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Homepage: <https://www.astrophoto.at>

Email: ms@astrophoto.at, Manfred Schwarz

User Group: <https://groups.yahoo.com/neo/groups/SbigControl/info>

Prefacing

I am working with a Shelyak LHires III spectrograph with 2400 lines/mm. Sometimes I take many images for a spectrum to get a better signal/noise ratio (S/N) and sometimes I have to monitor the lines over several hours to monitor a change of the line shapes (for example to analyse the pulsation of a star).

With my equipment, I got the experience that the wavelength can move more than 10 pixels over the night, caused by temperature shift. For that reason, I take always before and after each image of the spectrum a reference lamp image (except I will calibrate with water lines).

For that reason, I cannot add all spectra stripes before calibration without losing resolution! It would be possible if I take an alignment software to align the spectra stripes, but this take the risk, that the calibration images loose the exact position against the spectra.

For my opinion, the better way (and the way of more effort) is to calibrate all single spectra before making a sum of it. In addition, the calibration is done in a sub-pixel way with the resolution of 1/100 pixel.

My workflow is the same for each single spectra, before I start to add all spectra to get a better S/N:

- Master dark creation
- Master flat creation (depends on the used equipment)
- Dark frame subtraction of the spectrum
- Dark frame subtraction of the reference image
- Flat division of the spectrum (depends on the used equipment)
- Scan of the spectrum with rotation correction over more pixels in height if possible
- Scan of the related calibration images with exact the same parameters as before on the spectrum
- Generate an average of upper and lower background – polynomial 5th grade
- Subtract the background from the spectrum
- Fit a polynomial on the continuum and remove the continuum
- Average of the reference images before and after the spectrum
- Wavelength calibration of the reference image
- Copy the calibration data to the related spectra
- Add all calibrated spectra to get a better S/N (depends on the kind of project)
- Post processing, like crop, EW and S/N measure and/or heliocentric correction, etc.

Copyright

You are allowed to copy this program and share it free to other users! It is not allowed to sell this software!

Credits

Many thanks to my spectroscopic mentor and teacher Ernst Pollmann!
Many thanks to Roland Bücke for the algorithm of heliocentric correction!
Many thanks to Hartmut Bornemann for the FITs-IO library!

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Input file format

Input files have to be 2D images in FITs format or still scanned spectra in 1D FITs format!

Output file format and directory structure

Master dark, master flat and dark/flat corrected images are stored as “float” FITs.

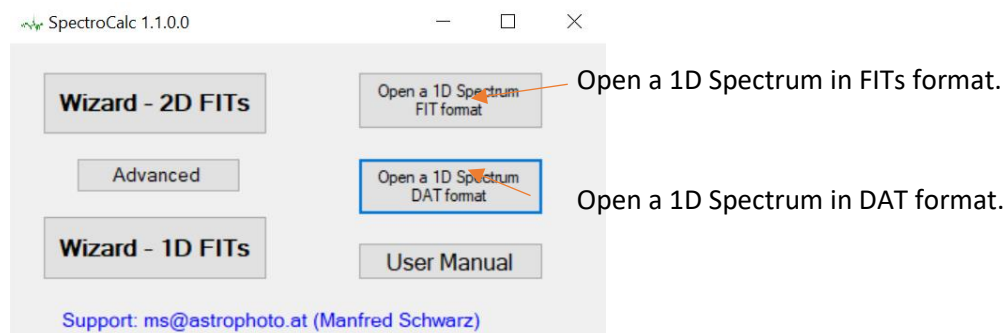
All files after scanning the spectra/calibration files are stored as 1D decimal DAT files or float FITs.

Under the directory of the spectra images, SpectroCalc creates following directory structure:

.\Spectro	Log-file and result spectrum (sum of all calibrated spectra: FIT)
.\Spectro\01_DarkFlatCorr	Master-dark, master-flat files
.\Spectro\02_Spec	dark/flat-corrected spectra
.\Spectro\03_Ref	dark/flat-corrected calibration images
----- following files are in 1D format -----	
.\Spectro\04_ScanSpec	scanned spectra (DAT & FIT)
.\Spectro\05_SkyBack	scanned and averaged sky background and polynomial of it (DAT)
.\Spectro\06_ScanSpecSkyCorr	scanned spectra - sky corrected (DAT & FIT)
.\Spectro\07_ScanRef	scanned reference images (DAT)
.\Spectro\08_Continuum	continuum polynomial (DAT)
.\Spectro\09_SpecConCorr	spectra with continuum removed (normalized contin. = 1) (DAT & FIT)
.\Spectro\10_RefCal	calibrated reference images (FIT)
.\Spectro\11_SpecCal	calibrated spectra (FIT)

All steps are stored separately to document the whole process. You are able to control if all processes have worked well.

Open 1D Spectra

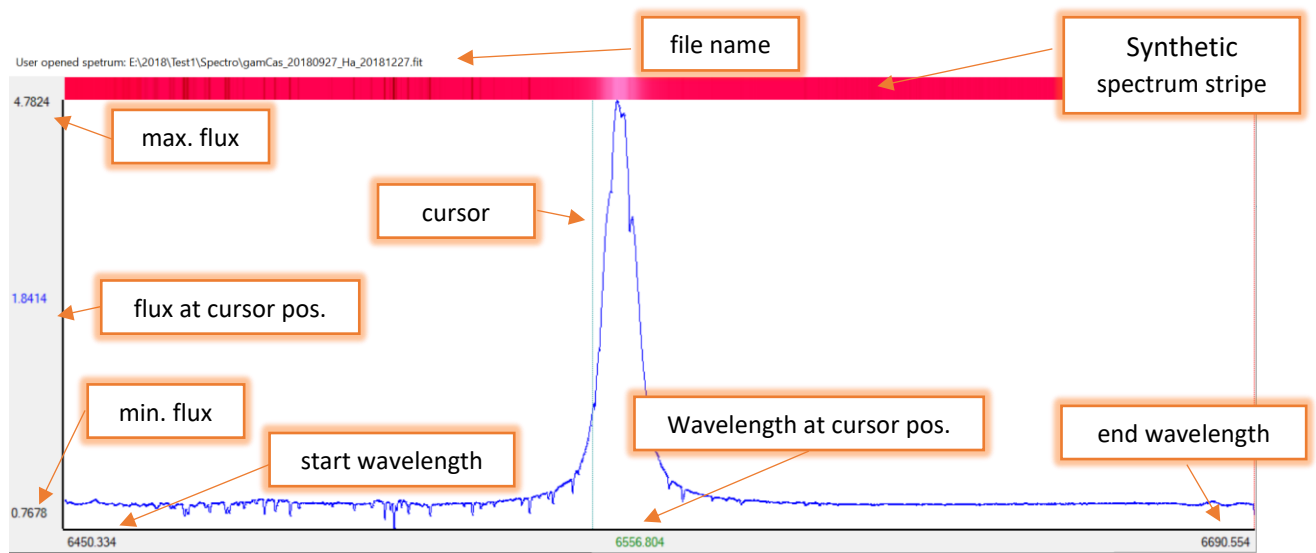


If you open a file in 1D-Fits format, you are able to process this file, like crop, measure S/N, measure EWA, etc. Look at chapter “**Post-Processing**”.

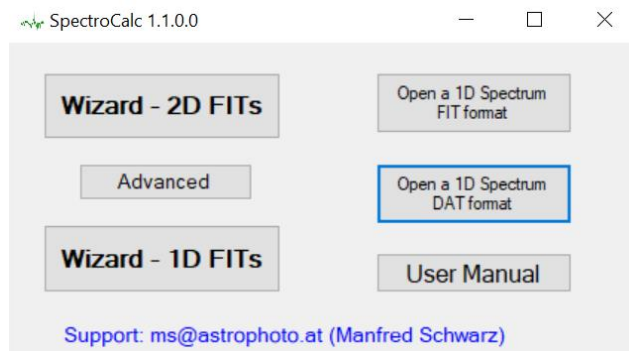
Graphical Representation of Spectra

SpectroCalc shows spectra always in the same way. It is stretched from the minimum value on the bottom line to the maximum value on the top line of the image. A turquoise line shows the current cursor position, the blue number left shows the Y value (flux) and the green number below shows the X value (wavelength) of the spectrum at the cursor position.

If there are more than one spectra in one window, you get the different Y values displayed at the right side in different colours.

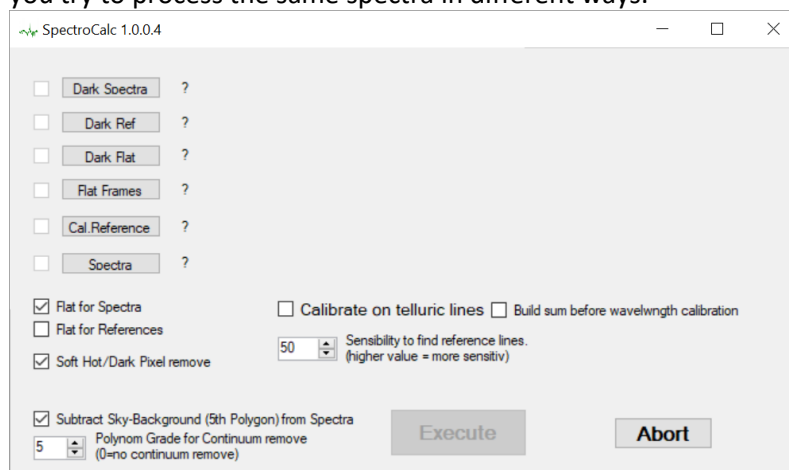


Wizard and Advanced



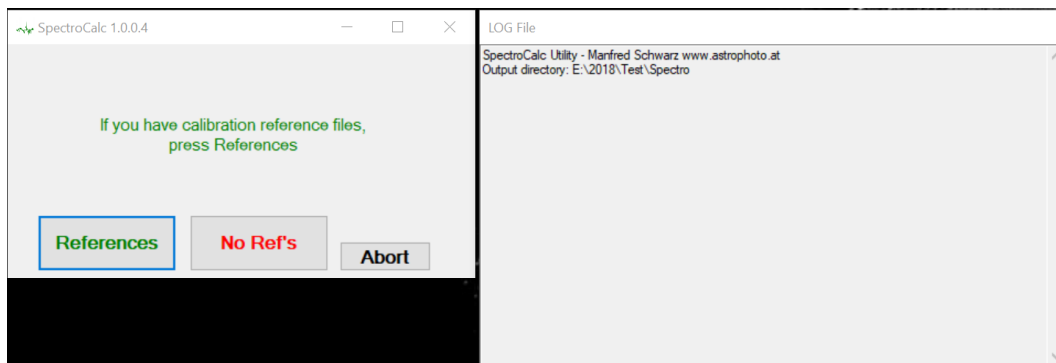
The “Wizard” button leads you step by step through the whole processing, starting by the definition of the different files for processing.

The “Advanced” button opens a configuration window where you can define the files and the parameters in advance before starting the processing. It can make sense to use the advanced feature if you try to process the same spectra in different ways.



Abort Button

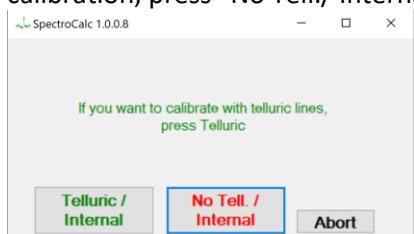
The “Abort” button bring you from each processing step back to the start window where you can start the “Wizard” or the “Advanced” function.



If you have no reference images and want to calibrate on telluric or internal lines or you don't want to calibrate, press "No Ref's".

Wizard: Select Calibration on Telluric or internal Absorption-Lines

If you have pressed "No Ref's" before, you can choose that you want to calibrate on tellurics or on known lines within the spectrum if you press "Telluric/Internal". If you don't want a wavelength calibration, press "No Tell./ Internal".

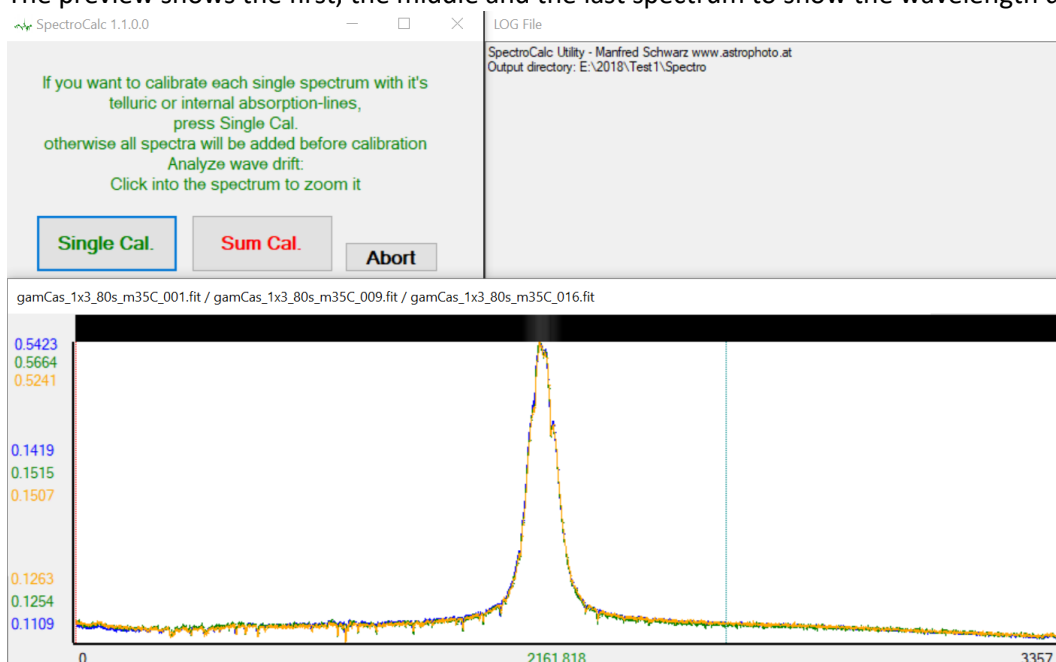


Wizard: Single or Sum of Telluric or internal Absorption-Lines

There are 2 possibilities to get a accurate result in wavelength calibration:

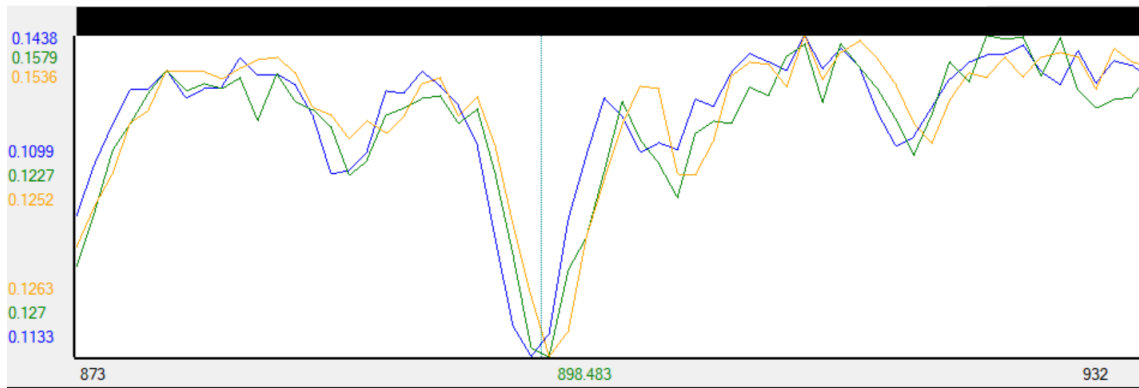
- Calibrate each single spectrum
- Align all spectra and calibrate the sum of all spectra

The preview shows the first, the middle and the last spectrum to show the wavelength drift.



Click on a telluric or calibration line into the spectrum to zoom this area.

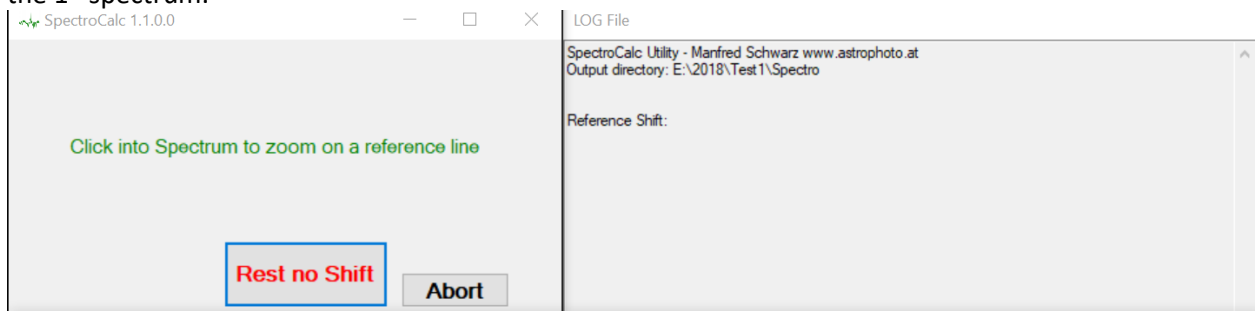
gamCas_1x3_80s_m35C_001.fit / gamCas_1x3_80s_m35C_009.fit / gamCas_1x3_80s_m35C_016.fit



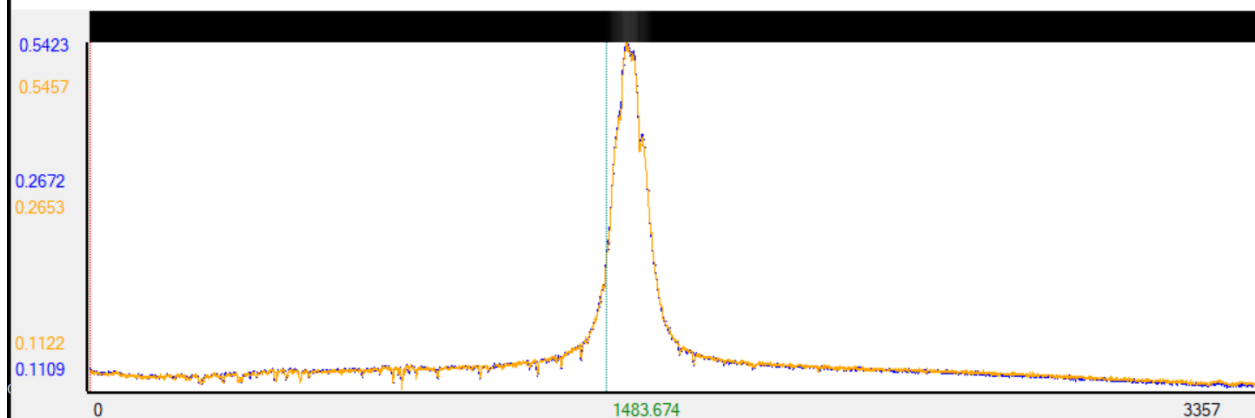
In this example, there is a small drift of about 1.5 pixel between the first (blue) and the last (orange) spectrum. I would decide to align and average the spectra before calibration because of better S/N for wavelength calibration. Another reason is, that I do not expect variations between the single exposures and I'm interested only in the averaged spectra.

Wizard: Sum of Telluric/Internal: Align the spectra

If you decided to generate a sum of all spectra before calibration, you have to align all spectra against the 1st spectrum.

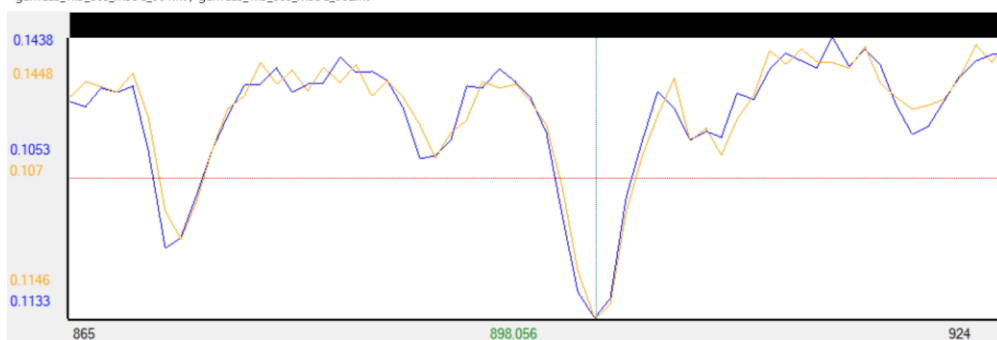


gamCas_1x3_80s_m35C_001.fit / gamCas_1x3_80s_m35C_002.fit

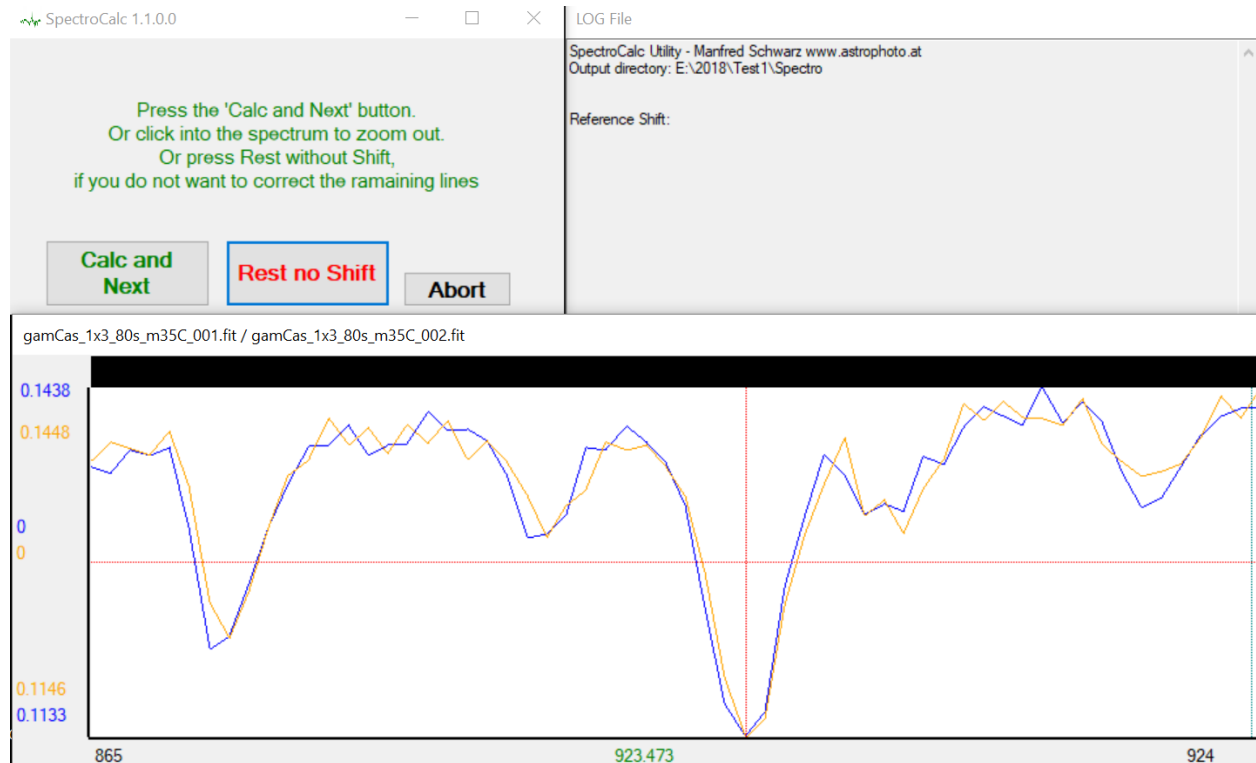


Click on a desired line to zoom it.

gamCas_1x3_80s_m35C_001.fit / gamCas_1x3_80s_m35C_002.fit



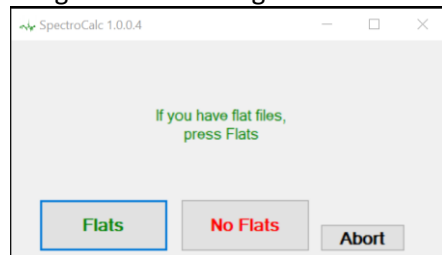
You can see the first spectrum in blue and the spectrum to shift in orange. The red middle line shows the level where the shift is measured as an average of the deviation of the left and right shoulder. Click in the middle of the line to select it.



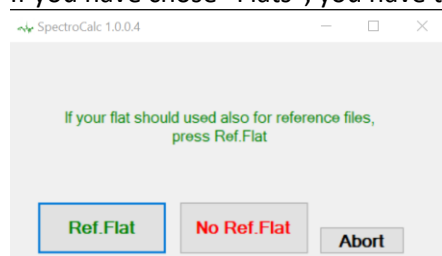
If you decide for another line, click again into the spectrum and repeat all previous steps.
 If you are lucky with the selected line press "Calc and Next" do calculate the wavelength shift and jump to the next spectrum.
 If you are sure that there is no shift between all the spectra, click "Rest no Shift".

Wizard: Flats

If you have flat field images, you can select one or more images to create a master-flat image. More images will be averaged.



If you have chose "Flats", you have to decide if the flats should be also used for reference images:



Formula of flat correction of a spectrum image:

a = average of all flat image pixels.

$\text{pixel_corr} = (\text{pixel_original} * a) / \text{pixel_masterFlat}$

The master flat image is stored in .\Spectro\01_DarkFlatCorr.

The dark and/or flat corrected spectra are stored in .\Spectro\02_Spec

The dark and/or flat corrected reference images are stored in .\Spectro\02_Ref

Wizard: Darks

If you have dark field images, you can select one or more images to create a master-dark image. More images will be averaged.

Depending what you have previous selected you will be asked for darks for spectra, reference images and flats.

Formula of dark correction:

a = average of all dark image pixels.

$\text{pixel_corr} = \text{pixel_original} + a - \text{pixel_masterDark}$

Limited to 0 to avoid negative values!

The master dark image is stored in .\Spectro\01_DarkFlatCorr.

The dark and/or flat corrected spectra are stored in .\Spectro\02_Spec

The dark and/or flat corrected reference images are stored in .\Spectro\02_Ref

Wizard: Select Remove Sky-Background

In this step you decide if you want an interactive remove of the sky background.

This function does not remove emission lines of street lamps etc. This function removes only the low frequency sky background differences.

From the spectra stripe up and down the background is searched and a stripe of 20 pixel in Y will be averaged. The upper and lower stripe will be also averaged to one 1D background stripe.

To avoid to add an additional noise of the background to the spectrum, it will be a polynomial of 5th grade done over the background stripe.

It is possible to move the stripes manually to another Y-position.

Wizard: Select Remove Continuum

For the most high resolution projects it is necessary to remove the continuum of the spectra and normalize it to 1, to be able to compare it. SpectroCalc provides an interactive tool to solve it.

Press "Remove Cont." to join this feature.

Wizard: Spectrum Scan

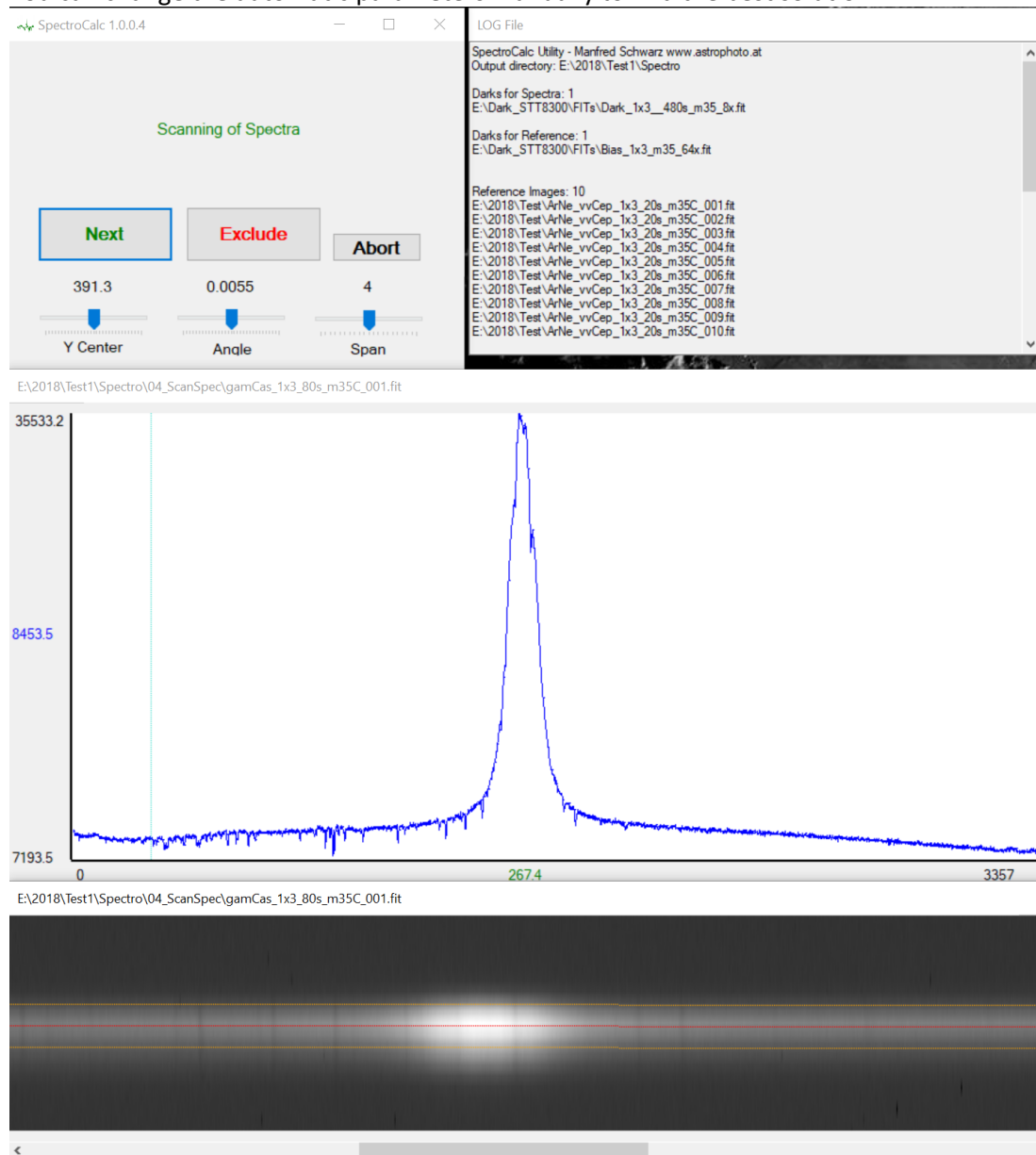
After all the selections, the automatic processing starts with:

- Generate Master-Darks
- Generate Master-Flat if defined
- Subtract of Dark frames from spectra, calibration images and flats if defined
- Division through Flat if defined

Next process is to scan the spectra stripes to 1D spectra.

SpectroCalc searches automatically for the spectra stripe and calculate the rotation angle, the center and the span (thickness of the stripe).

You can change the automatic parameters manually to find the best solution.



To estimate the best rotational angle, move the scroll bar of the spectrum stripe image to left and right. If the angle should be adapted, move the blue slider “Angle” to left or right.

The span (between the yellow lines) is calculated by the half value between the brightest Y-position and the background. You can change this value by moving the blue slider “Span”.

The centre of the scan can also be changed by moving the blue slider “Y Center”. Look at the maximum flux value on the right side of the spectrum diagram to estimate the best position of the centre. Normally a higher value is a better value.

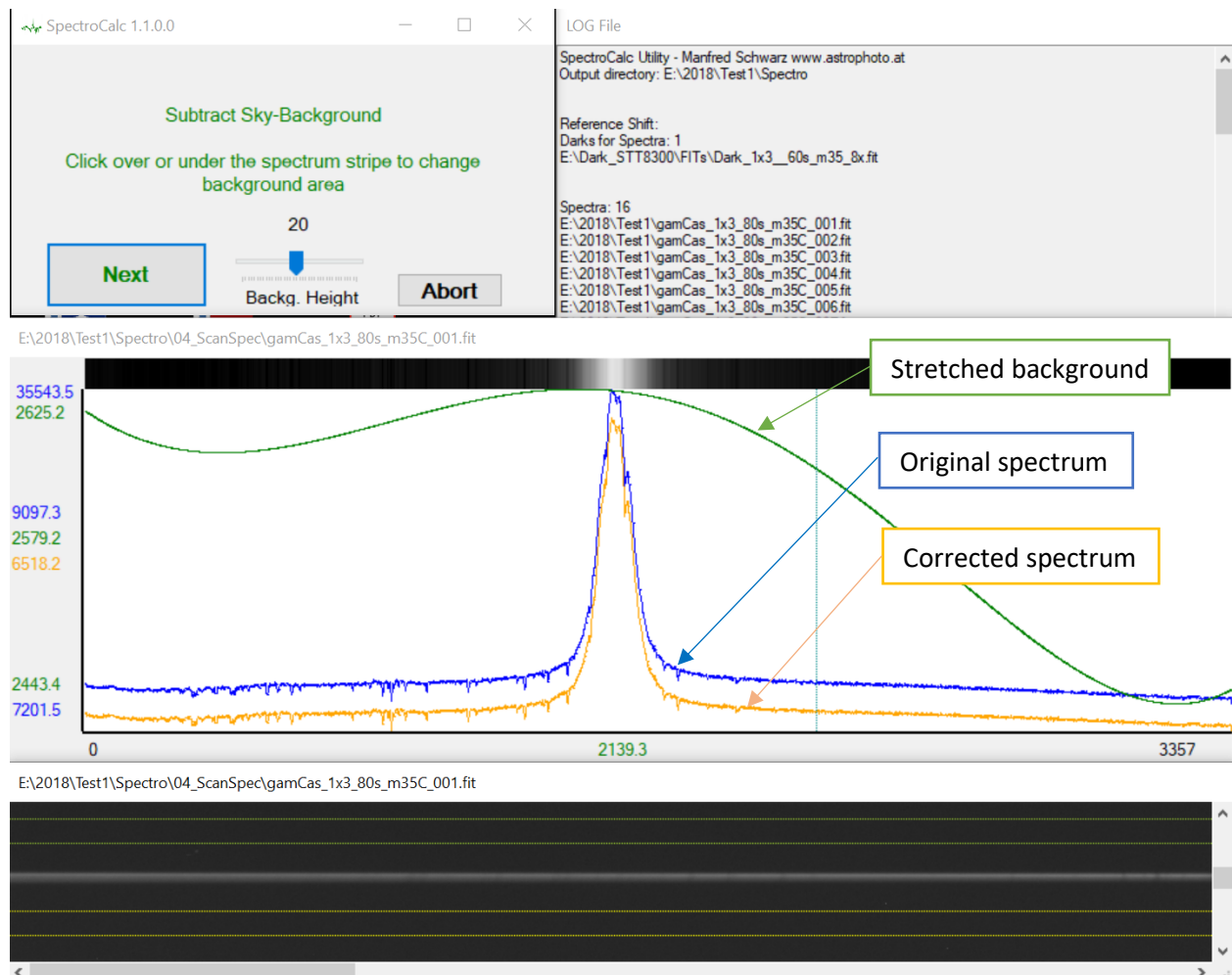
If you see that an image is too worse to use it for reduction, press “Exclude” and this image is disabled during the whole processing, also if you go back with the “Step Back” button. If you want to include an excluded image, you have to restart at the beginning by pressing “Abort”.

Press “Next” to save the scan of the current image and go to the next one.

The output of the spectra scan are 1D DAT files in the folder: .\Spectro\04_ScanSpec

Wizard: Remove Sky-Background

If you have previously selected “Remove Background”, you will get following graphic:



On the spectrum stripe image is a green area for upper sky region and a yellow area for lower sky region. If you click with the left mouse button above the stripe, you will move the upper area and if you click below the stripe, you will move the lower area. With the blue slider “Backg.Height” you can resize the background sky areas.

In the spectrum diagram, you see 3 curves.

The blue one is the original spectrum. The green one is the averaged sky-background (zoomed for better view) and the orange one is the result of the correction.

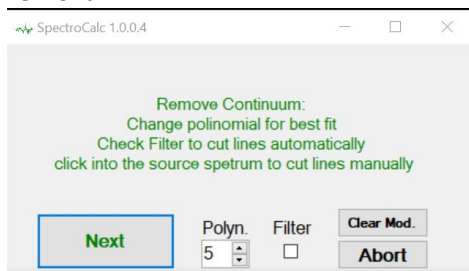
The output of the background and the polynomial files are 1D DAT files in the folder .\Spectro\05_SkyBack

The polynomial curve is subtracted from the spectrum: $\text{new_spec} = \text{spec} - \text{poly}$

The output file for the corrected spectrum is a 1D DAT file in the folder .\Spectro\06_ScanSpecSkyCorr

Wizard: Continuums remove and normalizing

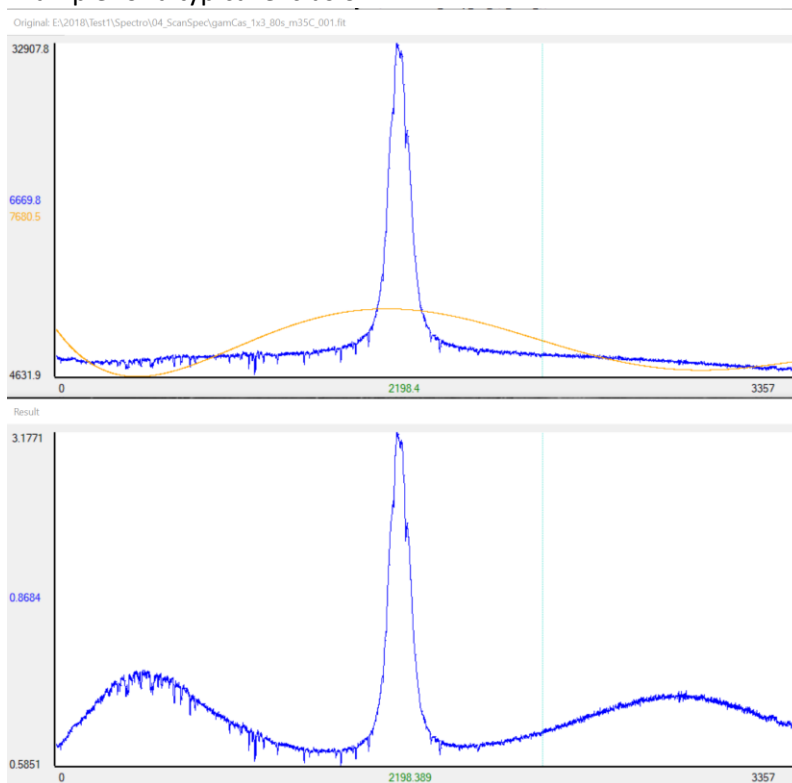
If you have previously selected “Remove Continuum”, you can now set the parameters for continuums removal.



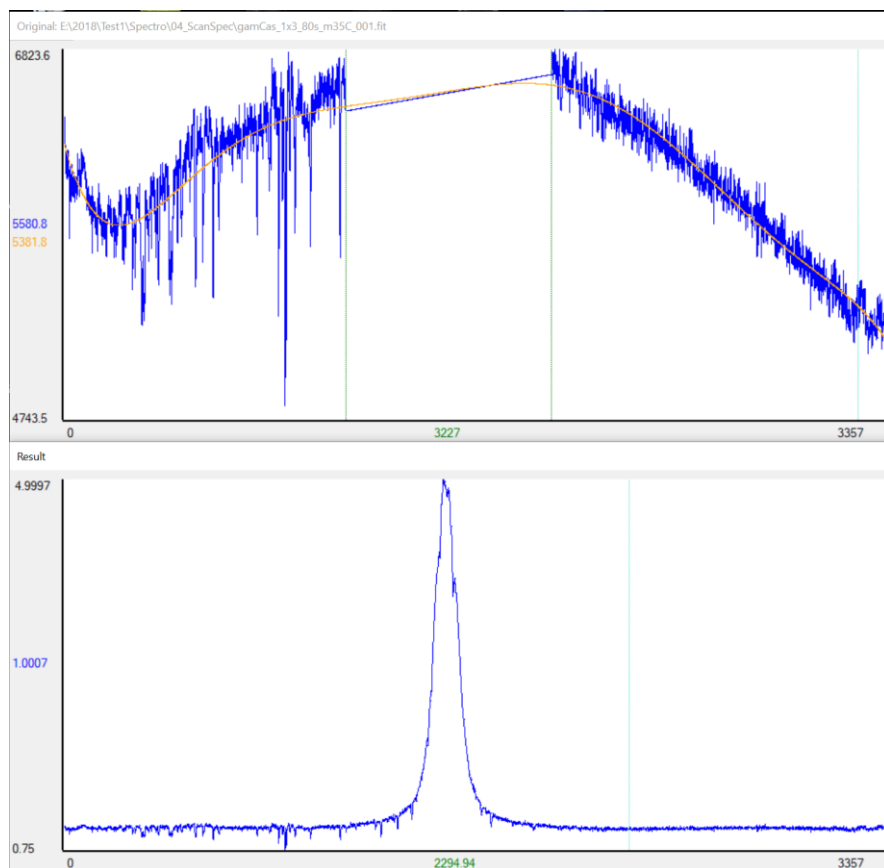
There are 3 parameters to change:

- Polynomial: the grade of polynomial
- Filter: cuts narrow absorption or emission lines automatically before the polynomial is used
- Exclusion of areas before the polynomial is used, by clicking into the graphic and define the left and right border of exclusion

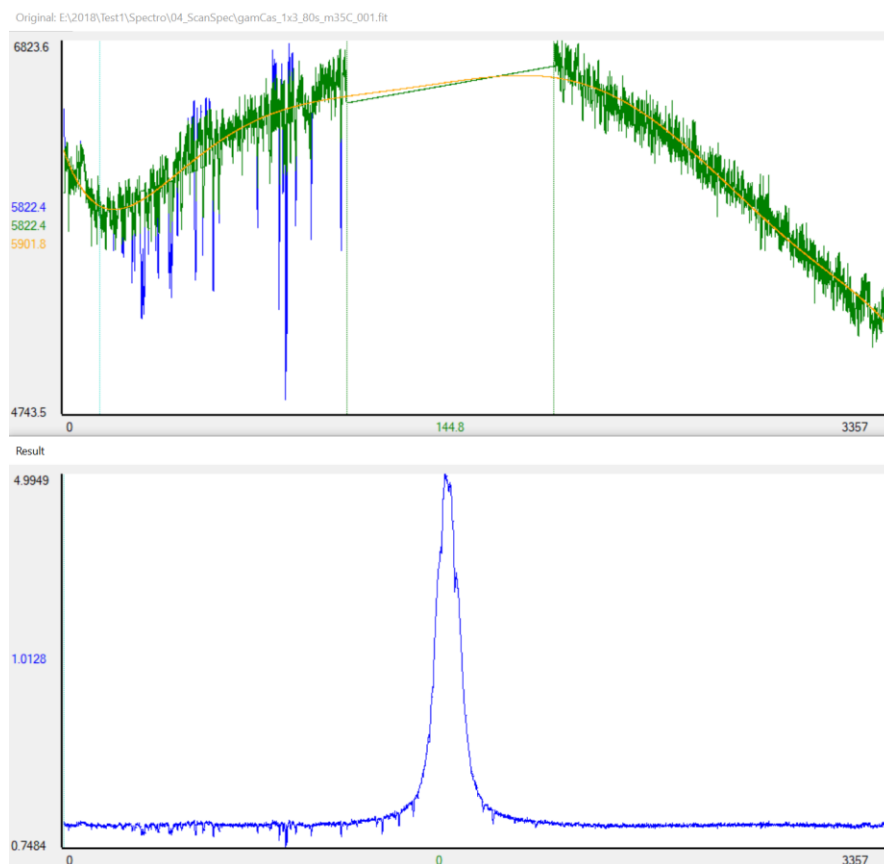
Example for a typical exclusion:



The big emission influences the polynomial. Click left and right of the emission in the original graph to cut the emission for continuums calculation.



If you use in this example the filter, the result turns a little bit better, because the big telluric lines will be cut off:



The output files for the continuum are 1D DAT files in the folder .\Spectro\08_Continuum

The output files for the continuum corrected spectra are 1D DAT files in the folder
.\Spectro\09_SpecConCorr

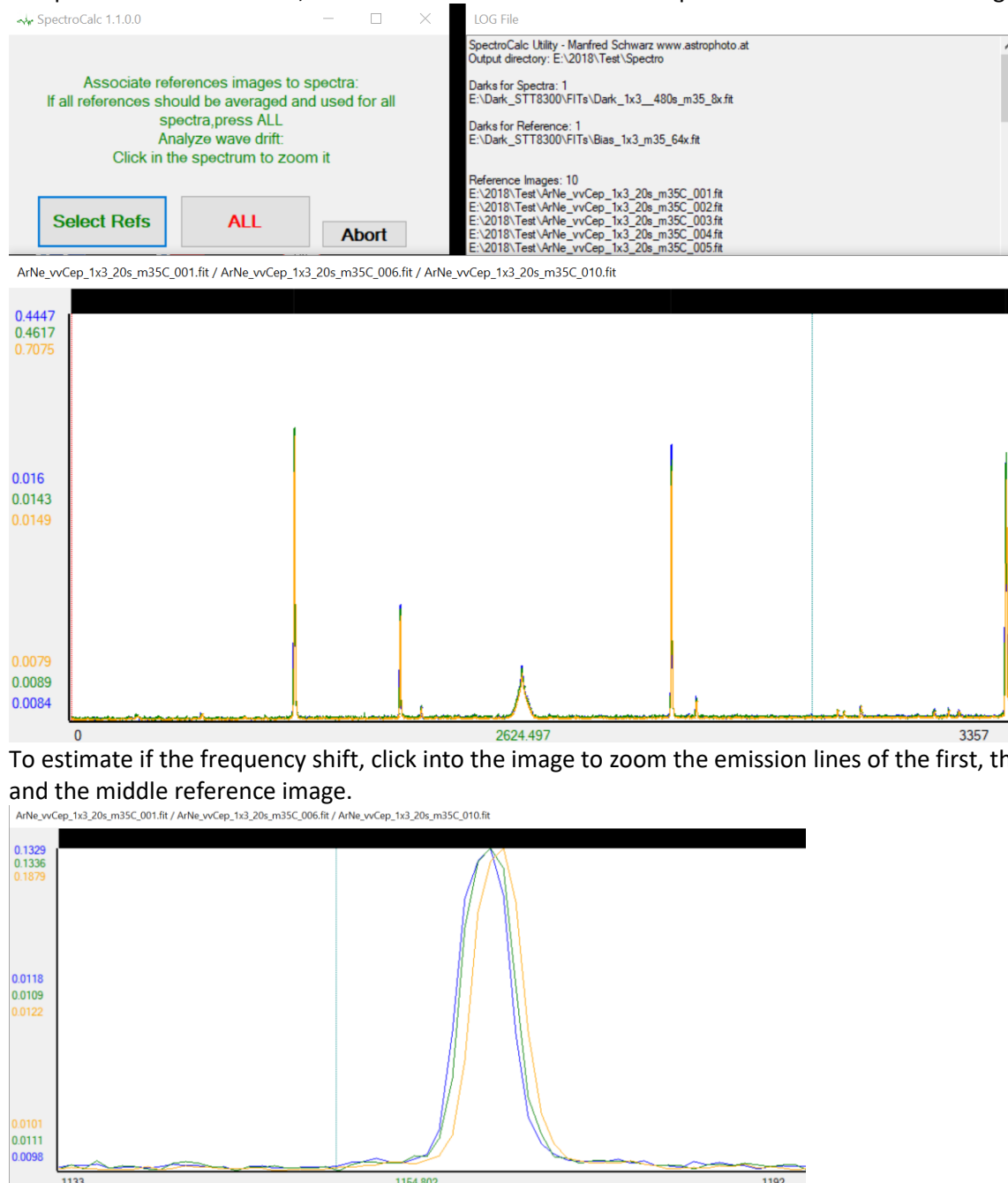
Wizard: Select References for your spectra

If you have taken a reference image between each spectrum, you should average the reference before and after the spectrum exposure to average the small frequency-shift over the temperature along one exposure. In this case press “Select Refs”.

There are 2 possibilities to get a accurate result in wavelength calibration:

- Calibrate each single spectrum (necessary, if you need each single spectra calibrated to recognize fast changes in the spectra)
- Align all spectra and calibrate the sum of all spectra (if you need only the sum of all spectra)

The preview shows the first, the middle and the last reference spectrum to show the wavelength drift.

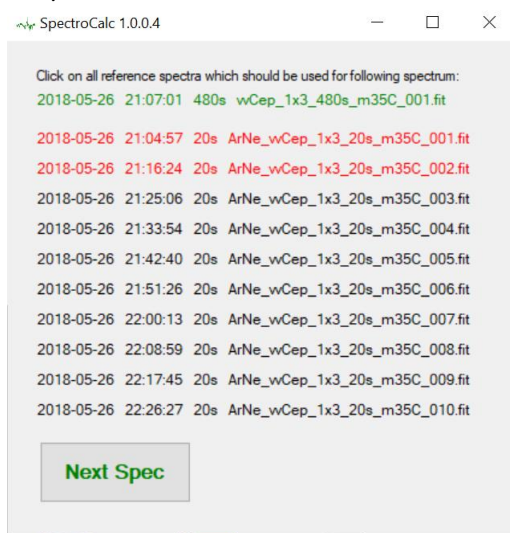


In this example, there is a drift of about 1,5 pixel between the first (blue) and the last (orange) reference spectrum.

If you need each single spectrum calibrated, press “Select Refs”, then you have to allocate the reference spectra for each single spectrum. You can select one or more reference images, which will be averaged to one reference image for the shown spectrum.

Normally I take one reference image before and one after the exposure of a spectrum. In this case, you have to select the reference image before and after.

SpectroCalc is looking for the best reference spectra and marks it automatically. You can deselect these and/or select additional references.



You get a list of reference files with date, start time, exposure time and name in black.

In green, you get the spectrum with the same dates. Look at the start time and choose the according reference files. In this example, the first two files.

Click on the desired files to turn it to red. If you have a wrong file selected, click again to turn it back to black.

After selecting all desired reference files, click on “Next Spec” and select the references for the next spectrum, and so on...

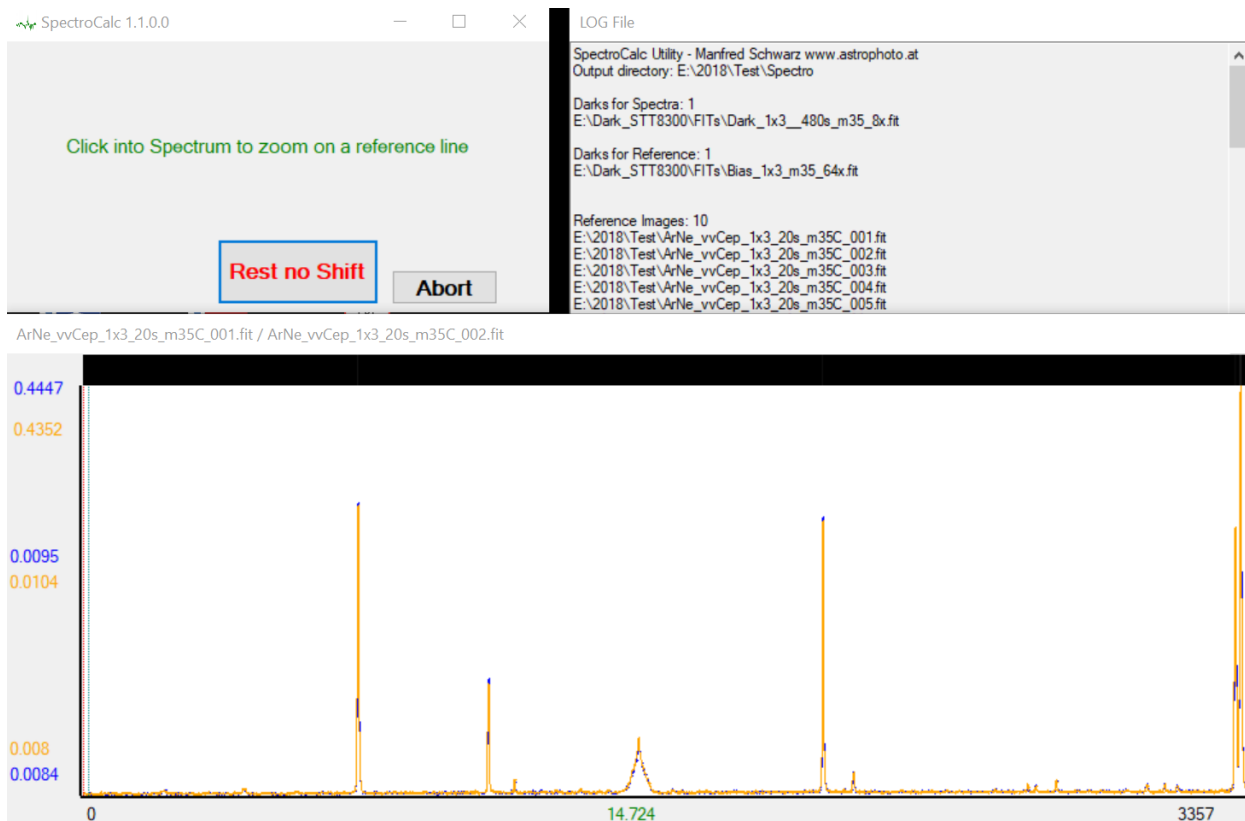
Scan of the References

The averaged references will be scanned with exact the same parameters as the allocated spectrum.

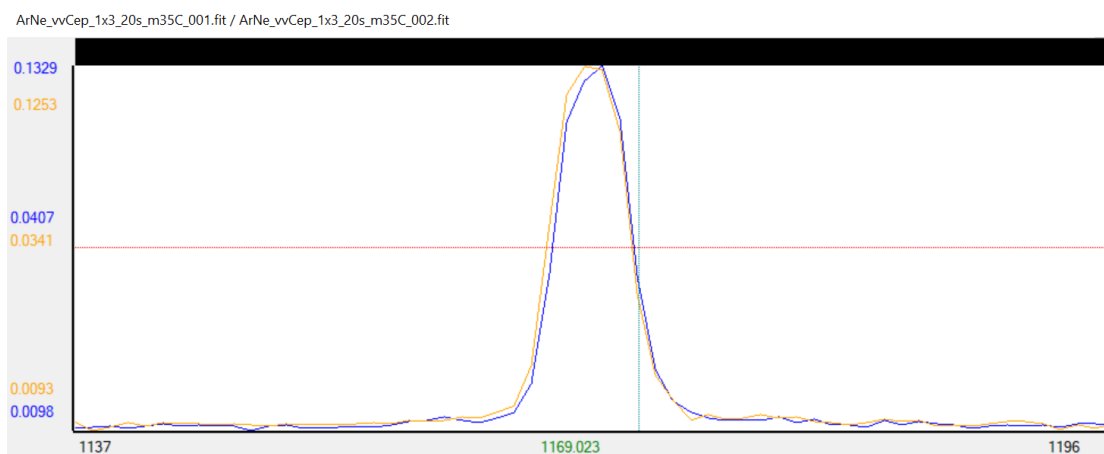
The output files for the averaged reference files are 1D DAT files in the folder .\Spectro\07_ScanRef

Wizard: Sum of all References: Align the references and spectra

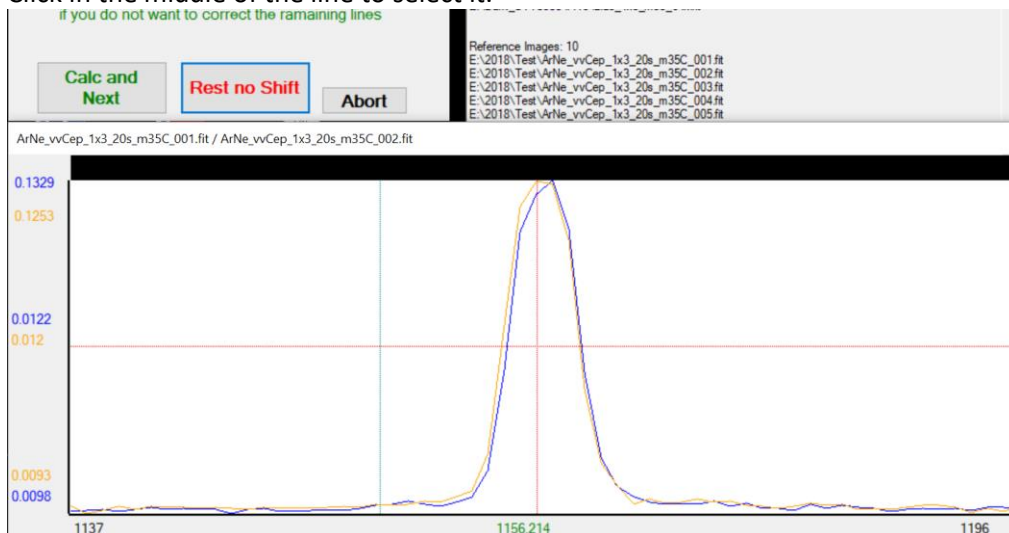
If you decided to generate a sum of all references before calibration, you have to align all references against the 1st reference spectrum.



Click on a desired line to zoom it.



You can see the first reference spectrum in blue and the reference to shift in orange. The red middle line shows the level where the shift is measured as an average of the deviation of the left and right shoulder. Click in the middle of the line to select it.



If you decide for another line, click again into the spectrum and repeat all previous steps.
If you are lucky with the selected line press “Calc and Next” do calculate the wavelength shift and jump to the next spectrum.

If you are sure that there is no shift between all the spectra, click “Rest no Shift”.

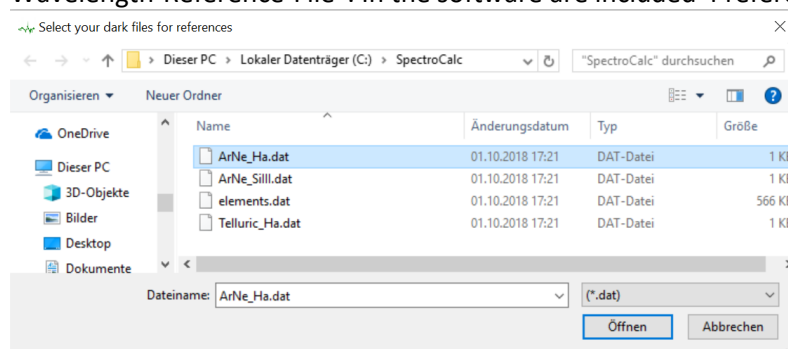
SpectroCalc is searching for the best corresponding reference files for each spectrum (best would be a reference before and on after the spectrum) and calculates the average of the wavelength shift. The spectrum is shifted before it will be averaged.

Wizard: Wavelength Calibration

If you have selected reference files, the calibration is done by the emission lines of the reference image(s).

Load the desired reference DAT file.

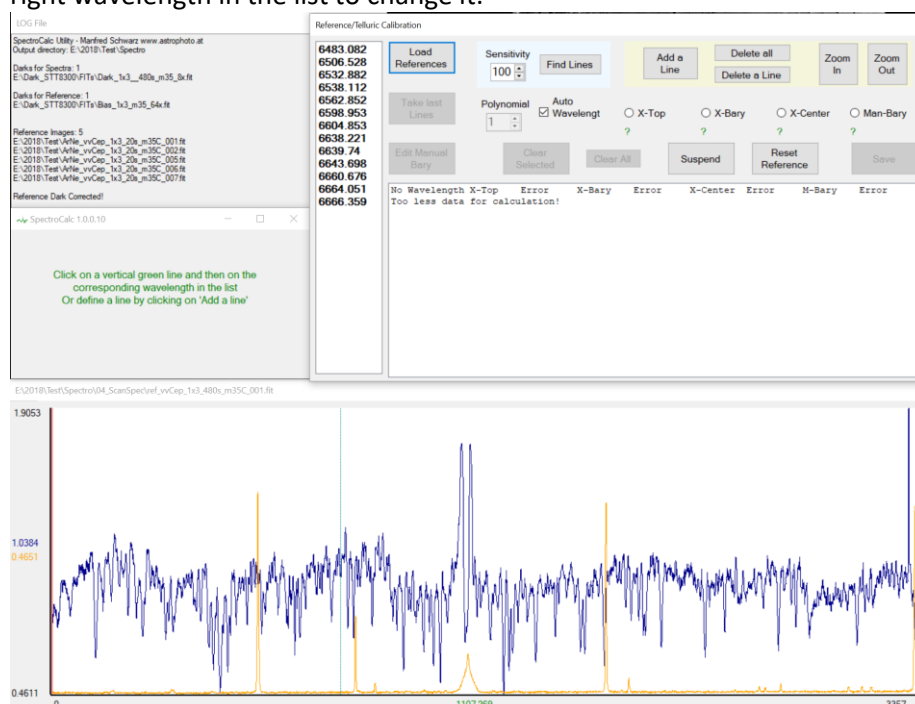
To make the life easier, generate special DAT files for your projects (look at chapter “Define a Wavelength-Reference-File”. In the software are included 4 reference files as examples:



- ArNe_Ha.dat ... Argon Neon lines in the area of Ha for 2400gr
- ArNe_SiIII.dat ... Argon Neon lines in the area of Si-triplet at 4560 Å for 2400gr
- Element_sort.dat ... big database of all elements. A good base to create your own ref-files
- Telluric_Ha.dat ... telluric lines around Ha for 2400gr

After loading the reference file, you see the wavelength on the right side.

If you check “Auto Wavelength proposal”, the system calculate the wavelength automatically after the first 2 manually defined lines. You should always check it. If the proposal is not the right one, click on the right wavelength in the list to change it.

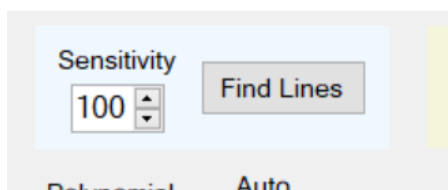


Now there are two possibilities to define reference wavelength at reference emission lines:

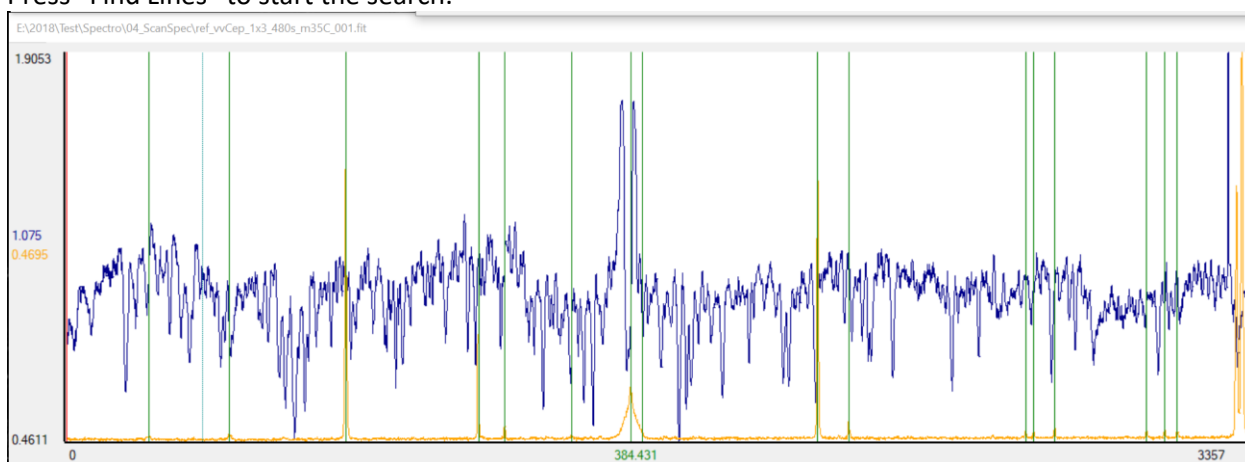
- Automatic find of emission lines
- Manual definition of emission lines

Both methods can be combined. That means, if you have searched automatically for lines and you miss some lines, you can define it manually. It is also possible to remove some of the lines, which are automatically found, if you do not need it.

Search for Lines automatically:

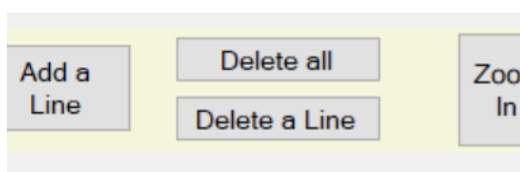


The sensitivity is a parameter to control the search algorithm. Higher values should result more lines. Press “Find Lines” to start the search.



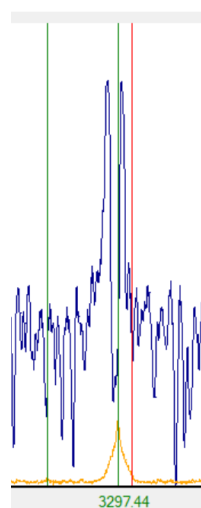
The green vertical lines mark the found emission lines. If too less numbers of lines appears, higher the sensitivity and press “Find Lines” again.

Delete one or all reference lines:

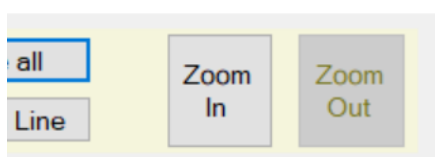


Select a line by clicking with the left mouse key on the line. The line will turn to red. Press “Delete a Line” to remove it.

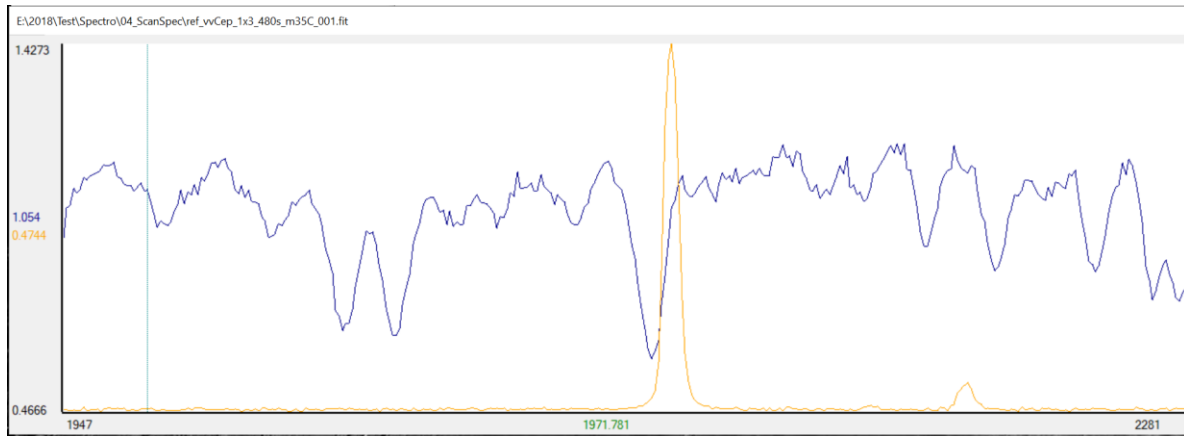
If you want to remove all visible lines, press “Delete all”.



Zoom In and Zoom Out:



You can zoom into the spectrum by pressing “Zoom In”, followed by a left mouse click to the center of the desired zoom area of the spectrum.



If you are already zoomed in, you can press “Zoom Out” to view the whole spectrum.

Add a Line manually:



Press “Add a Line”, if you want to define a reference line manually.

If you are in the “Zoom Out” view, you will be asked to click into the desired area of the spectrum to zoom it. Click on the left and then on the right side of the reference line, to define the border for the Gauss-fit to find the different line centres:

- X-Top: top of the Gauss curve
- X-Bary: bary centre
- X-Center: centre between your defined border lines
- M-Bary: best value of the previous values or manual defined bary centre (look at “Edit Manual Bary”)

Associate Lines with Wavelengths:

LOG File

SpectroCalc Utility - Manfred Schwarz www.astrophoto.at
Output directory: E:\2018\Test\Spectro

Darks for Spectra: 1
E:\Dark_STT8300\Fits\Dark_1x3_480s_m35_8s.fit

Darks for Reference: 1
E:\Dark_STT8300\Fits\Dark_1x3_m35_64s.fit

Reference Images: 5
E:\2018\Test\ArNe_vvCep_1x3_20s_m35C_001.fit
E:\2018\Test\ArNe_vvCep_1x3_20s_m35C_002.fit
E:\2018\Test\ArNe_vvCep_1x3_20s_m35C_008.fit
E:\2018\Test\ArNe_vvCep_1x3_20s_m35C_009.fit
E:\2018\Test\ArNe_vvCep_1x3_20s_m35C_010.fit

Reference Dark Corrected!

SpectroCalc 1.0.0.10

Click on a vertical green line and then on the corresponding wavelength in the list
Or define a line by clicking on 'Add a line'

Reference/Telluric: Calibration

6483.082
6506.528
6532.882
6538.112
6562.852
6598.953
6604.853
6638.221
6639.74
6643.698
6660.676
6664.051
6666.359

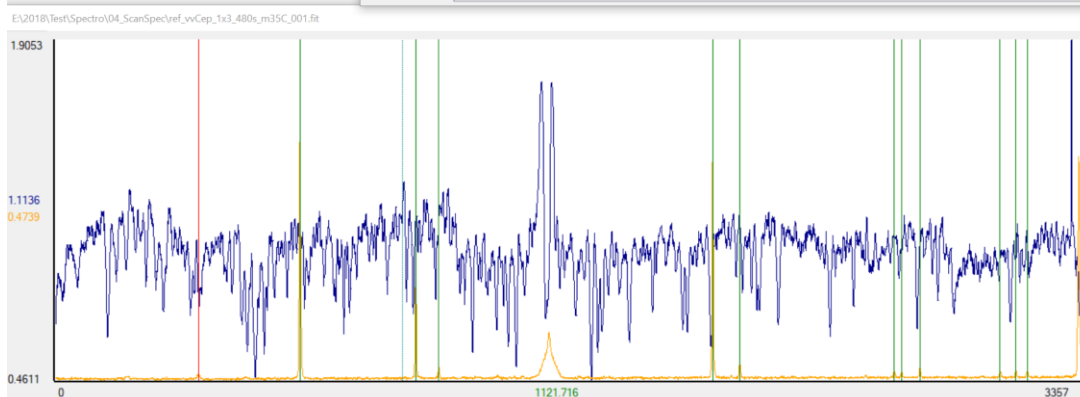
Load References
Sensitivity 100
Find Lines
Add a Line
Delete all
Delete a Line
Zoom In
Zoom Out

Take last Lines
Polynomial 1
Auto Wavelength
X-Top
X-Bary
X-Center
Man-Bary

Edit Manual Bary
Clear Selected
Clear All
Suspend
Reset Reference
Save

No	Wavelength	X-Top	Error	X-Bary	Error	X-Center	Error	M-Bary	Error
1	6483.082								

No Wavelength X-Top Error X-Bary Error X-Center Error M-Bary Error
1 6483.082
Too less data for calculation!



Select a line by clicking on it. The line turns to red. If no wavelength was defined before, click on the desired wavelength in the list (in above example: 683.082 Å).

If you have defined 2 lines manually and have checked “Auto Wavelength Proposal”, you can click line by line and the wavelength will be defined automatically.

Do not use lines which are not defined in your wavelength list!

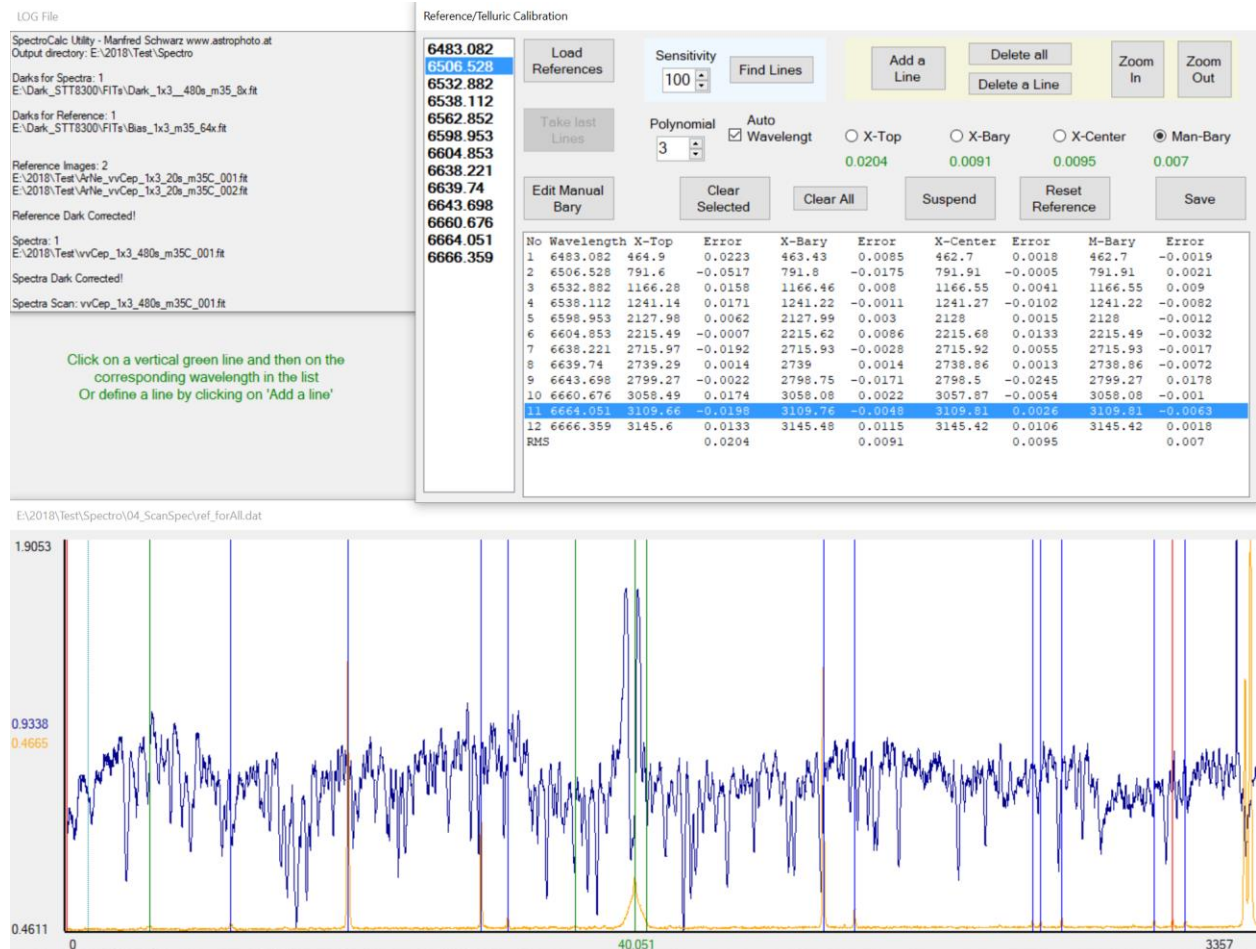
If there is a wrong interpretation, you will see it directly in the line error window. In this case the error increase too much.

If you want to change a value, click on the line again and choose another value of the list.

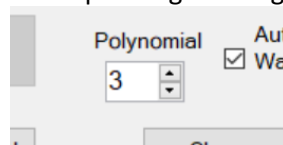
If you want to unassign a line, click on the line and press “Clear Selected”.

If you want to start from the beginning, press “clear All”.

If you have already calibrated the first spectrum, you can press “Take last Lines” to allocate the same lines with the same wavelength (without manual corrections).



The big text area shows the assigned lines, the wavelength the values of the pixel positions and the corresponding error against a polynomial curve with the grade defined by this parameter:



Following different line parameter are displayed for each assigned line:

- X-Top ... top-value of the gauss-fitted line
- X-Bary ... automated calculated bary center
- X-Center ... center between the left and right value of the automated bary-search or of the border lines defined by “Add a Line”
- M-Bary ... copy of the best value (X-Top, X-Bary or X-Center) which can be changed manually

Change the polynomial grade to improve the RMS error. But choose as maximum the number of (lines – 2) / 2. For 12 lines as in the example $(12 - 2) / 2 = 5^{\text{th}}$ grade. If you plan to delete some of the lines, choose a lower value. In this example I would choose 3rd grade.

Edit Manual Bary:

Take last Lines

Polynomial

Auto Wavelength ☒

☐ X-Top

☐ X-Bary

☐ X-Center

☒ Man-Bary

0.0204
0.0091
0.0095
0.007

Edit Manual Bary

Clear Selected

Clear All

Suspend

Reset Reference

Save

No	Wavelength	X-Top	Error	X-Bary	Error	X-Center	Error	M-Bary	Error
1	6483.082	464.9	0.0223	463.43	0.0085	462.7	0.0018	462.7	-0.0019
2	6506.528	791.6	-0.0517	791.8	-0.0175	791.91	-0.0005	791.91	0.0021
3	6532.882	1166.28	0.0158	1166.46	0.008	1166.55	0.0041	1166.55	0.009
4	6538.112	1241.14	0.0171	1241.22	-0.0011	1241.27	-0.0102	1241.22	-0.0082
5	6598.953	2127.98	0.0062	2127.99	0.003	2128	0.0015	2128	-0.0012
6	6604.853	2215.49	-0.0007	2215.62	0.0086	2215.68	0.0133	2215.49	-0.0032
7	6638.221	2715.97	-0.0192	2715.93	-0.0028	2715.92	0.0055	2715.93	-0.0017
8	6639.74	2739.29	0.0014	2739	0.0014	2738.86	0.0013	2738.86	-0.0072
9	6643.698	2799.27	-0.0022	2798.75	-0.0171	2798.5	-0.0245	2799.27	0.0178
10	6660.676	3058.49	0.0174	3058.08	0.0022	3057.87	-0.0054	3058.08	-0.001
11	6664.051	3109.66	-0.0198	3109.76	-0.0048	3109.81	0.0026	3109.81	-0.0063
12	6666.359	3145.6	0.0133	3145.48	0.0115	3145.42	0.0106	3145.42	0.0018
RMS			0.0204		0.0091		0.0095		0.007

If you are not satisfied with the calibration result (in this example the RMS looks Ok but some values are too high), you can delete some of the lines with bad values or unassign it. In the example I decided to remove the line number 9 (6343.698 Å). Click on the 9th line to select it (you can click on the line in the spectrum or on the line in the error-text list) and click on “Clear Selected”.

No	Wavelength	X-Top	Error	X-Bary	Error	X-Center	Error	M-Bary	Error
1	6483.082	464.9	0.0221	463.43	0.0073	462.7	0	462.7	-0.0027
2	6506.528	791.6	-0.0516	791.8	-0.0166	791.91	0.0008	791.91	0.0028
3	6532.882	1166.28	0.016	1166.46	0.0092	1166.55	0.0058	1166.55	0.0098
4	6538.112	1241.14	0.0173	1241.22	-0.0001	1241.27	-0.0087	1241.22	-0.0076
5	6598.953	2127.98	0.0059	2127.99	0.0002	2128	-0.0026	2127.99	-0.0039
6	6604.853	2215.49	-0.0011	2215.62	0.0055	2215.68	0.0088	2215.49	-0.0057
7	6638.221	2715.97	-0.0197	2715.93	-0.0065	2715.92	0	2715.92	-0.0054
8	6639.74	2739.29	0.001	2739	-0.0024	2738.86	-0.0041	2739.29	0.0191
9	6660.676	3058.49	0.0171	3058.08	0	3057.87	-0.0086	3058.08	-0.0017
10	6664.051	3109.66	-0.02	3109.76	-0.0066	3109.81	0	3109.81	-0.0066
11	6666.359	3145.6	0.0131	3145.48	0.01	3145.42	0.0085	3145.42	0.0019
RMS			0.0213		0.0076		0.0057		0.0077

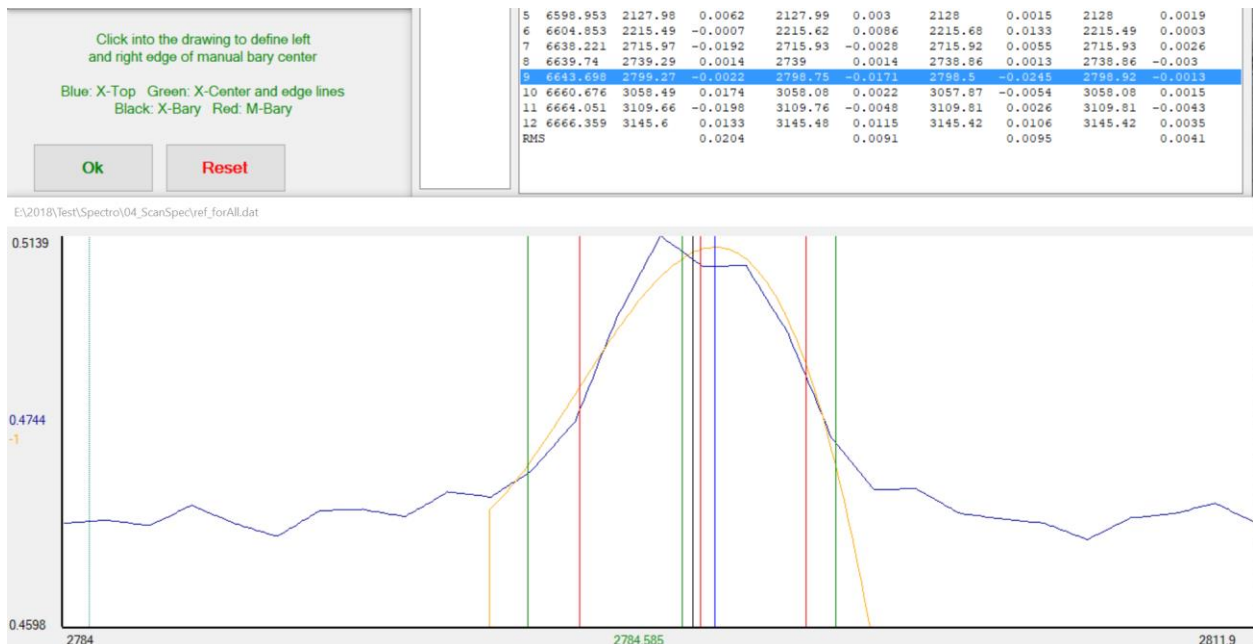
But you can see, that the result is worse as before. So I add the line again by clicking on it to select it and if you have selected “Auto Wavelength, it is automatically assigned. Otherwise you have to click on the wavelength in the list.

Another method is to edit the manual bary centre. Select a line to define your own bary center (M-Bary) by clicking “Edit Manual Bary”.

It is easy to find the desired line by clicking on a value in the error list. The corresponding line is automatically selected (red).

Then click on “Edit Manual Bary”. The selected area will be interpolated and zoomed 100 times!

In the example, I selected the line number 9 (6343.698 Å) and entered the manual bary centre editor:

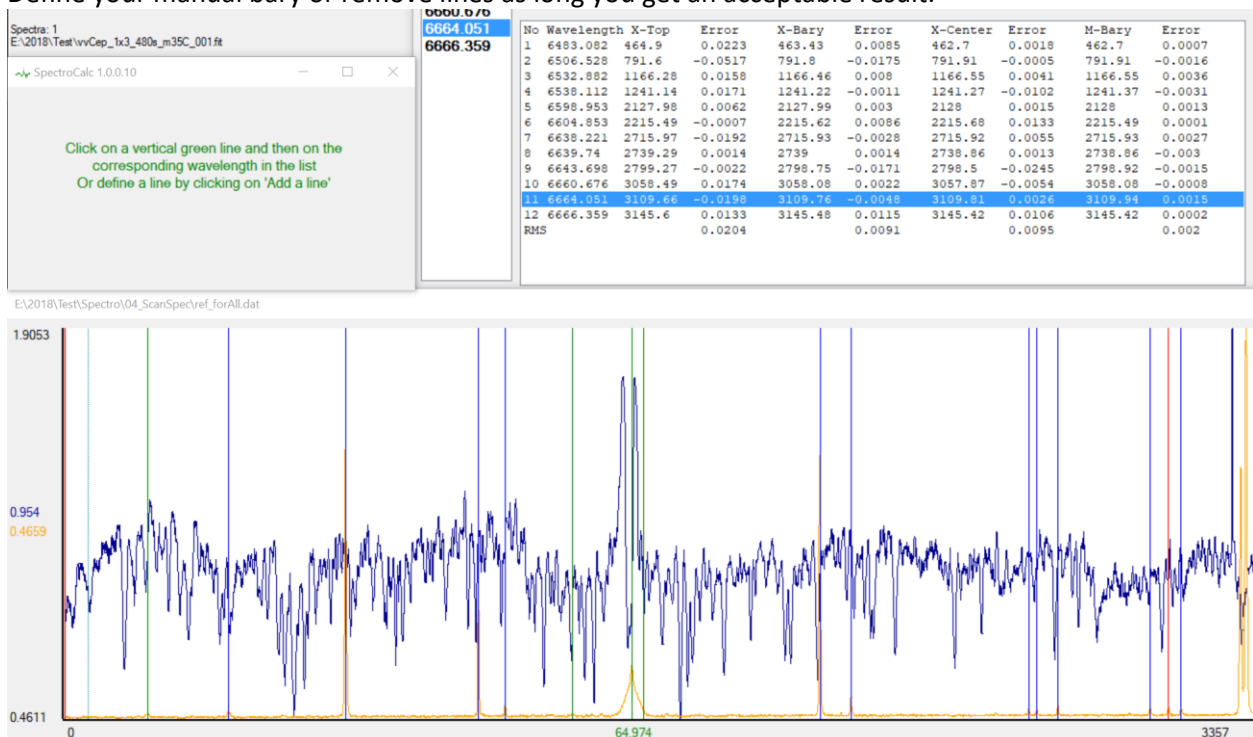


You can now define the left and the right border for calculating the bary centre (left and right red line)
On the error-text field you can see in life-time the change of the error.

Meaning of the different colors of lines:

- Blue: spectrum
- Brown: fit curve
- Blue: X-Top value
- Green: X-Center value and left and right limit of the automatic found X-Bary value
- Black: X-Bary value
- Red: M-Bary and limit-lines of new manual M-Bary

Define your manual bary or remove lines as long you get an acceptable result.



Before you store the result, you can choose one of the line fitting methods (X-Top, X-Bary, ..). The best result (normally M-Bary) is selected automatically.
Press "Save" to store the calibration.

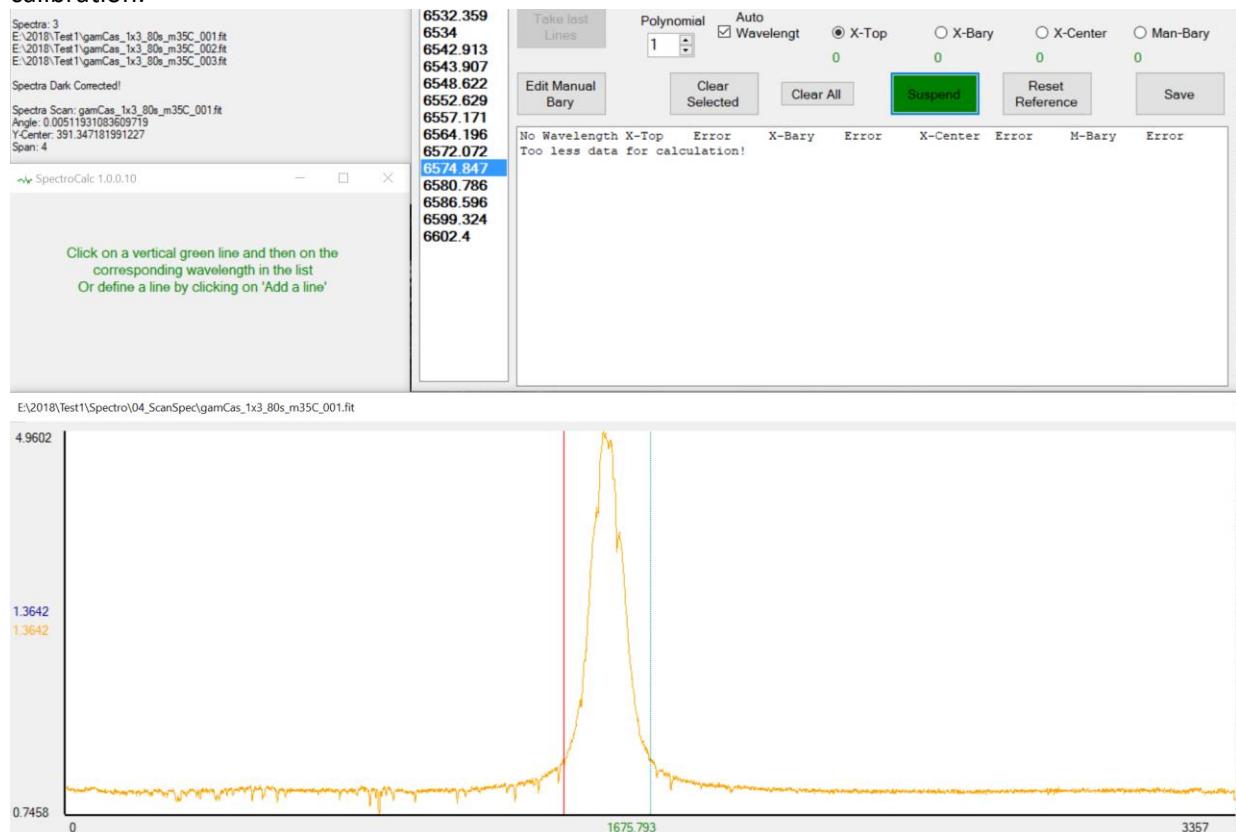
A new calibration window for the next spectrum appears. Normally the data should be very similar to the previous spectrum. You can press “Take last Lines” to take over the logic of the last calibration. But not the exact data are taken over, only the approximate location of the lines and the system calculates all parameters for new.

You can work with the selected lines or you can define not used lines again for this spectra. Important is to find an acceptable calibration result with much reference lines as possible.

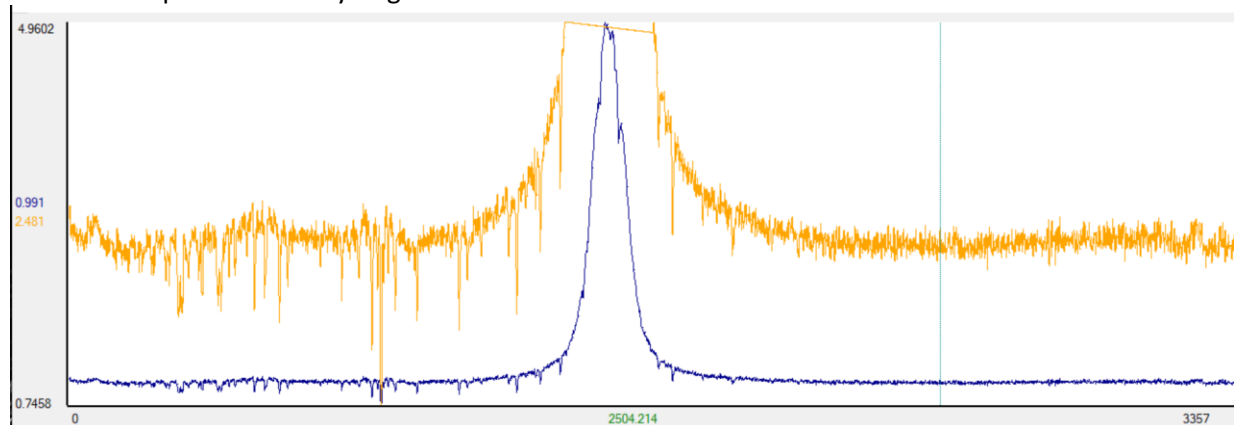
Wavelength Calibration with Telluric or Internal Absorption-Lines

If you have chosen calibration with telluric lines, you get a similar way for calibration as with reference lamp calibration. Instead of the reference file you have the spectrum itself for calibration and the system search for absorption lines and not for emission lines.

To get a better view for the telluric or internal lines, you can suspend the unneeded area of an emission or absorption by pressing “Suspend” and clicking left and right of the area you want to suspend for calibration:



After the suspend function you get a better view in Y direction:



The sum of uncalibrated files is a 1D DAT file and is stored:

In case of continuum remove: `.\Spectro\09_SpecConCorr`

Without continuum remove: `.\Spectro\06_ScanSpecSkyCorr` or `.\Spectro\04_ScanSpec`

The output files for the calibrated reference files are 1D FIT files in the folder `.\Spectro\10_RefCal`

The output files for the calibrated spectra files are 1D FIT files in the folder `.\Spectro\11_SpecCal`

Sum of all spectra

At the end of the routine, all calibrated spectra are averaged. If you need only the single calibrated spectra, you can ignore this file.

The output files for the averaged sum-spectra is `.\Spectro\sum.fit`

Processing of 1D Spectra “Wizard - 1D FITs”

If you have already scanned spectra in FITs format, you are able to process this data by pressing “Wizard - 1D FITs”.



Following processing steps are available:

- Continuum remove
- Calibration with internal or telluric lines
- Calibration with 1D reference spectra
- Wavelength calibration
- Average of spectra
- Post processing

It is not a problem, If your scanned spectra and reference files are not already wavelength calibrated.

If you have already made the wavelength calibration on the input files, SpectroCalc remove the wavelength information and exchange it to pixel values (0, 1, 2, 3, ...).

There is no problem to recalibrate a spectrum with internal lines or tellurics.

Attend you can get problems, if you try to recalibrate a calibrated spectrum with a reference file!

Because the calibrated spectrum is not any more pixel aligned with the reference file. The result could be wrong!

Log File

The log of all operations is shown on the right side of the main window. Also it is stored at `.\Spectro\LOG.TXT`

Post-Processing

The last processed file, normally the calibrated sum of all spectra is opened automatically after the processing is finished. Now you have the possibility to make additional processing steps.

Crop the spectrum

To cut the spectra approximately, you can press the “Set Crop Area with Cursor” button and click on the desired left and then at the right border for setting the crop values.

You can also enter the crop values in the wavelength fields.

Press “Crop” to cut the left and right border.

The crop is not physically done, only for the display. So it is possible to change the crop area dynamically by changing the border values.

If you press “Reset Crop Values”, the spectrum turns to the original size.

Save as

You can save the spectrum to a new FITs file. If you have cropped the spectrum, only the cropped area will be saved! All new parameters are saved into the FITs-header, like BeSS parameters or heliocentric corrections.

Signal to Noise Ratio

Click on “Set S/N Area with Cursor” and click on the left and right side on the desired area in the spectrum. Within this area the S/N value is calculated automatically.

You can also enter the area manually in the wavelength fields.

If you click into the spectrum before pressing “Set S/N Area via Cursor”, you get a zoomed view, which is mostly better to define the area.

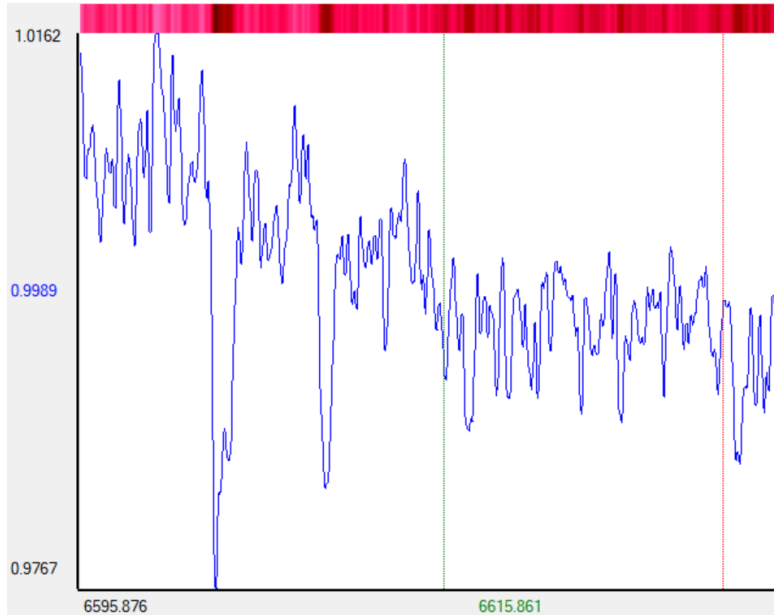
Attend:

- do not measure the S/N if an emission or absorption line is in the measure area
- do not measure the S/N on a steep slope or rise of the continuum

Example:

Set S/N Area via Cursor: 6605.069 S/N: 328 Heliocentric Correction: 12.243 km/s
 6612.083
 Set EWA Area via Cursor: EWA: ? Calculate HC Apply HC
 manual
 Set Normalize Area via Cursor: Normalize Remove Telluric Back to the Start Window
 manual

User opened spectrum: E:\2018\Test_ArNeShift\Spectro\gamCas_ArNe.fit



Measure the Equivalent Width

To measure the equivalent width approximately, you can press the “Set EWA Area with Cursor” button and click on the desired left and then at the right border for setting the EW values.

The EWA is calculated automatically.

It is possible to enter the desired area manually with entering the values in the EW fields.

You can predefine values for your objects and use the drop-down-box to select the predefined area.

Default there are 3 areas for gam Cas and one area for vv Cep defined (my individual values), but you can edit following file to change the values or add another stars:

C:\SpectroCalc\ew.txt

```
ew.txt - Editor
Datei Bearbeiten Format Ansicht ?
manual;;
gamCas 1;6525;6610
gamCas 2;6530;6605
gamCas 3;6535;6600
vvCep;6550;6575
```

Set EWA Area via Cursor: EWA: ?
 manual
 manual
 gamCas 1
 gamCas 2
 gamCas 3
 vvCep

First value of the line is the shown text in the drop-down-box.

It follows a “;” as separator

Second value is the lower border of the EW-area.

It follows a “;” as separator

Third value is the higher border of the EW-area.

If you change this file during SpectroCalc is open, you have to close the application and start it again to get the new values.

Attend:

- The continuum of the spectra has to be 1 (normalized)! Normally it is automatically done if you have used the “Remove Continuum” feature of SpectroCalc.

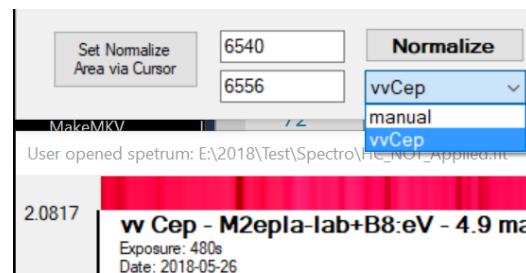
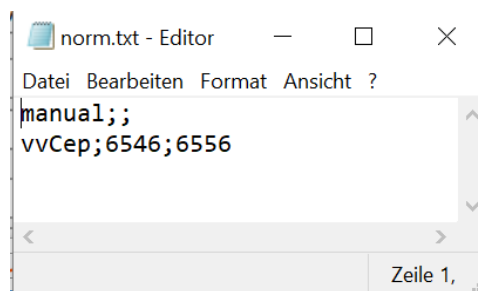
Normalize to 1

Normally, the spectrum is normalized by SpectroCalc through “Remove Continuum” feature. But it is possible to normalize the continuum at a defined wavelength area.

If you want to define the area approximately, you can press the “Set Normalize Area with Cursor” button and click on the desired left and then at the right border for setting the normalize wavelength values.

It is possible to enter the desired area manually with entering the values in the normalize fields. You can predefine values for your objects and use the drop-down-box to select the predefined area. Default there is areas for vv Cep defined (my individual values), but you can edit following file to change the values or add another stars:

C:\SpectroCalc\norm.txt



First value of the line is the shown text in the drop-down-box.

It follows a “;” as separator

Second value is the lower border of the normalize-area.

It follows a “;” as separator

Third value is the higher border of the normalize-area.

If you change this file during SpectroCalc is open, you have to close the application and start it again to get the new values.

Calculate the heliocentric correction

Press “Calculate HC” and a new window opens.

Post-Processing

Set Crop Area via Cursor: 6452.263, 6682.535 **Crop** **Save as** ☐ Titel ☐ Legend ☐ small text

Set S/N Area via Cursor: S/N: ? **Reset Crop and Telluric**

Set EWA Area via Cursor: EWA: ? **Calculate HC** **Apply HC** **BeSS Header** **Remove Telluric** **Back to the Start Window**

Set Normalize Area via Cursor: **Normalize** **manual**

Heliocentric Correction: **0 km/s**

Object: gamCas **Get data from Simbad** **Save Object as Preset**

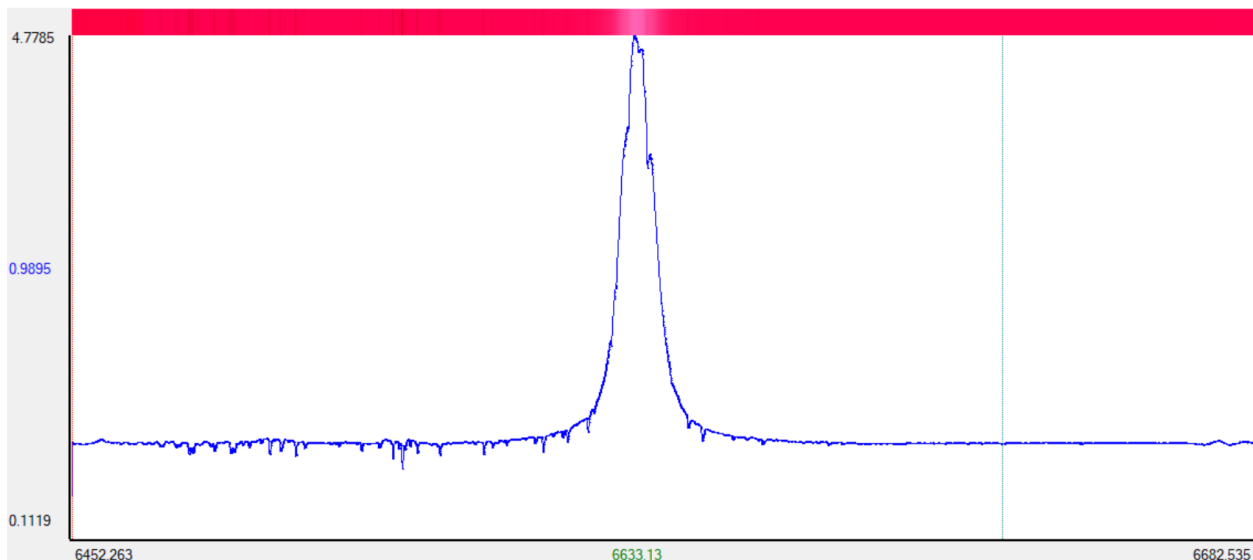
RA 2000 (°): h m s
DEC 2000 (°): ° ' "
JD (middle): 2458389.354057 Date: 2018-09-27 Time (UT): 20:29:51

Latitude (°): ° ' "
Longitude (°): ° ' "
Altitude (m): Location Name:

Preset Locat.: **Save Location as Preset**

Calculate Heliocentric Correction **Cancel**

User opened spectrum: E:\2018\Test_ArNeShift\Spectro\sum.fit



All parameters, which are relevant for calculating the heliocentric (HC) correction and are included in the FITs header, are shown automatically.

In the above example, there is only the object name defined and the exposure parameters (start time and exposure time). SpectroCalc calculates the center of the exposure time for the Julian date (JD) calculation.

If you have internet connection, you can press "Get data from Simbad" to fill out all object dates automatically.

Sometimes you have to press more than one time to get the connection to Simbad!

Heliocentric Correction

Object: gam Cas **Get data from Simbad**

RA 2000 (°): 14.177215 0 h 56 m 42.532 s

DEC 2000 (°): 60.71674 60 ° 43 ' 00.264 "

JD (middle): 2458389.354057 Date: 2018-09-27 Time (UT): 20:29:51

Latitude (°): ° ' "

Longitude (°): ° ' "

Altitude (m): Location Name:

Preset Locat.: **Save Location as Preset**

Calculate Heliocentric Correction **Cancel**

If you want to use this object data in future without Simbad, you can save the data by pressing "Save Object as Preset".

Next time you will find the object in the drop-down box:

Heliocentric Correction

Object	gamCas		Get data from Simbad		▼
RA 2000 (°)		h	m		gam Cas
DEC 2000 (°)		°	'	"	vv Cep
JD (middle)	2458389.354057		Date	2018-09-27	Time (UT) 20:29:51
Latitude (°)		°	'	"	

It is also necessary to enter the geo-position of the observation and the altitude.
You can also save the position into the location pre-set by pressing "Save Location as Preset".

Calculation of heliocentric correction value:

If all parameters are entered, press "Calculate Heliocentric Correction".

Object	gam Cas		Get data from Simbad		gam Cas ▼
RA 2000 (°)	14.177215	0 h	56 m	42.532 s	Save Object as Preset
DEC 2000 (°)	60.71674	60 °	43 '	00.264 "	
JD (middle)	2458389.354057		Date	2018-09-27	Time (UT) 20:29:51
Latitude (°)	16.28	N 16 °	16 '	48 "	
Longitude (°)	47.62	E 47 °	37 '	12 "	
Altitude (m)	700	Location Name Wiesmath			
Preset Locat.	Wiesmath ▼		Save Location as Preset		
Calculate Heliocentric Correction					Cancel

The calculation includes following influences:

- Orbit of earth at the entered JD
- Rotation of earth depending of the observe location and entered JD
- Influence of moon at the entered JD

SpectroCalc 1.0.0.13					
Post-Processing					
Set Crop Area via Cursor	6452.263	Crop	Save as	<input type="checkbox"/> Titel	Pos
	6682.535			<input type="checkbox"/> Legend	Pos
Set S/N Area via Cursor	6616	S/N: 396	Heliocentric Correction		
	6619		12.243 km/s		
Set EWA Area via Cursor	6530.003	EWA: -33.66 Å	Calculate HC	Apply HC	
	6604.983	gamCas 2 ▼	BeSS Header		
Set Normalize Area via Cursor		Normalize	Remove Telluric	Back to the Start Window	
		manual ▼			

Now you can see the calculated HC value in green. That means, it is only calculated and not applied to the spectrum.

You can apply the data to the spectrum by pressing "Apply HC". The HC value turns to red.

Attention: after applying the HC to the spectrum, it is not possible to reset the previous crop!

BeSS Header

If you want to store your spectrum to the BeSS data base:

<http://basebe.obspm.fr/basebe/>

you have to fill out all relevant data which are necessary. But anyway, you should fill out this data, because it is a good documentation for you or other people which want to work with your spectra. All the data will be stored into the FITS header when you press "Save as".

BeSS Header Information

Object	gam Cas		Get data from Simbad		gam Cas		
RA 2000 (°)	14.177215	0	h	56	m	42.532	s
DEC 2000 (°)	60.71674	60	°	43	'	00.264	"
Star Type	B0.5IVpe		Vmag		2.39		
JD (middle)	2458389.354057		Date	2018-09-27		Time (UT)	20:29:51
Latitude (°)	16.28	N	16	°	16	'	48
Longitude (°)	47.62	E	47	°	37	'	12
Altitude (m)	700		Location Name Wiesmath				
Preset Locat.	Wiesmath		Save Location as Preset				
Remove Cont.	normalized with SpectroCalc, Poly: 8						
Rem. Cosmics	none						Ok
Atmosph. Corr	none						
Helio Centric Velocity	12.243		<input type="checkbox"/> V-Hel is applied to the spectrum				
Observer	Manfred Schwarz		Camera		STT8300M		
Telescope	C11		Spectrograph		LHires3-2400		
Preset Name	C11 8300 Lhires		Inst. Resolution		18600		
	Save Preset		C11 8300 Lhires				

You see that the upper part of this window is exact the same as the HC-parameter window. All parameter you have entered there, are also entered in this window and opposite.

Additional you have several parameter:

Remove Continuum:

If you used the remove continuum feature of SpectroCalc, it is filled out automatically.

If you used another software, enter the method of normalization.

If the continuum is not removed, enter: **none**.

Remove Cosmics:

If you have removed cosmics, enter the method.

If you have removed cosmics but you don't know the method, enter: **corrected, no indication of method**

If you have not corrected the cosmics, enter: **none**

Atmospheric correction:

If you have removed the atmospheric lines (tellurics), enter the method.

If you have removed it but you don't know the method, enter: **corrected, no indication of method**

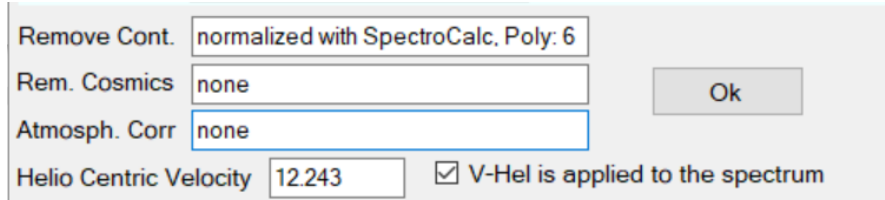
If you have not corrected it, enter: **none**

Helio Centric Velocity:

If you have calculated the HC with SpectroCalc, it is filled out automatically.

If you have calculated with another software, enter the value in km/s. Positive values are toward to the object.

If you have applied the HC to the spectrum, check the box "H-Vel is applied to the spectrum".



Instruments and observer:

All these data can be saved as pre-set to use it next times.

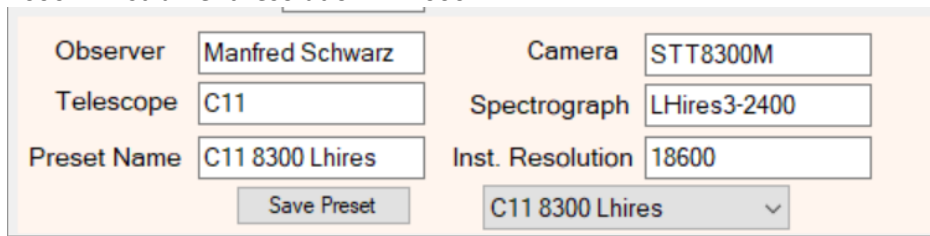
Please attend by the instrument resolution, that this value depends on the monitored wavelength.

It is a higher value in red areas and a lower value at blue area.

Example for my LHires III with 2400 l/mm grade:

6562 Å: instrument resolution = 18600

4600 Å: instrument resolution = 11000



Press "Ok" to close the window.

All parameters are saved into the FITs header by pressing "Save as".

Remove Telluric Lines

There is a important difference of SpectroCalc to other tools in case of dry a spectrum.

Like in other tools you can change parameters like strength, wavelength shift, etc. to the whole telluric reference spectrum.

SpectroCalc allows additional to edit these parameters to each single lines. This feature allows to get a much better result, with less artefacts caused by drying of the spectrum.

After pressing "Remove Telluric", a new window appears with the parameter sliders.

Post-Processing

Set Crop Area via Cursor

6452.263

Crop

6682.535

Reset Crop and Telluric

Save as

☐ Titel

Pos

☐ Legend

Pos

☐ small text

Set S/N Area via Cursor

6616

S/N: 396

Calculate HC

Apply HC

6619

Heliocentric Correction

12.243 km/s

BeSS Header

Remove Telluric

Set EWA Area via Cursor

6530.003

EWA: -33.66 Å

gamCas 2

▼

Back to the Start Window

Set Normalize Area via Cursor

Normalize

manual

▼

Remove Telluric

Strength

Wings

Width

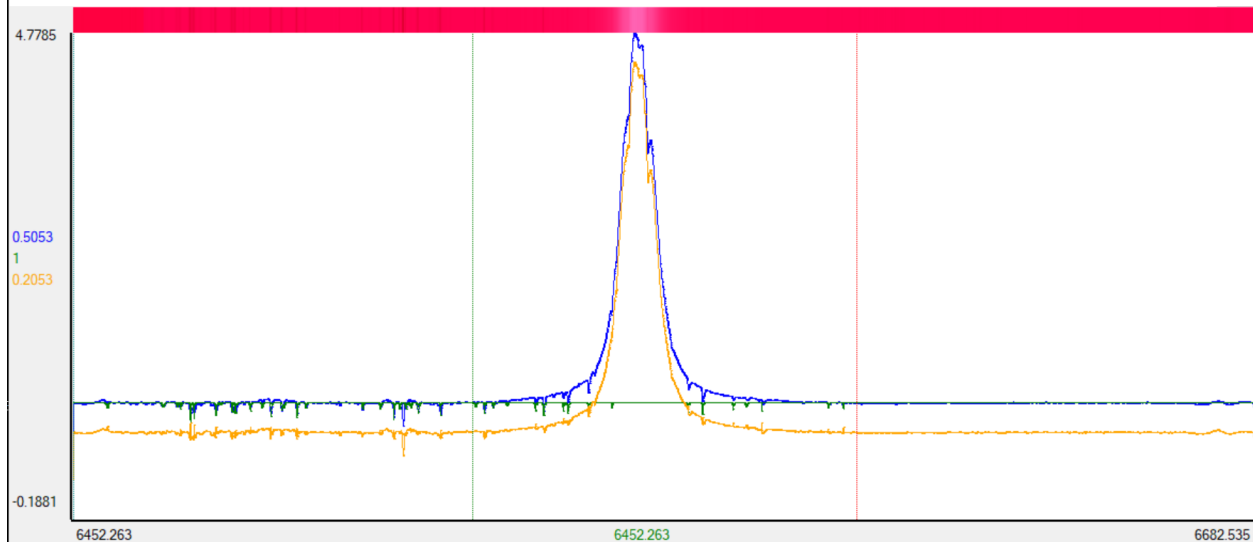
Shift

Apply

Modify single

Cancel

User opened spectrum: E:\2018\Test_ArNeShift\Spectro\sum.fit



The blue spectrum is the original spectrum.

The green spectrum is the telluric reference spectrum.

The orange spectrum is the preview to the result. It is shifted by -0.3 to get a better view.

You can click into the spectrum to zoom in (click again to zoom out).

Post-Processing

Set Crop Area via Cursor

6452.263

Crop

6682.535

Reset Crop and Telluric

Save as

☐ Titel

Pos

☐ Legend

Pos

☐ small text

Set S/N Area via Cursor

6616

S/N: 396

Calculate HC

Apply HC

6619

Heliocentric Correction

12.243 km/s

BeSS Header

Remove Telluric

Set EWA Area via Cursor

6530.003

EWA: -33.66 Å

gamCas 2

▼

Back to the Start Window

Set Normalize Area via Cursor

Normalize

manual

▼

Remove Telluric

Strength

Wings

Width

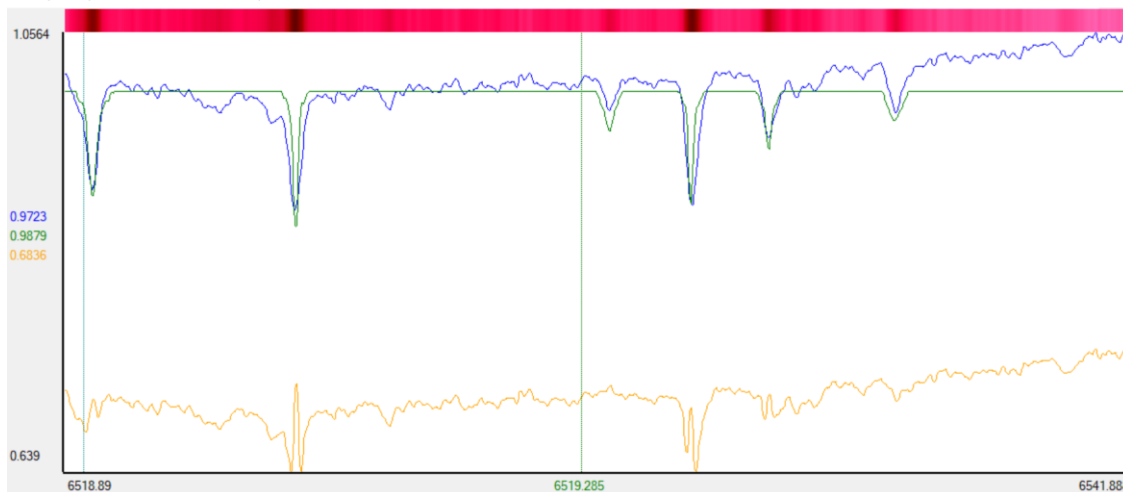
Shift

Apply

Modify single

Cancel

User opened spectrum: E:\2018\Test_ArNeShift\Spectro\sum.fit



Change the sliders to get a good result in average. The parameters have effects to the whole reference spectrum.

Post-Processing

Set Crop Area via Cursor

6452.263

Crop

Save as

☐ Titel

Pos

6682.535

Reset Crop and Telluric

☐ Legend

Pos

Set S/N Area via Cursor

6616

S/N: 396

Heliocentric Correction

12.243 km/s

Calculate HC

Apply HC

6619

BeSS Header

Remove Telluric

Back to the Start Window

Set EWA Area via Cursor

6530.003

EWA: -33.66 Å

gamCas 2

Normalize

manual

6604.983

Set Normalize Area via Cursor

Remove Telluric

Strength

Wings

Width

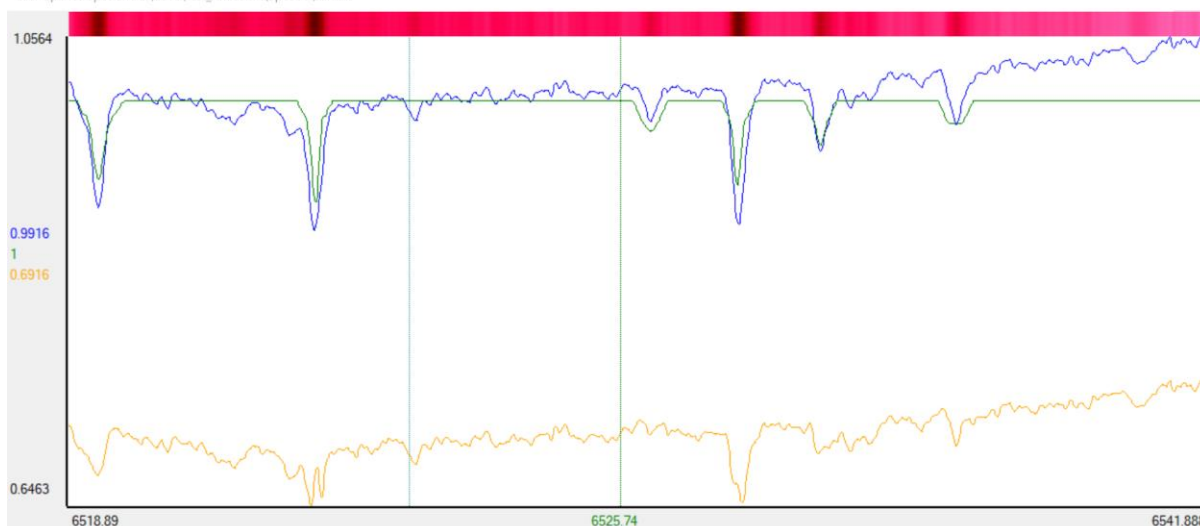
Shift

Apply

Modify single

Cancel

User opened spectrum: E:\2018\Test_ArNeShift\Spectro\sum.fit



Click on “Modifi single” and the Remove Telluric window turns to blue.

Click on the reference line you want to change and change the parameters only for this line.

Modify the single telluric line

Set Crop Area via Cursor

6452.263

Crop

Save as

☐ Titel

Pos

6682.535

Reset Crop and Telluric

☐ Legend

Pos

Set S/N Area via Cursor

6616

S/N: 396

Heliocentric Correction

12.243 km/s

Calculate HC

Apply HC

6619

BeSS Header

Remove Telluric

Back to the Start Window

Set EWA Area via Cursor

6530.003

EWA: -33.66 Å

gamCas 2

Normalize

manual

6604.983

Set Normalize Area via Cursor

Remove Telluric

Strength

Wings

Width

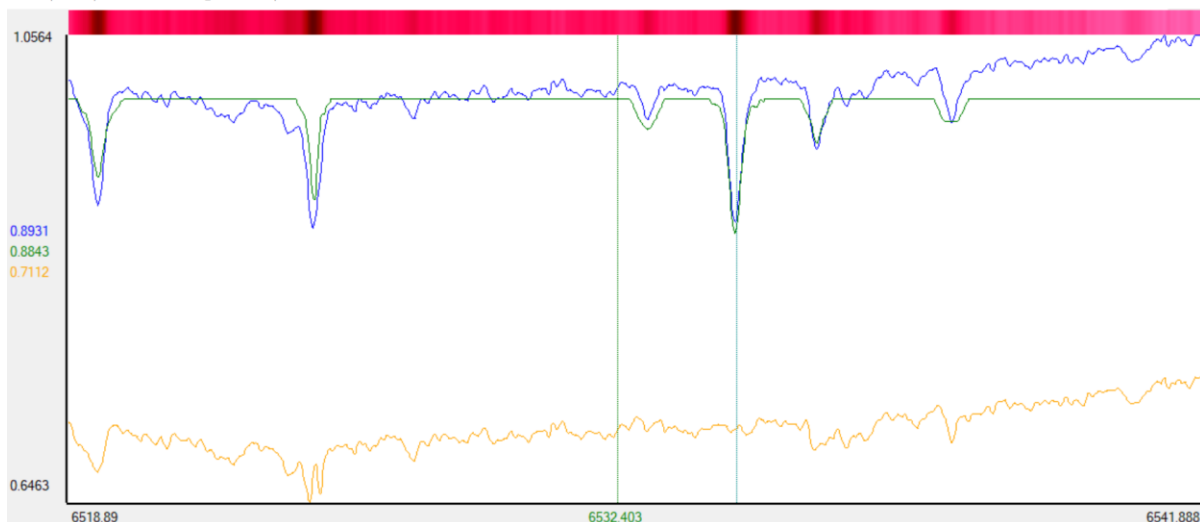
Shift

Apply

Ok

Cancel

User opened spectrum: E:\2018\Test_ArNeShift\Spectro\sum.fit



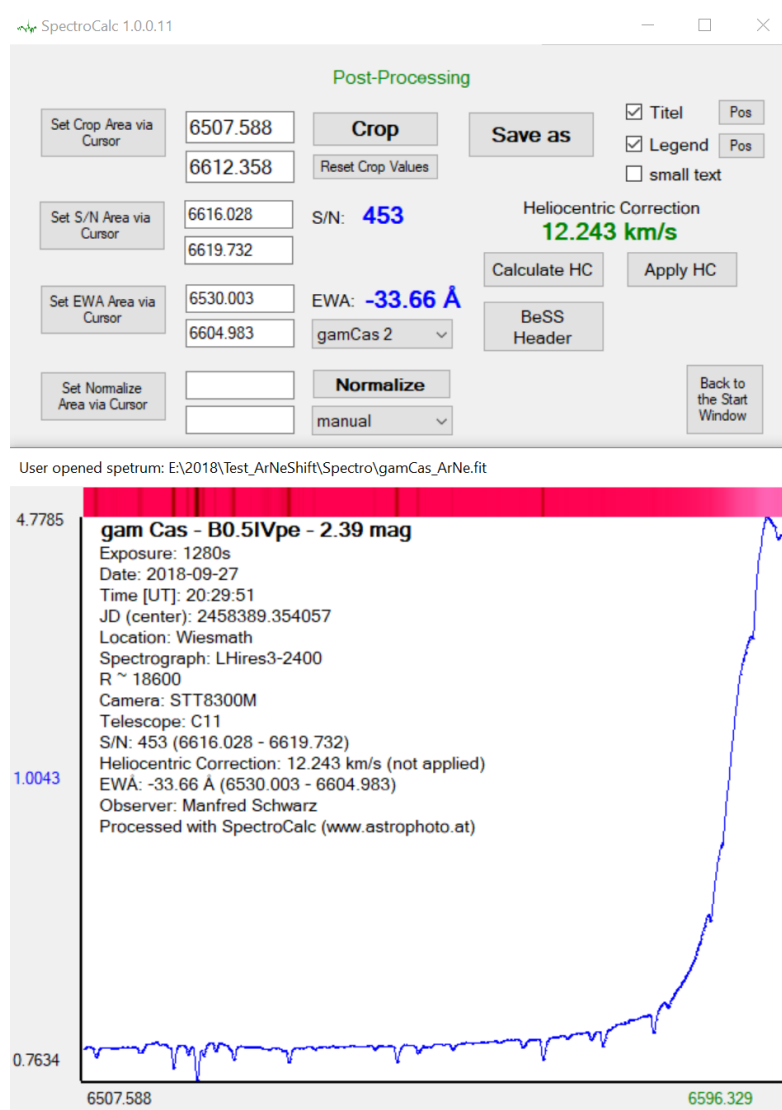
Go through the spectrum and fit all lines.

Press “Apply” to correct the spectrum and dry it from telluric lines.

Attention: Change in the crop size will remove the telluric correction!

For that reason, crop the spectrum first and then make the telluric correction!

Titel and Legend



Title and legend can be displayed if the corresponding checkbox is selected.

“small text” turns the legend to a smaller font.

The title is automatic generated of the object name, the object type and the magnitude.

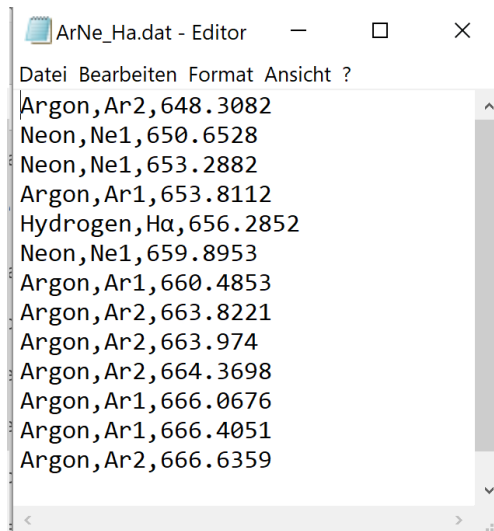
The legend is automatic generated from several parameters of the FITs header.

With the corresponding buttons “Pos”, you can change the position of the title or the legend.

Define a Wavelength-Reference-File

There are different reference files included, like ArNe_Ha.dat or Telluric_Ha.dat, etc.

You can define your own reference file. The file extension has to be .dat.



You can see the structure on this example.

First value of a line is the element name.

It follows a “,” as separator.

Second value is the element sign with the ionisation state.

It follows a “,” as separator.

Third value is the wavelength in nanometre (nm)!

There is also included the file C:\SpectroCalc\elements.dat. You can use this as base for a new reference file, take only the desired lines.

Conclusion

For me, SpectroCalc is a really important tool which speed up my workflow extremely. For example 35 pcs of epsPer spectra exposed in one night needs about 6 hours work to get calibrated and continuum removed spectra, now it takes about 10 to 20 minutes. Further features are planned.

For all bugs and your proposals, please contact me: ms@astrophoto.at

Software Installation and Updates

Environment:

- Windows 7 or higher
- 4GB Memory
- For optimal handling: Full-HD or better resolution
-

SpectroCalc is available at: <https://www.astrophoto.at>

On each start of the software, it is looking for updates and ask you for installation, if an update is found.

Software Version Release Notes

V1.1.0.6- 2019-07-02

- Improvement of the spectra-scan feature, now SpectroCalc should find always the optimum parameters for scan

V1.1.0.5 - 2019-06-29

- Bug-fix in the area of heliocentric correction

V1.1.0.4 - 2019-05-05

- Message, if the path of specs and references are different
- Bug-fix of repeated log messages of “Spectra Scan” in case of changing scan parameters

V1.1.0.3 - 2019-04-21

- Remove of feature Hot-Dark-Pixel remove, because of creation of too much artefacts

V1.1.0.2 - 2019-04-20

- Bug-fix of BeSS data in FITs header

V1.1.0.0 - 2019-04-13

- Calculate frequency shift in case of average the spectra before wavelength calibration
- 1st official version

V1.0.1.1 - 2019-02-10

- Processing of 1D FITs files

V1.0.1.0 - 2019-01-06

- Post-Processing: Remove Telluric
- Bug-fix: Windows 7 problem at start application

V1.0.0.12 - 2018-12-30

- Bug-fix: FITs file read

V1.0.0.12 - 2018-12-30

- Titel and Legend
- Post-Processing: Normalize

V1.0.0.10 - 2018-12-29

- Wavelength calibration: Extreme improvement of accuracy of reference line finding
- Wavelength calibration: Manual add line support
- Wavelength calibration: line delete support
- Wavelength calibration: Zoom In/Out support
- Post-Processing: Heliocentric correction
- Post-Processing: BeSS Header Data
- Synthetic spectrum stripe on the top of the graphic

V1.0.0.8 - 2018-12-10

- Add of Post-Processing feature
- Post-processing: Crop
- Post-processing: S/N
- Post-processing: EWA

V1.0.0.7 - 2018-11-30

- changes in the spectra colours for better preview
- Extend the log file with calibration parameter

V1.0.0.6 - 2018-11-10

- Window overlapping on small screens
- Sky background area can be resized

- Sky background spectrum is zoomed for a better view

V1.0.0.5 - 2018-11-01

- Window sizes depending screen resolution

V1.0.0.4 - 2018-10-27

- Non official Beta Version

April 2018

- start of the development