baseline and intensity values are saved together with their respective wavenumbers in the 'ifors_fitted_values.fit'-file. **The value must be a string. Options: 'yes' or 'no' (default: no)**

[Readout_opts]

- *mineral_phases*: This parameter controls whether the curve-fit results should be corrected for Raman bands of mineral phases. Applies only to results acquired with the 'Readout_type' 'Cm_readout'. **The value must be a string. Options: 'yes' or 'no' (default: no)**
- *plot_results*: This parameter controls if the curve-fit results should be plotted or not. If set to 'yes' a '.png'- and '.pdf'- file of the curve-fits is saved. **The value must be a string. Options: 'yes' or 'no' (default: yes)**
- *print_mode*: This parameter applies to the 'Readout_types' 'Cm_readout' and 'Peak_parameters'. If set to 'line' all pV-function parameters of an evaluation are written in one line in the corresponding '.fit'-file. If set to 'block' the parameters of each pV-function are written line by line, i.e. one set of pV-function parameters per line. **The value must be a string. Options: 'line' or 'block' (default: block)**
- *STA_range_start*: This parameter defines the start value of the wavenumber interval from which the STA values are computed. **The value must be an integer. (default: 1000)**
- *STA_range_stop*: This parameter defines the stop value of the wavenumber interval from which the STA values are computed. **The value must be an integer. (default: 1800)**

[Ignored_peak_ranges]

- This section contains intervals of Raman shift values between which 'Non-CM'-Raman bands (for instance of transparent minerals like quartz, calcite, dolomite, plagioclase) are present. If the 'Readout_opts' 'mineral_phases' is set to 'yes' any pseudo-Voigt function is excluded from further evaluation during readout if it has a center value coinciding with any of the values from the intervals. The start and stop values of the ranges/intervals can be modified by the user. The number of ranges/intervals can also be modified by the user by extending the section. **The start and stop values must be integers (default: 0, 0). The range name must be a string (default: range_1, range_2, etc.) avoid spacebars.**

[Estimate_temp]

- *pl* = This parameter sets the confidence level of the confidence interval. **The value must be a float. (default: 0.95)**

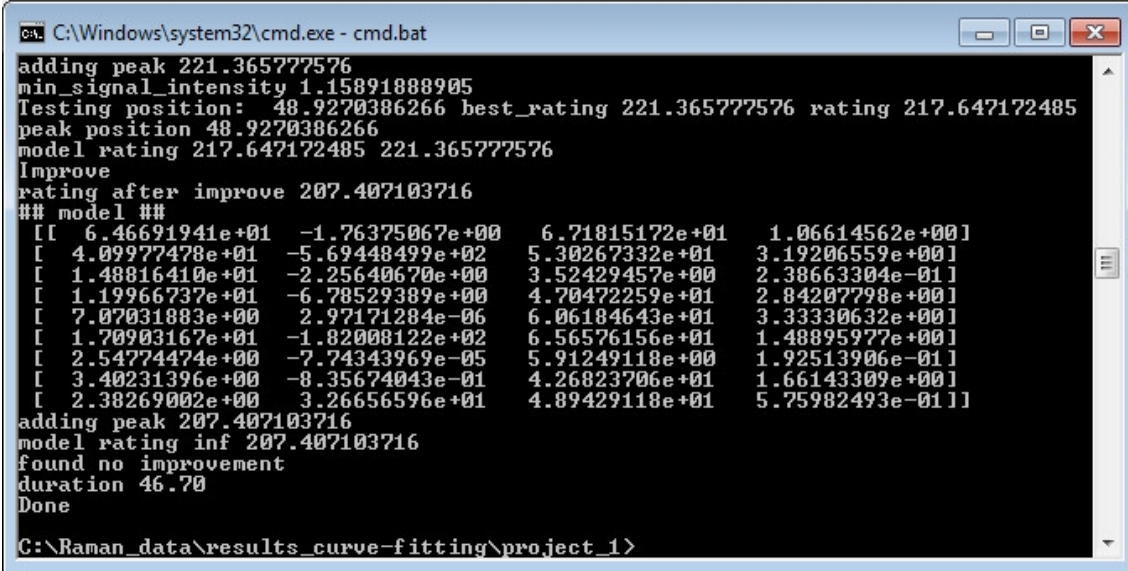
- *p2* = This parameter sets the confidence level of the prediction interval. **The value must be a float. (default: 0.9)**
- *model*: This parameter determines the model used during orthogonal distance regression. If set to '*cubic*' a third order polynomial is used if set to '*linear*' a linear function is used. **The value must be a string. Options: 'cubic' or 'linear'. (default: cubic)**
- *plot*: If set to 'yes' a plot of the reference data (metamorphic temperature vs. STA) together with the orthogonal distance regression line, confidence and prediction interval is shown. **The value must be a string. Options: 'yes' or 'no' (default: yes)**

1.3 Generating Output

The purpose of the live-view curve-fit mode is to quickly check different curve-fit behavior when parameters in the config_file are changed, e.g. control and constraint parameters. This is necessary, because no universal set of constraint/control parameter values exists. The config_file allows you to define control/constraint parameter value sets for different spectra. You are supposed to copy the 'ifors_default_config.cfg'-file, change its name according to your project (e.g. 'ifors_project_1_config.cfg') and to save it in the 'ifors_aux'-folder.

When you have found a satisfying set of control/constraint values, you will have to start the 'ifors_run' command:

- Open the 'ifors_default_config.cfg'-file with notepad++
- In the [Control]-section change the parameter 'Gui' from 'yes' to 'no'
- In the [Control]-section change the parameter 'Cli' from 'no' to 'yes'
- Save the 'ifors_default_config.cfg'-file as 'ifors_project_1_config.cfg' in the 'ifors_aux' folder
- In the command prompt navigate to the folder in which you want to save the results of the curve-fit, in this example C:\Raman_data\results_curve-fitting\project_1. (Follow the steps in section 1.1)
- Once you are in the correct folder, type in the command prompt and press enter (Figure 3):
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o cf [...]`
`-f c:\Raman_data\spectra\project1\KL2-19_2.txt`



```
C:\Windows\system32\cmd.exe - cmd.bat
adding peak 221.365777576
min_signal_intensity 1.15891888905
Testing position: 48.9270386266 best_rating 221.365777576 rating 217.647172485
peak position 48.9270386266
model rating 217.647172485 221.365777576
Improve
rating after improve 207.407103716
## model ##
[[ 6.46691941e+01 -1.76375067e+00 6.71815172e+01 1.06614562e+00]
[ 4.09977478e+01 -5.69448499e+02 5.30267332e+01 3.19206559e+00]
[ 1.48816410e+01 -2.25640670e+00 3.52429457e+00 2.38663304e-01]
[ 1.19966737e+01 -6.78529389e+00 4.70472259e+01 2.84207798e+00]
[ 7.07031883e+00 2.97171284e-06 6.06184643e+01 3.33330632e+00]
[ 1.70903167e+01 -1.82008122e+02 6.56576156e+01 1.48895977e+00]
[ 2.54774474e+00 -7.74343969e-05 5.91249118e+00 1.92513906e-01]
[ 3.40231396e+00 -8.35674043e-01 4.26823706e+01 1.66143309e+00]
[ 2.38269002e+00 3.26656596e+01 4.89429118e+01 5.75982493e-01]]
adding peak 207.407103716
model rating inf 207.407103716
found no improvement
duration 46.70
Done
C:\Raman_data\results_curve-fitting\project_1>
```

Figure 8: The command prompt window after curve-fitting finished with the 'Control'-parameter 'Cli' activated.

- When the curve-fitting process is completed, the duration is reported and you can again execute commands in command prompt window (Figure 8).
- When finished, three files are saved in the 'results_curve_fitting\project_1' folder which have the name of the spectrum-file added with the prefix 'fit_'. In this case the three files are 'fit_KL2-19_2.npz', 'fit_KL2-19_2.pdf' and 'fit_KL2-19_2.png'.

- The npz-file contains all curve-fitting results, i.e. optimized pseudo-Voigt function parameters, baseline values, and the spectrum itself.
- The pdf-file shows the plot of the spectrum with the optimized pseudo-Voigt functions, the baseline, etc. and can be modified in any vector-graphic program (e.g. Inkscape or Adobe Illustrator).
- The png-file shows the same as the pdf but can be modified in any pixel-graphic program (e.g. Gimp or Adobe Photoshop).

1.4 Fitting multiple spectra

If you want to apply curve-fitting for several spectra, you have to move all your spectrum-files into the same folder (here *Raman_data\spectra\project_1*) and proceed as outlined in section 1.3:

- Once you are in the folder where you want your results to be stored (here *Raman_data\results_curve-fitting\project_1*), type in the command prompt and press enter:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o cf [...] -f c:\Raman_data\spectra\project1*.txt`
 - '*.txt' passes a list of all txt-files present in the indicated directory to the 'ifors_run' command.
- For each spectrum-file a pdf-, npz- and png-file is created (see section 1.3)
- You can quickly evaluate the quality of your curve-fits by browsing through the curve-fit plots in the png files.

2. Working with the curve-fit results

The results of a curve-fit done by IFORS are stored in the npz-file (see section 1.3 & 1.4). The following steps concern the results of Raman spectra of carbonaceous material (CM).

2.1 Structuring your output

To keep your 'project' folders clearly arranged it is suggested:

- Inside the 'project_1' folder create a folder for the npz-files and a folder for the plots, i.e. '*results_curve-fitting\project_1\npzs*' and '*results_curve-fitting\project_1\plots*'
- Move the npz-, pdf- and png-files in their respective folder.

2.2 Extracting the results from the npz-files

- In the command prompt window, navigate to the 'project_1' folder.
- In the command prompt window type and press enter:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o ro [...] -f npzs\fit_KL2-19_2.npz`

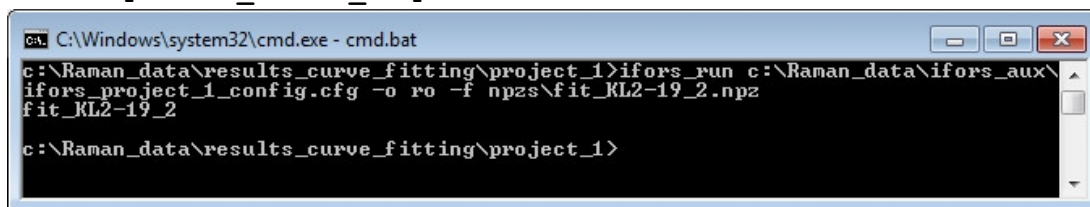


Figure 9: Invoking the 'ifors_run'-command with the 'ro' option.

- Notice that you have to change the option '*cf*' of the '*ifors_run*'-command to '*ro*' for readout. In this mode the '*ifors_run*'-command will generate three files in the '*project_1*' folder, i.e. '*ifors_peaks.fit*', '*ifors_all_data.fit*' and '*ifors_averaged_data.fit*'. These files are **space-delimited txt-files** and can be imported into LibreOffice 5 Calc, Microsoft Excel or any other spreadsheet calculator.

In the following section we will examine the contents and structure of the generated '.fit' files.

2.3 Contents of the '*ifors_peaks.fit*' file

To open any of the '.fit' files in Excel, set Excel to show all files in the open-file-dialog and select the '.fit' file, in this case '*ifors_peaks.fit*'. In the 'Textconverter-wizard' select the delimited option, hit next and in the following step select space as delimiter and hit 'done'.

	A	B	C	D	E	F	G
1	sample	scaled_intensity	shape	area	hwhm_[cm ⁻¹]	center_[cm ⁻¹]	
2	fit_KL2-19_2_eval_1_func_1	14.882	0.693	92.114	4.296	463.734	
3	fit_KL2-19_2_eval_1_func_2	2.548	0	9.732	3.465	506.223	
4	fit_KL2-19_2_eval_1_func_3	3.402	0.455	134.82	29.906	1168.67	
5	fit_KL2-19_2_eval_1_func_4	11.997	0.872	925.444	51.157	1245.923	
6	fit_KL2-19_2_eval_1_func_5	2.383	0.97	39.513	10.368	1280.687	
7	fit_KL2-19_2_eval_1_func_6	40.998	0.998	3673.94	57.457	1354.077	
8	fit_KL2-19_2_eval_1_func_7	7.07	0	467.62	60	1491.202	
9	fit_KL2-19_2_eval_1_func_8	17.09	0.995	728.213	26.801	1581.974	
10	fit_KL2-19_2_eval_1_func_9	64.669	0.638	1763.492	19.191	1609.013	
11							
12	fit_KL2-19_2_eval_2_func_1	14.657	0.479	86.85	4.436	463.734	
13	fit_KL2-19_2_eval_2_func_2	1.803	0	4.918	2.475	479.185	
14	fit_KL2-19_2_eval_2_func_3	2.566	0	9.986	3.53	506.223	
15	fit_KL2-19_2_eval_2_func_4	3.525	0.362	141.413	31.37	1170.601	
16	fit_KL2-19_2_eval_2_func_5	11.873	0.952	883.905	48.071	1245.923	
17	fit_KL2-19_2_eval_2_func_6	2.491	0	37.054	13.494	1280.687	
18	fit_KL2-19_2_eval_2_func_7	41.423	0.999	3765.75	58.316	1354.077	
19	fit_KL2-19_2_eval_2_func_8	7.11	0	470.282	60	1491.202	
20	fit_KL2-19_2_eval_2_func_9	18.602	0.997	793.087	26.797	1583.906	
21	fit_KL2-19_2_eval_2_func_10	63.079	0.747	1721.837	18.492	1609.013	
22	fit_KL2-19_2_eval_2_func_11	3.854	0	16.911	3.98	1622.532	
23							
24	fit_KL2-19_2_eval_3_func_1	14.876	0.691	92.101	4.3	463.734	
25	fit_KL2-19_2_eval_3_func_2	2.547	0	9.734	3.467	506.223	
26	fit_KL2-19_2_eval_3_func_3	3.137	0.106	107.853	29.786	1168.67	
27	fit_KL2-19_2_eval_3_func_4	12.292	0.981	994.475	51.928	1247.854	
28	fit_KL2-19_2_eval_3_func_5	2.407	0.986	39.739	10.269	1280.687	
29	fit_KL2-19_2_eval_3_func_6	40.763	0.998	3642.424	57.284	1354.077	
30	fit_KL2-19_2_eval_3_func_7	7.06	0	466.943	60	1491.202	
31	fit_KL2-19_2_eval_3_func_8	17.376	0.994	745.298	26.985	1581.974	
32	fit_KL2-19_2_eval_3_func_9	64.371	0.639	1749.215	19.118	1609.013	
33							

Figure 10: The content of the '*ifors_peaks.fit*' file after importing into Excel.

Figure 10 shows the content of the '*ifors_peaks.fit*' file after successfully importing into Excel. Each line below the header contains the parameters of a pseudo-Voigt function, i.e. the scaled intensity, shape (Gauss/Lorentz ratio), area, half width at half maximum in cm⁻¹ and the center value, also in cm⁻¹. In this case on spectrum-file (KL2-19_2) has been evaluated three times ('*repetition*' parameter is set to be 3 by default (section 1.2)). Thus, all functions with the same eval-number (Figure 10) belong to the same evaluation. Within each evaluation-block the functions are sorted by ascending center-value.

2.4 Contents of the '*ifors_all_data.fit*' file

To open the '*ifors_all_data.fit*' file with Excel proceed in the same way as in section 2.3. Figure 11 shows the contents of '*ifors_all_data.fit*' after opening it in Excel.

	A	B	C	D	E	F	G
1	sample	D_STA	G_STA	G_shape_factor	Dmax_pos	Gmax_pos	Dmax/Gmax-ratio
2	fit_KL2-19_2_eval_1	210.934	122.787	0.789	1354.077	1607.082	0.582
3	fit_KL2-19_2_eval_2	211.006	122.722	0.79	1354.077	1607.082	0.582
4	fit_KL2-19_2_eval_3	211.062	122.723	0.789	1354.077	1607.082	0.582
5							

Figure 11: Contents of the 'ifors_all_data.fit' file.

In this file the results, in terms of D_STA, G_STA, G_shape_factor, Dmax_pos, Gmax_pos and the Dmax/Gmax -ratio, are shown for each evaluation (**i.e. one line equals one evaluation**). For details on the STA- values and the G_shape_factor see Lünsdorf (2016), Lünsdorf & Lünsdorf (2016) and Lünsdorf et al. (2017).

2.5 Contents of the 'ifors_averaged_data.fit' file

This file is used later for the temperature estimation, see section 3. To open the 'ifors_averaged_data.fit' file proceed in the same way as in section 2.3. Figure 12 shows the contents of the 'ifors_averaged_data.fit' after opening it in Excel.

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	sample	D_STA(mean)	std	G_STA(mean)	std	G_shape_factor(mean)	std	Dmax_pos(mean)	std	Gmax_pos(mean)	std	Dmax/Gmax-ratio(mean)	std
2	fit_KL2-19_2	211	0.052	122.744	0.03	0.789	0	1354.077	0	1607.082	0	0.582	0
3													

Figure 12: Contents of the 'ifors_averaged_data.fit' file after opening it in Excel.

The 'ifors_averaged_data.fit' contains essentially the same data as the 'ifors_all_data.fit' file, but here the data of each evaluation, which is given in 'ifors_all_data.fit', is averaged in the 'ifors_averaged_data.fit' file and the mean values with their associated standard deviation are reported. Thus, each line in this file represents the averaged evaluation results of one spectrum-file.

2.6 Extracting results from non-CM samples

If you recorded, for instance, a mineral Raman spectrum and you are only interested in the pseudo-Voigt function parameters, you have to proceed as in section 2.2.

- Open the 'ifors_project_1_config.cfg'-file, or your own config-file, with notepad++
- In the [Readout_type]-section change the parameter 'Cm_readout' from 'yes' to 'no'
- In the [Readout_type]-section change the parameter 'Peak_parameters' from 'no' to 'yes'
- Save the 'ifors_project_1_config.cfg'-file
- In the command prompt window, navigate to the 'project_1' folder and type:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o ro [...] -f npzs\fit_KL2-19_2.npz`
- This will start the 'ifors_run'-command and only the 'ifors_peaks.fit' file will be generated.

2.7 Extracting the results from multiple curve-fits

If you have curve-fits (i.e. npz-files) of multiple spectrum-files, you can extract the results of each curve-fit from the respective npz-file (in this case we are only interested in the function parameters).

- In the command prompt window, navigate to the 'project_1' folder and type:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o ro [...] -f npzs*.npz`
- In the command prompt the name of each npz-file, that the 'ifors_run'-command is working on, is displayed; here KL2-19_2 and KL2-8_HS_1_ics.txt (Figure 13).

```

C:\Windows\system32\cmd.exe - cmd.bat

c:\Raman_data\results_curve_fitting\project_1>ifors_run c:\Raman_data\ifors_aux\
ifors_project_1_config.cfg -o ro -f npzs\*.npz
fit_KL2-19_2
fit_KL2-8HS_1_ics

c:\Raman_data\results_curve_fitting\project_1>

```

Figure 13: Starting the 'ifors_readout.py', using the '-Peak_parameters' option, for multiple npz-files.

- Open the saved 'ifors_peaks.fit' file in Excel and each pseudo-Voigt function parameter of each evaluation for the KL2-19_2 and KL2-8HS_1_ics spectrum-files is presented (Figure 14).

	A	B	C	D	E	F	G
1	sample	scaled_intensity	shape	area	hwhm_[cm-1]	center_[cm-1]	
2	fit_KL2-19_2_eval_1_func_1	14.882	0.693	92.114	4.296	463.734	
3	fit_KL2-19_2_eval_1_func_2	2.548	0	9.732	3.465	506.223	
4	fit_KL2-19_2_eval_1_func_3	3.402	0.455	134.82	29.906	1168.67	
5	fit_KL2-19_2_eval_1_func_4	11.997	0.872	925.444	51.157	1245.923	
6	fit_KL2-19_2_eval_1_func_5	2.383	0.97	39.513	10.368	1280.687	
7	fit_KL2-19_2_eval_1_func_6	40.998	0.998	3673.94	57.457	1354.077	
8	fit_KL2-19_2_eval_1_func_7	7.07	0	467.62	60	1491.202	
9	fit_KL2-19_2_eval_1_func_8	17.09	0.995	728.213	26.801	1581.974	
10	fit_KL2-19_2_eval_1_func_9	64.669	0.638	1763.492	19.191	1609.013	
11							
12	fit_KL2-8HS_1_ics_eval_1_func_1	0.956	0	31.004	38.905	423.287	
13	fit_KL2-8HS_1_ics_eval_1_func_2	1.118	0.996	68.24	40.297	628.988	
14	fit_KL2-8HS_1_ics_eval_1_func_3	1.165	0	16.952	13.26	1156.824	
15	fit_KL2-8HS_1_ics_eval_1_func_4	6.793	0.995	630.055	60	1203.397	
16	fit_KL2-8HS_1_ics_eval_1_func_5	13.721	0.887	1232.62	59.999	1315.951	
17	fit_KL2-8HS_1_ics_eval_1_func_6	79.774	0.999	4246.876	33.734	1358.643	
18	fit_KL2-8HS_1_ics_eval_1_func_7	8.46	0.719	653.924	54.315	1494.483	
19	fit_KL2-8HS_1_ics_eval_1_func_8	14.165	0.166	681.067	40.934	1574.047	
20	fit_KL2-8HS_1_ics_eval_1_func_9	1.671	0	7.546	4.116	1593.453	
21	fit_KL2-8HS_1_ics_eval_1_func_10	69.401	0.475	2081.097	22.546	1605.096	
22	fit_KL2-8HS_1_ics_eval_1_func_11	6.315	0	46.649	6.733	1620.621	
23							
24							
25							

Figure 14: Content of the 'ifors_peaks.fit' file generated from multiple npz-files. Only one evaluation was performed for this example.

- The same procedure is valid if you activate the other 'Readout_type' parameters. Note, it is advised to only have on 'Readout_type' active at one time.

2.8 Extracting the spectrum data, fitted function values and baseline values

If you want to work with the values of the fitted pseudo-Voigt functions, baseline values or Raman intensity values (for instance plotting in Excel or alike), you can extract these values from the npz-file. To do this, open the 'ifors_default_config.cfg'-file and change the 'Readout_type' parameter 'Fitted_values' to 'yes'.

- In the command prompt window, navigate to the '*project_1*' folder and type:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o ro [...] -f npzs\fit_KL2-19_2.npz`
- This will generate a new file named '*ifors_fitted_values_fit_KL2-19_2.fit*'
- The first column in this file contains the Raman shift values of the spectrum, followed by the scaled Raman intensity, baseline values of the first evaluation (eval_1_bl), values of function one of evaluation one (eval_1_f1), values of function two of evaluation one (eval_1_f2), and so forth (Fig. 15).
- To extract these data from multiple npz-files type in the command prompt window:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o ro [...] -f npzs*.npz`
- For each npz-file present in the '*project_1\npzs*' folder a '*ifors_fitted_values_filename.fit*' file will be created for further use.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Raman_shift [cm-1]	Intensity [a.u.]	eval_1_bl	eval_1_f1	eval_1_f2	eval_1_f3	eval_1_f4	eval_1_f5	eval_1_f6	eval_1_f7	eval_1_f8	eval_1_f9	eval_2_bl	eval_2_f1
2	400	21.7799	21.1461	0.0471	0	0.0023	0.038	0.0003	0.1478	0	0.0087	0.0104	21.1473	0.0342
3	401.9313	21.3883	21.1435	0.0501	0	0.0024	0.0382	0.0003	0.1484	0	0.0088	0.0104	21.1445	0.0363
4	403.8627	21.2159	21.1409	0.0533	0	0.0024	0.0384	0.0003	0.149	0	0.0088	0.0105	21.1418	0.0387
5	405.794	21.2597	21.1383	0.057	0	0.0024	0.0385	0.0003	0.1496	0	0.0088	0.0105	21.139	0.0414
6	407.7253	20.7286	21.1357	0.061	0	0.0024	0.0387	0.0003	0.1502	0	0.0089	0.0105	21.1363	0.0443
7	409.6567	20.3438	21.1332	0.0654	0	0.0024	0.0389	0.0003	0.1508	0	0.0089	0.0106	21.1337	0.0475
8	411.588	21.0614	21.1307	0.0703	0	0.0024	0.0391	0.0003	0.1514	0	0.0089	0.0106	21.131	0.051
9	413.5193	21.0689	21.1283	0.0758	0	0.0024	0.0393	0.0003	0.152	0	0.0089	0.0106	21.1284	0.055
10	415.4506	21.1424	21.1258	0.082	0	0.0024	0.0394	0.0003	0.1527	0	0.009	0.0107	21.1258	0.0595
11	417.382	21.0438	21.1234	0.0889	0	0.0025	0.0396	0.0003	0.1533	0	0.009	0.0107	21.1233	0.0646
12	419.3133	21.4987	21.1211	0.0968	0	0.0025	0.0398	0.0003	0.1539	0	0.009	0.0107	21.1207	0.0703
13	421.2446	20.9718	21.1188	0.1058	0	0.0025	0.04	0.0003	0.1545	0	0.0091	0.0108	21.1183	0.0768
14	423.176	20.7931	21.1165	0.1161	0	0.0025	0.0402	0.0003	0.1552	0	0.0091	0.0108	21.1158	0.0843
15	425.1073	20.621	21.1142	0.1279	0	0.0025	0.0404	0.0003	0.1558	0	0.0091	0.0108	21.1134	0.0929
16	427.0386	20.8376	21.112	0.1417	0	0.0025	0.0406	0.0003	0.1565	0	0.0092	0.0109	21.111	0.1028
17	428.97	21.102	21.1098	0.1577	0	0.0025	0.0407	0.0003	0.1571	0	0.0092	0.0109	21.1087	0.1145
18	430.9013	20.9518	21.1077	0.1767	0	0.0025	0.0409	0.0003	0.1578	0	0.0092	0.0109	21.1064	0.1283
19	432.8326	20.5048	21.1056	0.1992	0	0.0026	0.0411	0.0003	0.1584	0	0.0092	0.011	21.1042	0.1446
20	434.7639	19.922	21.1036	0.2264	0	0.0026	0.0413	0.0003	0.1591	0	0.0093	0.011	21.102	0.1643
21	436.6953	21.0608	21.1016	0.2594	0	0.0026	0.0415	0.0003	0.1598	0	0.0093	0.0111	21.0998	0.1882
22	438.6266	21.2115	21.0996	0.3002	0	0.0026	0.0417	0.0004	0.1604	0	0.0093	0.0111	21.0977	0.2178
23	440.5579	20.9198	21.0977	0.3512	0	0.0026	0.0419	0.0004	0.1611	0	0.0094	0.0111	21.0957	0.2547
24	442.4893	21.3679	21.0958	0.4162	0	0.0026	0.0421	0.0004	0.1618	0	0.0094	0.0112	21.0936	0.3018
25	444.4206	21.2084	21.094	0.5007	0	0.0026	0.0423	0.0004	0.1625	0	0.0094	0.0112	21.0917	0.363
26	446.3519	21.5351	21.0922	0.6132	0	0.0027	0.0425	0.0004	0.1632	0	0.0095	0.0112	21.0897	0.4446
27	448.2833	22.4671	21.0905	0.7679	0	0.0027	0.0427	0.0004	0.1639	0	0.0095	0.0113	21.0878	0.5578
28	450.2146	22.6415	21.0888	0.9909	0	0.0027	0.0429	0.0004	0.1646	0	0.0095	0.0113	21.086	0.7286
29	452.1459	22.0768	21.0872	1.3419	0	0.0027	0.0431	0.0004	0.1653	0	0.0096	0.0113	21.0842	1.0286
30	454.0773	22.4703	21.0856	1.9644	0	0.0027	0.0434	0.0004	0.166	0	0.0096	0.0114	21.0825	1.646
31	456.0086	24.2821	21.084	3.1593	0	0.0027	0.0436	0.0004	0.1667	0	0.0096	0.0114	21.0808	2.9584
32	457.9399	26.746	21.0825	5.3783	0	0.0027	0.0438	0.0004	0.1674	0	0.0097	0.0115	21.0791	5.437

Figure 15: Contents of the '*ifors_fitted_values_fit_KL2-19_2.fit*' file.

3. Estimating peak-metamorphic temperature from computed STA-values

To estimate the peak-metamorphic temperature from the STA-value of a sample with unknown temperature, you have to prepare first a calibration line.

In order to do this you will need to measure the reference samples described in Lünsdorf et al. (2017). The samples are available (email to: kluensd@gwdg.de) and of course, you can extend this reference sample set with your own samples of known temperature.

As an example, the data of the reference sample series described in Lünsdorf et al. (2017), is provided in the 'reference_series_data.xls' file (Figure 16).

	A	B	C	D	E	F	G	H	I	J
1	Reference sample	Peak temperature [°C]	uncertainty	D_STA	std	G_STA	std	G_shape_factor	std	n
2	KL14_5A	162	30	240.980	5.359	135.033	3.091	0.939	0.020	28
3	KL14_7	178	30	230.192	13.727	132.535	8.991	0.873	0.052	25
4	KL14_21	228	30	222.967	10.846	120.875	4.577	0.907	0.035	20
5	KL14_16	236	30	216.891	7.176	114.694	3.003	0.885	0.030	30
6	KL16_31	236	30	196.782	10.704	105.918	3.232	0.798	0.026	30
7	KL16_35	240	30	204.389	6.775	110.206	2.428	0.827	0.022	30
8	KL14_17	256	30	177.202	4.112	100.581	2.278	0.775	0.025	30
9	KL16_43B	260	30	180.670	6.683	102.574	3.845	0.813	0.036	30
10	KL14_13A	267	30	172.870	5.614	100.324	2.736	0.756	0.028	30
11	KL14_1A	295	25	132.480	3.829	127.790	3.461	1.095	0.098	30
12	KL14_19	299	23	162.090	2.714	123.994	3.095	1.041	0.076	27
13	KL16_8B	325	25	106.257	9.164	138.379	6.983	0.986	0.073	20
14	KL16_19B	350	25	87.449	4.733	149.956	3.990	1.323	0.088	15
15	KL14_58B	370	50	79.448	2.595	123.739	8.477	1.803	0.079	15
16	KL16_10B	375	35	74.857	2.395	139.442	4.431	1.621	0.073	20
17	KL16_11B	375	35	78.804	4.436	138.261	7.907	1.584	0.087	20
18	KL16_14	415	35	89.819	6.961	68.405	7.460	3.257	0.283	21
19	KL14_59	420	50	78.586	9.158	71.535	7.313	3.318	0.307	20
20	KL16_29	420	30	85.178	8.944	56.125	5.954	4.083	0.395	15
21	KL16_27	440	30	110.581	27.634	37.726	5.366	6.682	1.005	20
22	KL14_56B	450	30	101.475	17.806	42.078	4.199	5.874	0.594	20
23	KL16_23	480	40	132.136	18.813	30.821	2.518	8.078	0.710	20
24	KL16_15	490	40	94.610	11.034	38.774	4.656	5.872	0.711	19
25	KL16_16B	490	40	151.970	29.045	28.526	3.985	7.696	1.144	10
26	KL14_52	520	25	158.510	54.119	28.069	3.161	9.208	1.308	20
27	KL14_49C	610	50	199.934	69.140	21.506	2.366	11.698	1.618	20

Figure 16: Temperature values and the associated STA-values of the reference series samples.

3.1 Creating the calibration line

- Measure the reference samples and evaluate the recorded spectrum-files using the 'ifors_run'-command with the 'Cli' control parameter activated in the config_file and extract the results from the generated npz-files with the 'ifors_run'-command using the 'ro' option (section 1.3, 2.2 & 2.5).

- Open the 'reference_series_data.xls' file in Excel or LibreOffice Calc and insert your D_STA, G_STA and G_shape_factor (Figure 16). NB: remember to use the correct excitation wavelength.
- Save the updated 'reference_series_data.xls' file and save it also as a 'tab-delimited.txt' file in the 'Raman_data\reference_data' folder.
- In the command prompt navigate to your 'Raman_data\results_curve-fitting\project_1' folder.
- To create only the calibration line from the reference data, type in the command prompt and press enter:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o et [...] -rd c:\Raman_data\reference_data\reference_series_data_488.txt`
 - If the '[Estimate_temp]'-parameter 'plot' in the config_file is set to 'yes' a plot of the reference data (Temperature vs. STA) is shown (Figure 17).
 - Perform a temperature point estimate (*optional*).
 - If you answer with no, the script will stop, if you answer with yes, you must enter a STA value (the range of possible STA values can be seen in the plot-window) and the estimated temperature will be printed in the command prompt window (Figure 19).
 - A txt-file 'calib_curve_coefs.txt' will be stored in your 'results_curve-fitting\project_1' folder. In the case of a 'linear' model (see section 1.2), the slope and intercept of the regression line and their respective standard errors are saved, in the case of 'cubic' model the coefficients of the polynomial and their standard errors are saved (Figure 18).

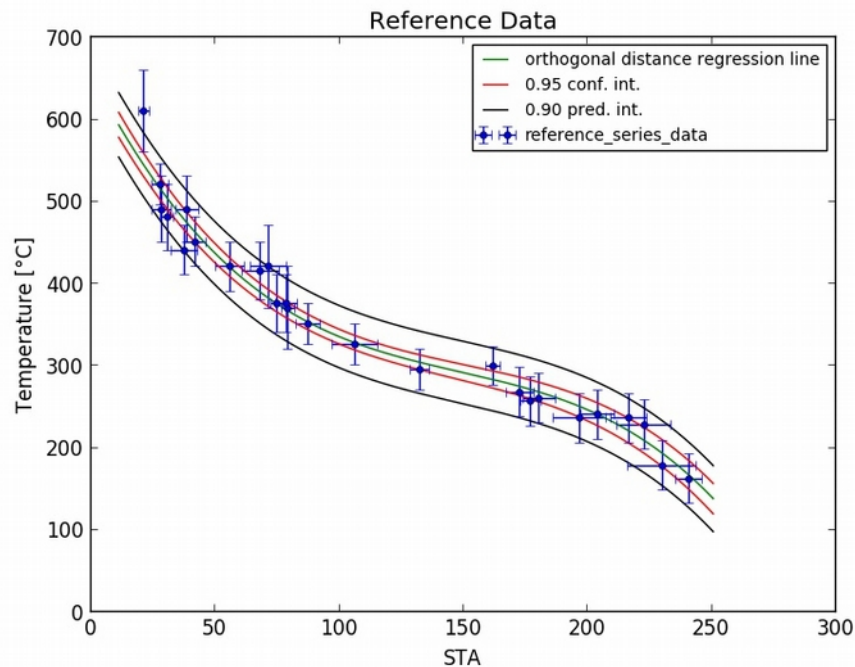


Figure 17: The calibration line (orthogonal distance regression line), reference data, confidence and prediction interval.

	A	B	C	D	E	F	G	H
1	Slope	SE	Intercept	SE				
2	-145.15	5.93	1004.57	28.09				
3								
4								

Figure 18: Contents of the 'calib_curve_coefs.txt' file for a linear model.

- If you change/extend your reference data, the 'ifors_run'-command will automatically compute a new calibration line.

```

C:\Windows\system32\cmd.exe - cmd.bat

c:\Raman_data\results_curve_fitting\project_1>ifors_run c:\Raman_data\ifors_aux\
ifors_project_1_config.cfg -o et -rd c:\Raman_data\reference_data\reference_seri
es_data_488.txt

regression coefficients:

coefficients: [ -7.90538136e-05  3.53402641e-02 -5.95832482e+00  6.56165289e
+02]
standard errors: [ 1.55474491e-05  6.15300817e-03  7.16756530e-01  2.267358
93e+01]

unweighted r2: 0.966

Do you want a temperature point estimate? (y/n): y
Type your STA value here: 200
Estimated temperature: 245.7 +- 38 (based on 0.90 pred. int.)
c:\Raman_data\results_curve_fitting\project_1>

```

Figure 19: Output of the 'ifors_estimate_temperature.py' script.

3.2 Estimating the temperature of unknown samples

You can use the 'ifors_run'-command together with the 'et' option to estimate the temperature for multiple samples. If you evaluated multiple spectrum-files and extracted the results with the 'ifors_run'-command using the 'ro' option, you can then use the 'ifors_averaged_data.fit' file with the 'ifors_run'-command and 'et' option.

- In the command prompt navigate to your 'Raman_data\results_curve-fitting\project_1' folder.
- To estimate the temperature from multiple samples, type in the command prompt:
 - `ifors_run c:\Raman_data\ifors_aux\ifors_project_1_config.cfg -o et [...] -rd c:\Raman_data\reference_data\reference_series_data_488.txt -f [...] ifors_averaged_data.fit`
 - Once the script is finished, a txt-file 'temperature_estimates.txt' is stored in the 'results_curve-fitting\project_1' folder. In this file the estimated temperatures are stored for each sample (Figure 20).

	A	B	C	D	E
1	sample	est. Temp.[°C]	uncertainty	conf_int_lvl:0.95	pred_int_lvl:0.90
2	fit_KL2-19_2	229	39		
3	fit_KL2-8HS_1_ics	307	37		

Figure 20: Contents of the 'temperature_estimates.txt' file.

References

- Lünsdorf, N. K. (2016). Raman spectroscopy of dispersed vitrinite – Methodical aspects and correlation with reflectance. *International Journal of Coal Geology*, 153, 75-86.
- Lünsdorf, N. K. and Lünsdorf, J. O. (2016). Evaluating Raman spectra of carbonaceous matter by automated, iterative curve-fitting. *International Journal of Coal Geology*, 160-161, 51-62.
- Lünsdorf, N. K., Dunkl, I., Schmidt, B. C., Rantitsch, G., von Eynatten, H. (2017). Towards a higher comparability of geothermometric data obtained by Raman spectroscopy. Part 2: A revised geothermometer. *Geostandards and Geoanalytical Research*, DOI: 10.1111/ggr.12178