

# Manual for MagicSERS3

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last Update: 25. Nov. 2005





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## 2. About this program

MagicSERS3 is a Program to view and convert spectra which are produced by the Winspec-Software from Roper Scientific. All known versions of the software and produced files are supported from Winspec32 and Winspec16.

It is also possible to load Tab separated textfiles but then some features are disabled.

The main problem when you measure tons of spectra is the fast overview over all of them. With this Program its possible to load a large numbers of files into a list and then scroll very fast through the spectra, also if there are spectra series with thousands of spectra in one file it is possible to view every single spectra separately and save or copy it to an other program.

An other use should be to find peaks in the spectra (work only with small peaks like raman or low temperature fluorescence bands).

If you prefer to use an other program to view or analyse the spectra its also possible to only convert all spectra into a Tab separated textfile

For this Manual:

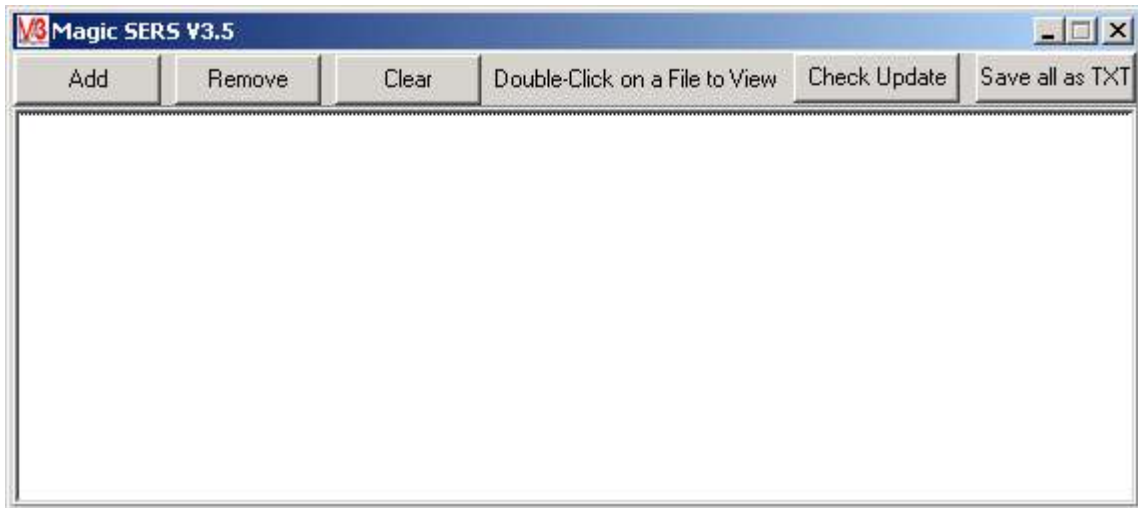
*italic* - Means buttons or text in the program.

**Bold** - Means keys you can use for shortcuts

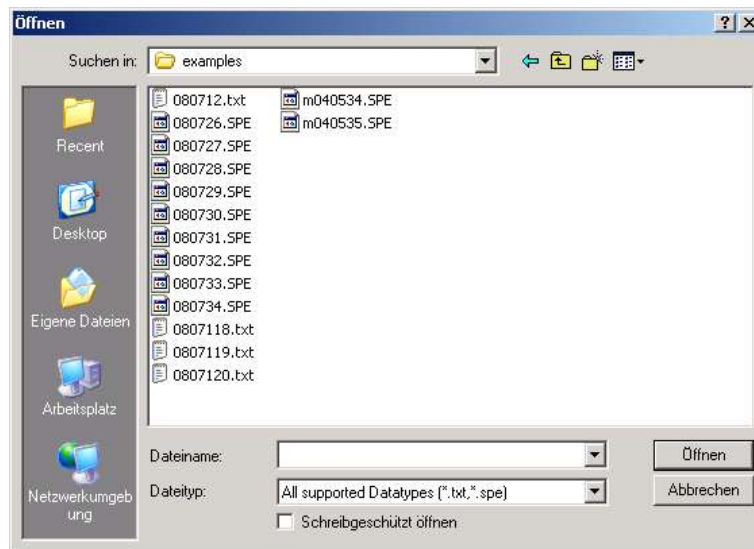
### 3. The windows

#### 3.1. The main window

When open the program the main window will open (Picture 1). The most important things in this



Picture 1: Main window



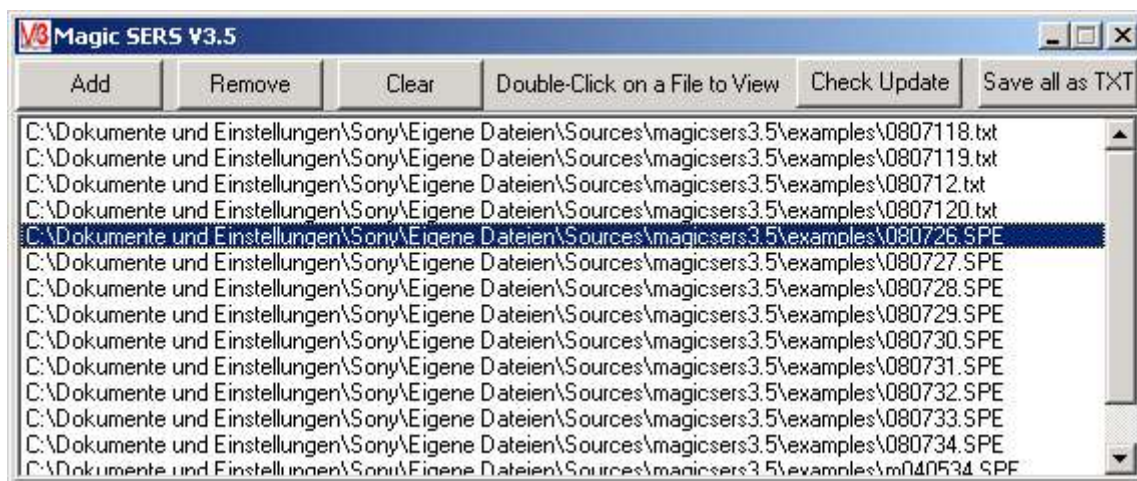
Picture 2: Open-requester of Windows XP

window are the *Add*, *Remove* and *Clear* buttons and the file list under this buttons. A press on *Add* button opens a standard windows open-requester to add some files into the file list (Open-requester of Windows XP for example shown in Picture 2). As default only supported file extensions are shown, for Winspec files “.SPE” for textfiles should be “.TXT”. With a click on *All supported Datatypes* it

### 3. The windows

can be changed to show only Winspec or textfiles or all files (especially useful for textfiles with other extensions). In this requester now can be marked one or more files (add more then one by hold **shift** or **control** key). SPE and TXT files can be mixed. After click on *Open* the files are added to list (like in Picture 3). The files are automatically sorted in the list.

An other way to add files to the list is Drag'n'Drop simply drag a file over the list and let it fall then it will be added and sorted in.



Picture 3: Main window with loaded files

With a single click on a name you can select a file and remove this file from the list with the *Remove* button. The *Clear* button clears the whole list (back to Picture 1).

The button *Check Updates* performs a check if there is a new Version available in Internet. For this a Internet connection (to website <http://www.alb42.de>) is mandatory. The Program only gets the number of the newest version and compares with the current version no data is send to the webserver. If function works a window appear and show both version numbers the current installed and the version number available in Internet. If there is a newer version available please update fast as possible to the newer version, especially if you found and error and want write a bugreport. Go to <http://www.alb42.de/projekte> and click on the MagicSERS3 Logo to get the new Version.

The *Button Save all as TXT* converts the whole list into tab separated textfiles with a 3 lines header. The files are converted into the directory which you can choose by a requester which open after click on this button. The files have the same name like the original file but with a .TXT extension. After conversation a message shows how many files are successfully are converted.

==> **BE CAREFULLY:**

**If this filename already exist the file will be simply overwritten without question before, especially dangerous if TXT files are in the list and the same Folder is selected like the original file.**

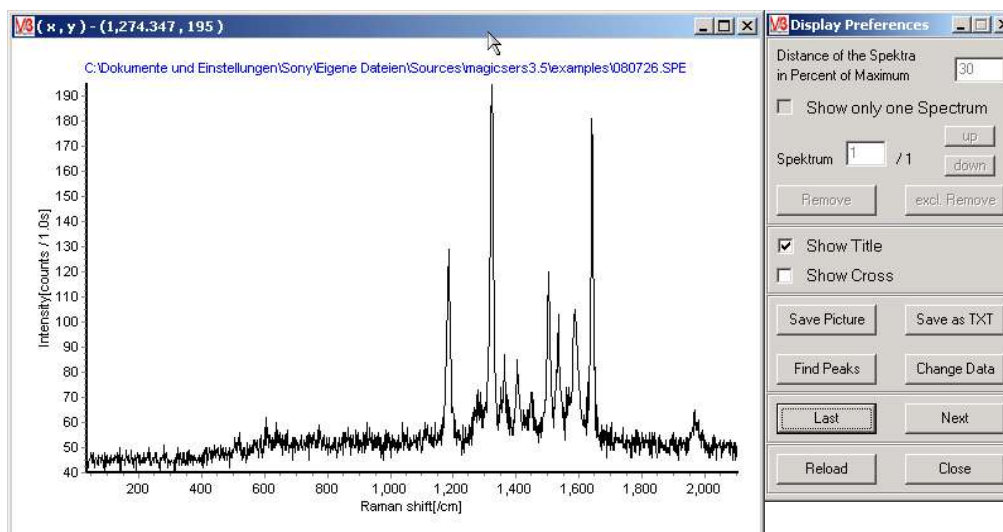
The header included the original name of the file the x- and y-axis. For example for x-axis: “Intensity [counts/10s]” and for y-axis: “raman shift [1/cm]” so in this case the integration time is 10 seconds below 0.1s its converted to milliseconds.

Close this main window will close the whole program and all other open windows.

A double click to a file in the list try to read this file and show the spectrum. If it fails a message will appear. If everything works fine two windows will appear, the *Display* and the *Display preferences* window (Picture 4).

### 3.2. Display and Display Preferences

Both windows comes always together so if you close one the other will be closed also.



Picture 4: Display and display preferences window

The *Display* window shows the current spectrum the window is free resizable and can be also maximised to full screen. The graphic will be automatically scaled with the window. In the titlebar of the window the current co-ordinates of the mouse position is shown if the mouse is situated in the spectrum.

To zoom the spectrum simply click with left mouse button into the window hold the button and drag the frame to the size you wish. If you want zoom in first choose the upper left point and drag the frame down right. If you want reset the zoom and back to normal view first choose lower right point and then drag the frame up to left. When you release the button the operation will be done.

The spectrum is also moveable simply click and hold right mouse button in the window and move the mouse then the spectrum will move in the same way.

A click on the x- or y-axis will open the axis window to change the scaling and names of axis. (see in chapter 3.3).

The name of the file belongs to this spectrum is shown as title over the spectrum self, can be hidden in *Display Preferences* window with the checkmark named *Show Title*. If it is a single file the Standard is that he name is shown. If multiple files are loaded and shown in the window the title is hidden (see chapter 3.5).

The checkmark *Show Cross* adds additional lines to the cursor when moving in the spectrum so its



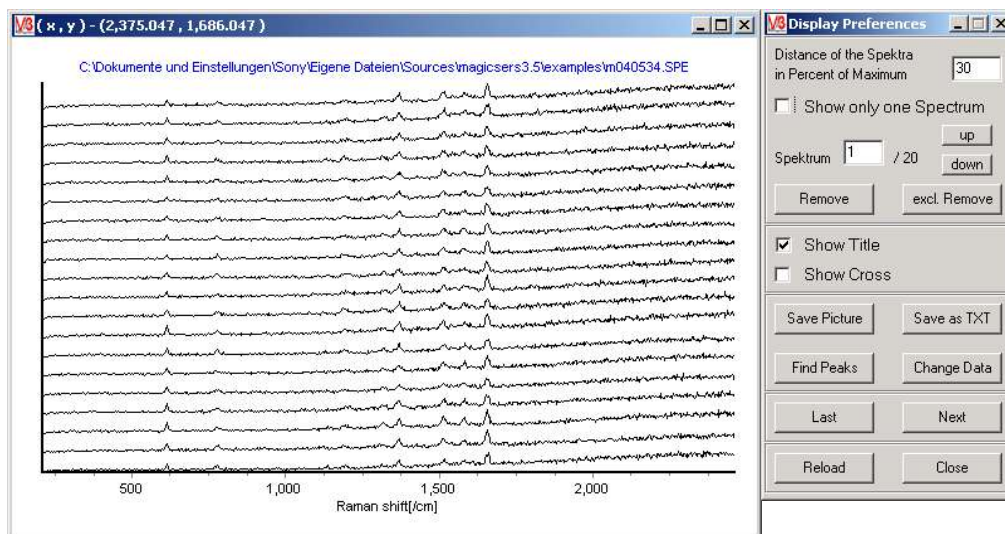
### 3. The windows

easier to point to maxima or other features.

A file can be also dragged and dropped on the *Display* window then this file will be showed but not be added to the list in *main window* to add this file to the list drag and drop it to *main window*.

All buttons over this two checkmarks belongs to multiple spectra (so they are disabled if only one spectrum shown).

If multiple spectra shown in one window the main problem is to see the spectra if they have very similar range of data. One way to show them together is to move one of the spectrum a little bit higher (means add an offset to the spectrum). How much is controlled by the value *Distance of the Spectra in Percent of the Maximum* standard is 30 and a good value for most spectra. The name explains what it do. It calculate the maximum of the spectrum and calculate a percentage of this maximum given by this value and adds this to the 2<sup>nd</sup> spectrum and to the 3<sup>rd</sup> double and so on.



Picture 5: Display and display preferences with a spectra series

If you click directly onto one spectrum the number will be shown in the field behind the label *Spektrum* there is also the absolute number of all spectra shown. If you now click on *Remove* this spectrum will be remove from the window (can be restored with *Reload*). With *excl. Remove* all other spectrum except this selected one will be removed.

The number of the spectrum can be also typed by hand into this field or changed by the buttons *up* and *down* on the right side of the field.

Its also possible to let only one spectrum draw from a spectra series. From multiple display to single display can be switched by the checkmark *Show only one Spectrum*. With *up* and *down* is it possible to scroll through the spectra of this series. Instead of using the buttons you can use the keys **q** for switch between single view of spectra and multiple display, **w** for *up* and **s** for *down*.

If the series contains more then 100 spectra its not possible to switch to the multiple mode only single mode available. When scroll over the 100. spectrum the program load the next 100 spectra to display so there is a little break.

There are multiple ways to save this picture. You can use the Button *Save Picture* a save requester appears then give in a name and a extension .BMP or .WMF the program will automatically choose the corresponding format. With *Save as TXT* is it possible to save the current shown dataset as a textfile. You can also use the clipboard to export the picture, with **Ctrl+T** you copy the current shown dataset as tab separated text into the clipboard from there you can paste directly to Origin or Excel.

For copy the picture into the Clipboard you have two ways one is **Ctrl+C** then it will be copied as a Bitmap (so you should first change the size of the window to the size you need) the other way is **Ctrl+X** then the Picture is copied as EMF to clipboard so you can scale it free later.

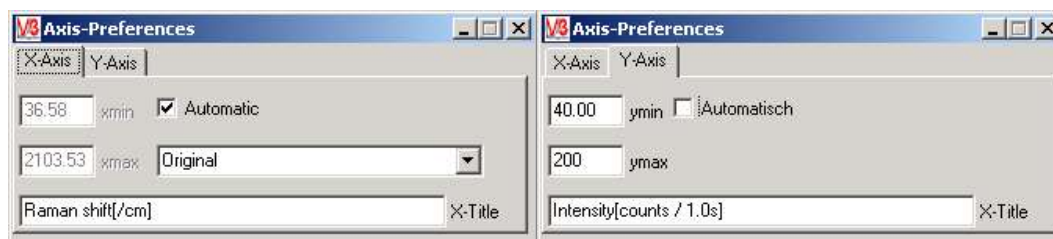
The next two Buttons are *Find Peaks* and *Change Data* the first search for peaks and show them, this is exactly explained in chapter 3.4. With *Change Data* it is possible to create a multiple display of spectra from different files, its exactly explained in chapter 3.5.

With *Next* and *Last* you can go to the next or previous spectrum file in the list in *main window*(chapter 2.1). You can also use keys for it. Press **d** for *Next* and **a** for *Last*.

The last line of buttons contains the *Close* button which do the same like close the *Display* or *Display Preferences* window and the *Reload* button which performs a complete reload of the file and redisplay very useful if you found and error or to remove all markers or so on.

### 3.3. Axis window

The Axis window (Picture 6) opens when you click on an axis in the display. Its not important if you click the x-axis or the y-axis you get always the same window but the tab belongs to the axis you clicked on.



Picture 6: Axis window with tab for x- and y-axis

In this tabs you can set the scaling of the graphic by type in the minimum and maximum value for each axis or let the program choose automatic the best values by turn the checkmark *Automatic* on.

You can also change the title of the axis in the last field in this window.

A special thing is in X-Axis tab there you can choose which unit the x-values are shown. This Option is only available if a SPE file is loaded. The standard is *Original* this use the same unit like in the SPE file is written (should be the same like shown at the measurement).

Other possibilities are:

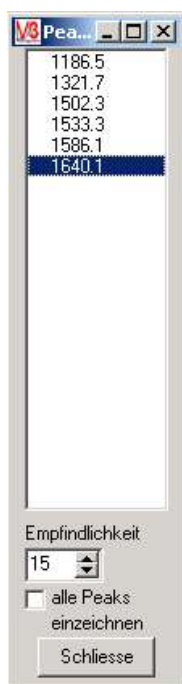
*Pixel* then the number of the CCD Pixel is shown, in principle is this the raw-data,

*Wavelength [nm]* then the wavelength  $\lambda$  in nm is shown.

*Wavenumber [1/cm]* means the reciprocal of the wavelength  $1/\lambda$  in  $\text{cm}^{-1}$

*Raman shift [cm]* then relative wavenumber to the laser-wavelength is used  $(1/\lambda_{\text{laser}})-(1/\lambda)$  in  $\text{cm}^{-1}$   
if the window is closed the *Display* window will not be closed, but if the *Display* window is closed this window will be closed also.

### 3.4. Peaksearch

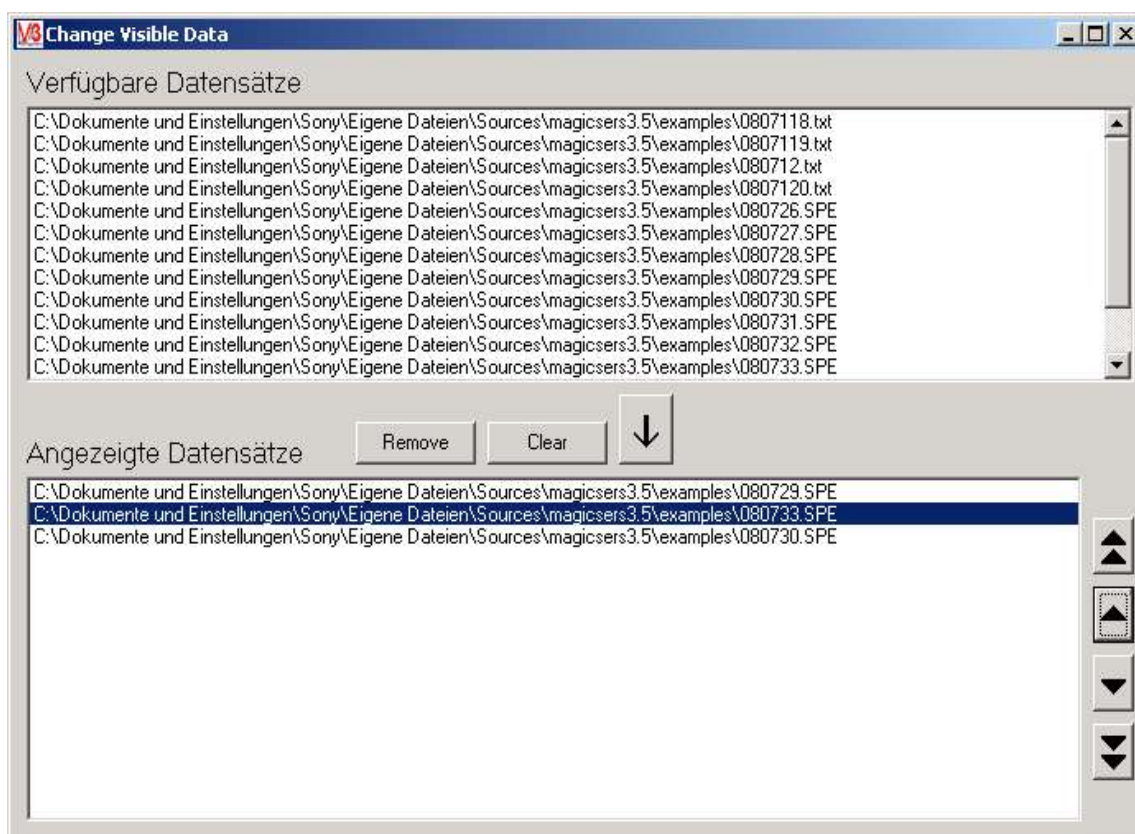


Picture 7:  
Peaksearch  
window

The program is able to search for peaks in a given spectrum simply click on *Find Peaks* in *Display Preferences*. For an easier finding of peaks a smoothing is done for the whole spectrum (only for finding, not shown) and then a calculation of gradient is done. The highest founded peaks are shown in a list in the *Peaksearch* window (Picture 7). The sensitivity of choosing the peaks can be changed by type a number in the field *Sensitivity* or use the up and down arrow next to this field. When you click on one entry in the list of peaks this peak will be marked in the spectrum by a black vertical line. If you click on a already marked peak the mark will be deleted again. You can also mark all peaks in every spectrum you load into the display by set the checkmark at *Mark all Peaks*. The peak search works quiet well for raman spectra or other spectra with small line width broad bands like in fluorescence spectra cant be found exactly. The *Close* button closes the *Peaksearch* window but let the *Display* window open. When the *Display* window is closed this window is closed also.

### 3.5. Change Data

If you want combine some single spectrum files to a series you can use the function *Change Data* in *Display Preferences* window. It will open a new window named *Change Visible Data*. There are two



Picture 8: Create series with Change Data

lists the upper one shows all available files (in principle a copy of the list in *main window* . The lower one shows the files which are shown in the *Display*. To add new files to the display list simply double click on a file in the upper list or use the big down arrow. By choosing one file in the lower list and press the *Remove* button you can remove files from this list. The *Clear* button clears the whole display list. On the right side of the display list are four little arrows to adjust the order of the files in the display list. Click on one file and use the single up arrow to move the file down or the double arrow to set this file as first file. Same for down arrows.

.SPE and .TXT can be mixed, one file can be some times in the display list. The drawing of this list is performed when the window is closed. The dataset will be handled like a series of spectra in one file with some exceptions:

The title is disabled in *Display* window and a reload will destroy the dataset back to a single spectrum but can be restored with a open of *Change Data* and close again.

### 3.6. Shortcuts

A summary of all shortcuts usable in the *Display* or *Display Preferences* Window

- a** - load previous spectrum in list (like click on *Last*)
- d** - load next spectrum in list (like click on *Next*)
- q** - switch between single display or multiple display of a series of spectra
- s** - show the previous spectrum of a series of spectra (like click on *down*)
- w** - show the next spectrum of a series of spectra (like click on *up*)
- Ctrl+c** - copy the current display as bitmap into the clipboard (for use in graphic programs)
- Ctrl+t** - copy the dataset as a tab separated text into the clipboard (useful for Excel or Origin)
- Ctrl+x** - copy the current display as scaleable vector picture to clipboard (for vector based draws)
- Alt+F4** - close the *Display* and *Display Preferences* window

## 4. Greetings and Thanks

Thanks goes to the many people who help to improve this program by wishes and bug reports especially Christian Blum and Tim Vosgróne.

Special thanks goes to Andreas Lieb who wrote a script to load SPE files into SXM it was very helpful to learn how SPE files work, even I used later a completely different method.

Thanks to Mathias Steiner for gave me a file with 20.000 spectra (size 51.1 MB) to develop and test the loading of very large files and improve the speed of loading and display.

I'm also very thankful for the interesting discussion with Friedrich Menges the programmer of Spekwin32 (<http://www.agdal.chemie.uni-konstanz.de/menges/spekwin/>).