SpecPlot — NMR Spectrum Plot File Generator

User Manual

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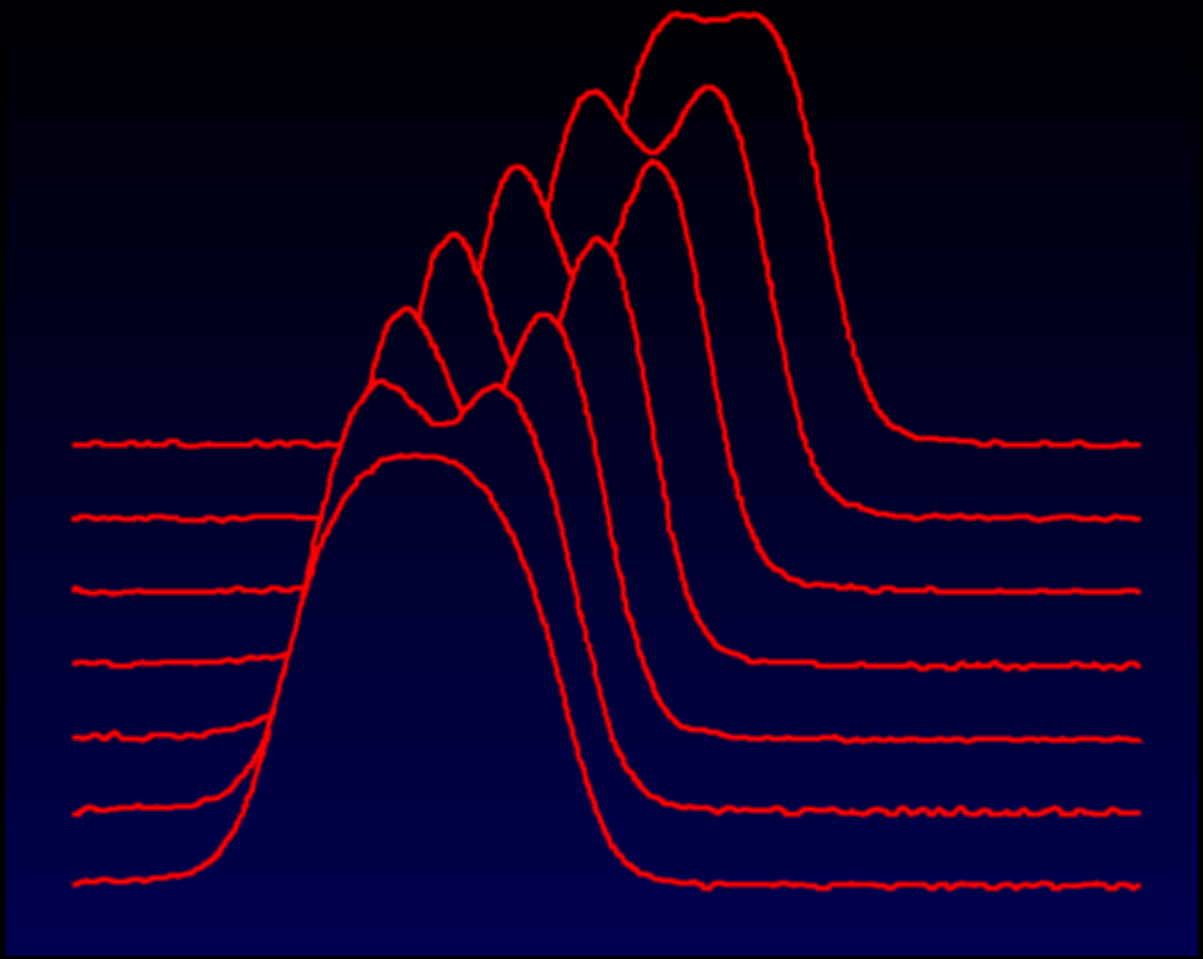

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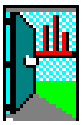
1 Getting Started

This chapter covers the following topics:



Introduction (p. 5)	An introduction to SpecPlot
Overviews (p. 8)	An overview of some of the common tasks and actions
Revision History (p. 6)	Summary of changes versus previous versions
Acknowledgements (p. 10)	Credits for important contributions etc.

1.1 Introduction

1.1.1 Purpose of the Program

The name of the program, SpecPlot, is pretty generic and indicates its use: read an NMR spectrum and create a vector graphic file that can be imported into most decent graphics programs and desktop publishing programs. Initially, the output format was a file compatible to Hewlett-Packard's Graphics Language, HPGL. In the nineties of last century this was a vector graphics format supported by many different programs and had the advantage that it is very easy to program. Nowadays, this support is a little lacking (for example, CorelDraw 4 had a very nice import filter, but version 11 does a poor job; even Microsoft's PowerPoint does better but will require to separately download and install the import filter, HPGLIMP32.FLT, from their web site).

Recently, the default output format has been switched to PostScript while maintaining the option to produce HPGL. Personally, I am using these postscript files in combination with MiKTEX or convert them to PDF format using MiKTEXś `epstopdf` tool. The resulting PDF can be enhanced using InkScape. Microsoft Office (2003, 2007) is also able to handle the postscript files.

SpecPlot has been written in C++ using Borland C++ 4.52 and has been developed to run on IBM-compatible personal computers under the MS-Windows environment. For the 32-bit version, Borland C++ 5.0 has been used initially. The current version has been produced using Microsoft Visual C++ 2008 Express Edition. A lot of the code is based on experience I gained by writing and working with the DOS programm SOLIDS (written in FORTRAN). The current program is actually a spin-off of a larger package, WSolids, aimed at simulating solid-state NMR spectra for a variety of nuclear spin interactions and experimental conditions, and is planned to interface with that package

1.1.2 Features

- read a NMR spectrum in any of the file formats supported by WSolids
- plot this spectrum into a HPGL or postscript file
- a wide variety of parameters are available to customize the output; more control of the layout is possible than with most NMR programs
- the resulting plot file can be copied to a HP plotter, HP printer, or imported into a variety of software programs for further enhancements. So far, the following programs have been tested:

- WordPerfect 6-8
- Corel Presentations 8
- Corel Draw 4-10
- Micrografx Designer 7
- Microsoft Word 97 and Microsoft Powerpoint 97 (works better than Word)
- InkScape

1.1.3 License

This program package can be used by any individual or organization without any fee, as detailed in the Copyright (p. 11) statement.

1.1.4 Troubleshooting

Although SpecPlot has been tested and used both in-house and by others, it is always possible that errors still exist. Some errors may become apparent after detailed use. It is the responsibility of the user to determine the correctness of the results. As stated in the Disclaimer (p. 11), we disclaim all warranty. If errors are noticed, please notify us of your problems, and the prescribed or suggested corrections, so that others may benefit from the improved code. Also, suggestions for improvements are always welcome. You can address your correspondence to:

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1.2 Revision History

This page summarizes changes made compared to previous versions of SpecPlot. Experienced users may use this information as a quick update on new program features.

1.2.1 New in Version 1.2.29 (20.05.2021)

- Neither bug nor feature: determination of the Adobe Acrobat version looks up now a registry key to determine the proper version of the Acrobat DDE server

1.2.2 New in Version 1.2.24 (19.06.2015)

- New feature: the location of the INI file has changed: in the pogram's directory for the portable version, or in the user's documents/WSolids directory.
- New feature: the documentation in PDF format supports context sensitive help for the following PDF viewers: PDF-XChange Editor (by Tracker Software Products, Ltd., `http://www.tracker-software.com`), **currently my prefered PDF viewer**, the successor of PDF XChange Viewer (by

Tracker Software Products, Ltd., http://www.tracker-software.com), Sumatra PDF Viewer (http://blog.kowalczyk.info/software/sumatrapdf), also deal with Adobe Reader X and pre-X versions of Adobe Reader.

- New feature (or bug?): for postscript output, we deal with the `plot speed` every time to allow for different line widths; because there is only one global speed setting, this will also affect the axes etc., if plotted together with the spectrum.
- Bug fix: toggling the absolute intensity mode did not reinitialize.
- Bug fix: for small spectra (small SI), the spectrum end was drawn too far to the right.
- Bug fix: fixed a bug when plotting the axis for part of an FID.
- (Bug fix): some programs export spectra to JCAMP file format with XUNITS of PPM, although the IUPAC standard specifies Hz; we are more relaxed on that issue now.

1.2.3 New in Version 1.2.20 (08.02.2011)

- basically a build to synchronize with my other NMR programs
- bug fix: reading JCAMP-DX files

1.2.4 New in Version 1.2.19 (25.05.2010)

- added absolute maximum to skip modes
- added layout parameters for scaling CY to highest peak absolutely or within range
- some minor bug fixes

1.2.5 New in Version 1.2.11 (29.05.2009)

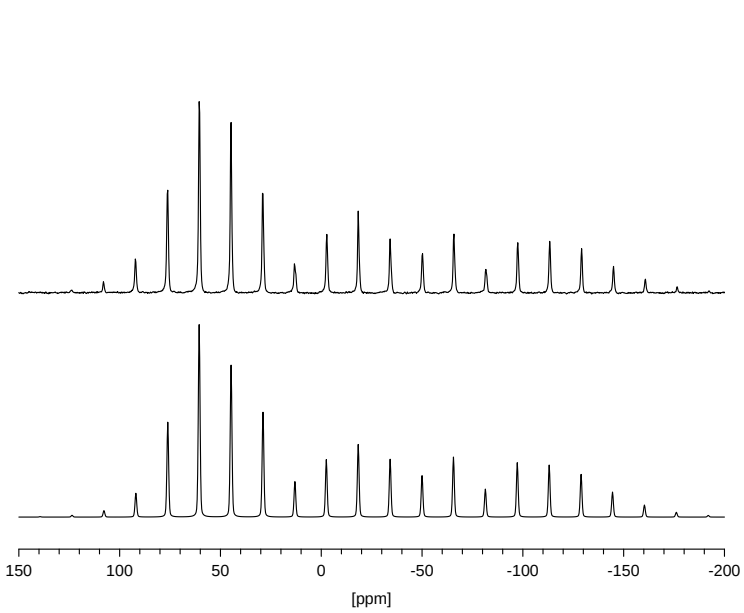
- added plot text option
- added plot logo option
- use PDF instead of WinHelp
- added skip modes
- added handling of postscript format
- adjusted handling of FID, especially the calculation of digits to avoid problem with log10(0)
- increased the resolution (number of digits) in the HPGL output
- deal with normalization constants of Bruker Xwinnmr spectra
- added checkbox for HPGL command IW on single spectrum plot layout dialog
- added parameters for plotting in absolute intensity mode, to generate WMF output, and to divide the labels by a divisor

1.2.6 New in Version 1.0.5 (22.05.2001)

This is the first documented release.

1.3 Overview

Because SpecPlot does not have a graphical interface the production of a decent plot file can be difficult for a new user. This short guide might be helpful. It explains how to plot an experimental and calculated spectrum to the same file. The layout is best for an experimental and calculated MAS spectrum showing chemical shift anisotropy; a text file coming from the program HBA is added to the plot to provide the parameters:



WSolids

```
*================================*
     Herzfeld-Berger Analysis
     Fitting Results HBA V1.6.9
     Wed Jun 10 19:39:17 2009
*================================*

data source:
F: mrKOOPH2BU 001.PP

Iterations:                     6
Chisq:                      0.209
lsq:                        0.015
Mu:                        14.070
Rho:                        1.000

SF:                        81.023
Rot:                     1277.000
Shift:                     -2.540

Delta_11:                  76.107
Delta_22:                  76.107
Delta_33:                -159.834

Shift:                     -2.540
Span:                     235.941
Skew:                       1.000
Red. anisotropy:         -157.294
Anisotropy:              -235.941
Asymmetry:                 -0.000

SSB    Exp.      Calc.    Calc.-Exp.
=========================================
 15   0.0000   0.0000   0.0000
 14   0.0000   0.0000   0.0000
 13   0.0000   0.0000   0.0000
 12   0.0000   0.0001   0.0001
 11   0.0000   0.0003   0.0003
 10   0.0000   0.0017   0.0017
  9   0.0000   0.0075   0.0075
  8   0.0436   0.0313  -0.0123
  7   0.1863   0.1123  -0.0740
  6   0.5841   0.4147  -0.1694
  5   1.8009   1.6523  -0.1486
  4   3.3439   3.3493   0.0053
  3   2.9462   2.6424  -0.3037
  2   1.7918   1.8234   0.0315
  1   0.5024   0.6157   0.1132
 -1   1.3984   1.2641  -0.1343
 -2   0.9281   1.0058   0.0857
 -3   0.6769   0.7205   0.0437
 -4   1.0157   1.0452   0.0295
 -5   0.3978   0.4865   0.0887
 -6   0.8573   0.9463   0.0890
 -7   0.8802   0.9053   0.0251
 -8   0.7526   0.7431  -0.0094
 -9   0.4498   0.4360  -0.0137
-10   0.2331   0.2109  -0.0222
-11   0.1023   0.0837  -0.0186
-12   0.0000   0.0287   0.0287
-13   0.0000   0.0086   0.0086
-14   0.0000   0.0023   0.0023
-15   0.0000   0.0005   0.0005
=========================================
```

1. start SpecPlot, select ”File—Plot single spectrum”
2. for the purpose of illustration, I have created a layout file containing the parameters for the experimental spectrum:
   press the button ”Load” and select the file **specplot_expe.ini**
3. select the required experimental spectrum by entering the path or use the appropriate ”select” button
   (the current preset assumes that experimental and calculated spectra have the same limits and should be plotted in total; if this assumption is not valid, unselect ”update F1,F2 upon reading” and enter the correct values for F1 and F2)
4. select or provide the name of an output file
5. press ”OK”, this should create the output file
6. select the layout file for the calculated spectrum:
   ”File—Plot single spectrum”
   ”Load”
   select **specplot_calc.ini**
7. select the calculated spectrum
8. same output file as for the experimental spectrum (note that the option ”append to data, if file exists” is activated)
9. ”OK”
10. select ”Add logo to postscript file”
11. select ”Add text to postscript file”, as file select **iterate.txt** in the HBA directory
12. exit SpecPlot

With some practice, one will not use two different layout files but will change the parameters directly. If you found some useful parameter settings satisfying your preferences, press ”as Default” to store them.

1.4 Acknowledgements

This section covers the following topics:

Credits (p. 10)	Credits for important contributions
Trademarks (p. 10)	Trademark acknowledgements
Copyright (p. 11)	The obligatory copyright statement
Disclaimer (p. 11)	The obligatory disclaimer message

1.4.1 Credits

- the HPGL output is based on the manual *HP 7475A — Interfacing and Programming Manual* by Hewlett-Packard Company, San Diego, CA, 1987
- the Postscript output is based on the "bluebook" *PostScript Language — Tutorial and Cookbook* by Adobe Systems Inc., 1987, and the "redbook" *PostScript Language — Reference Manual* by Adobe Systems Inc., 1987.
- Microsoft for providing `Visual C++ 2008 Express Edition` for free
- Jordan Russell for making `Inno Setup` available (`http://www.jrsoftware.org/`)
- Jochen Kalmbach for demonstrating how to statically link against the Microsoft CRT and thus get rid of `VCREDIST_X86.EXE` (`http://blog.kalmbach-software.de`)
- "chicks" for demonstrating in his `pdfp` PDF tools how to establish Dynamic Data Exchange (DDE) with Adobe Acrobat (Reader) (`http://www.esnips.com/web/PDFTools`, website not available anymore).
  Here are some "substitute kudos" pages: `http://www.quickpdf.org/forum/printdocument-blank-pages_topic688.html` or `https://www.techrepublic.com/forums/discussions/want-to-print-pdfs-from-access-form/`.
- This manual has been produced using the MiKTEX (`http://www.miktex.org`) distribution of LATEX in combination with the TeXstudio editor (`http://texstudio.sourceforge.net/`), or TeXnicCenter editor (`http://www.ToolsCenter.org`) initially.
- **Irfan Skiljan**'s `IrfanView` (`http://www.irfanview.com/`) has been used to process bitmapped images, and `Inkscape` (`www.inkscape.org`) for dealing with vector graphics.

1.4.2 Trademark Acknowledgements

- *Microsoft (MS)* is a registered trademark and *MS-DOS* and *MS-Windows* are trademarks of Microsoft Corporation.
- *WIN-NMR* is a product of Bruker-Franzen Analytik GmbH.
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1.4.3 Copyright Information

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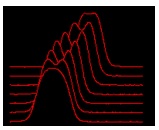

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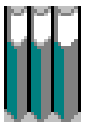
2 Reference

This chapter contains information on the following topics:



Help on Menu Items (p. 13)	Explains the meaning of specific menu items
Known Problems (p. 23)	Summarizes known problems

2.1 Help on Menu Items

Category	Menu Item	Action
File	Plot single spectrum (p. 14)	Plot a single spectrum to a file
	Add logo to postscript file (p. 22)	Add the WSolids logo to the postscript file
	Add text to postscript file (p. 22)	Add the content of a text file to the postscript file
	Exit (p. 22)	Exit the program
Help	Content (p. 23)	Calls a PDF Reader and displays the contents page for this help file
	Search for help on (p. 23)	Opens a dialog box to search for a specific keyword
	About (p. 23)	Displays version information

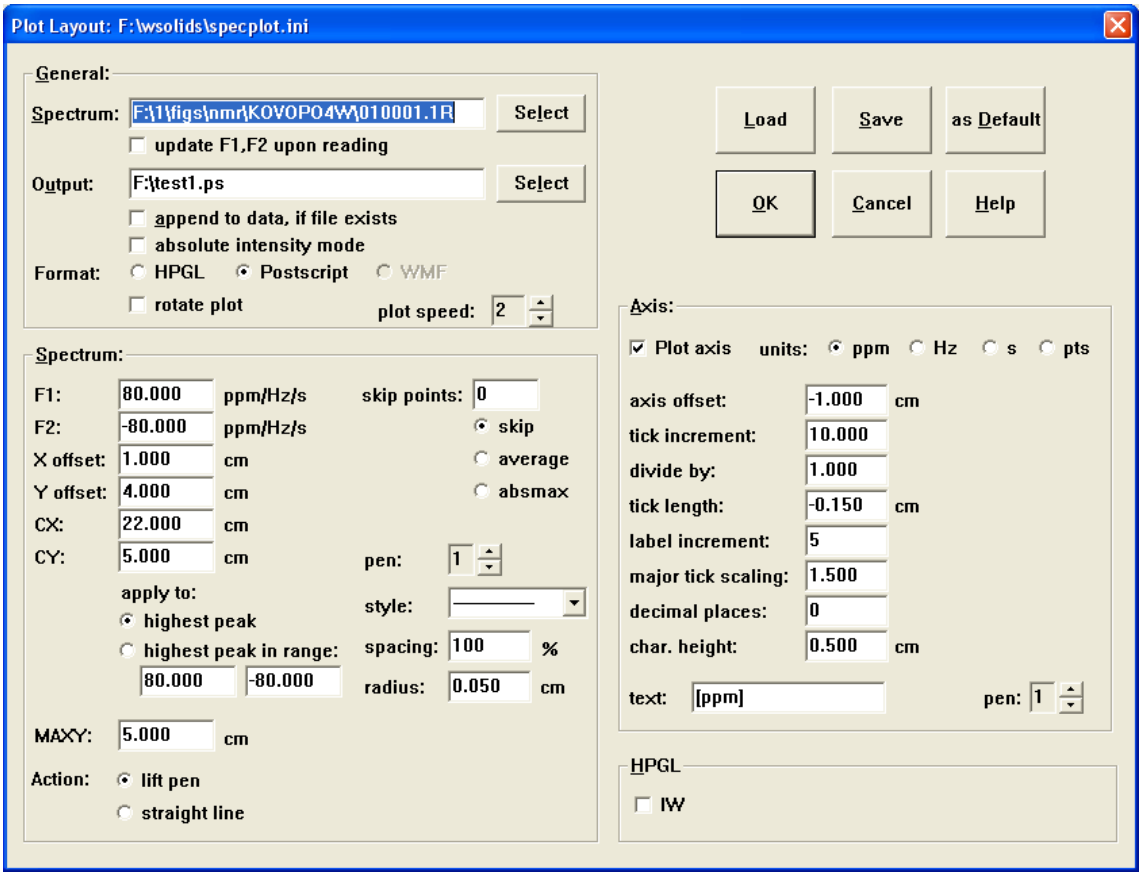
2.2 Plot Single Spectrum

The option to plot a single NMR spectrum is available from:

- the menu via **File|Plot single spectrum**

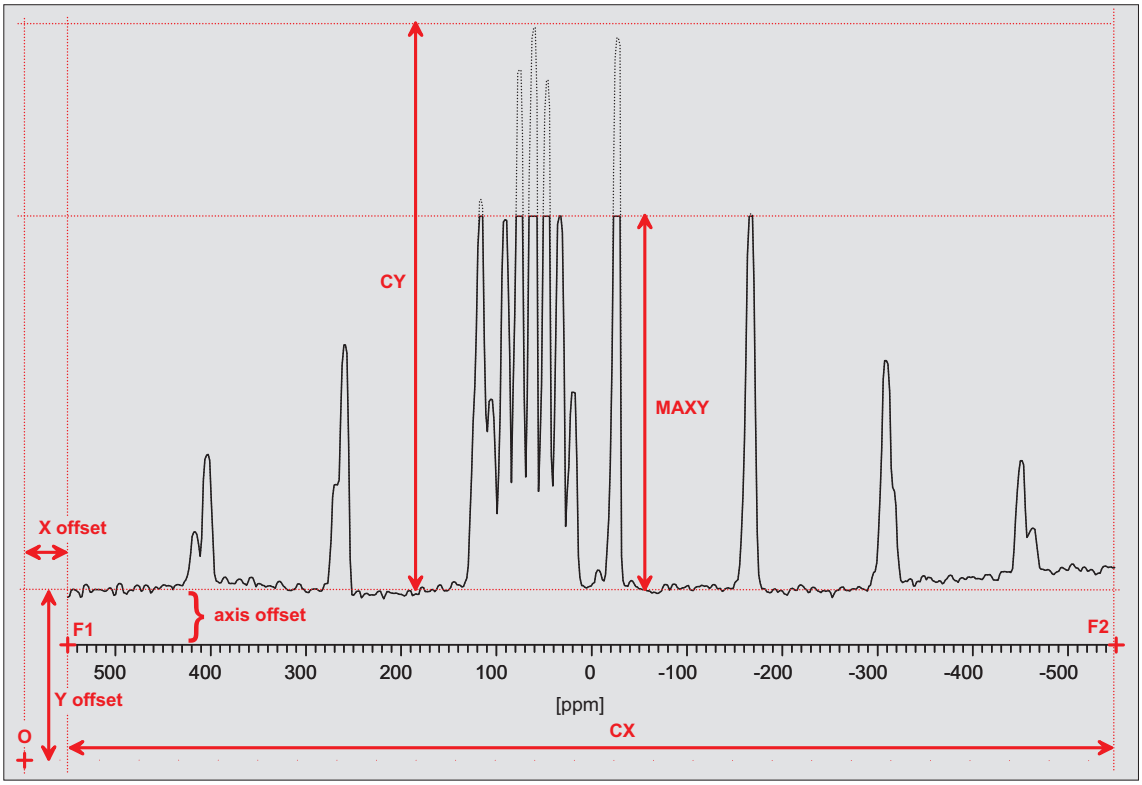
Purpose

The dialog box allows to customize to a high degree the outcome of plotting the spectrum. The layout can be loaded, saved, and set as default. A wide variety of parameters lets the user control the individual elements of the plot.



Category	Parameter	Comment
General	Spectrum (p. 17)	Enter full name of spectrum or select a file using the select button
	update F1,F2 upon reading (p. 17)	adjusts F1 and F2 according to spectrum settings
	Output (p. 17)	Enter full name of output file or select a file using the select button
	append to data, if file exists (p. 17)	overwrite output file or append at end
	absolute intensity mode (p. 17)	use this spectrum as scaling reference for the following spectra
	Format (p. 17)	format of output file: HPGL or Postscript (WMF is planned)
	rotate plot (p. 17)	rotate output by 90 degrees
	plot speed (p. 17)	plot speed for HPGL or line thickness for Postscript
Spectrum	F1 (p. 18)	left limit of plot range
	F2 (p. 18)	right limit of plot range
	X offset (p. 18)	x coordinate of first plot point (F1)
	Y offset (p. 18)	y coordinate of first plot point (F2)
	CX (p. 18)	width of plot
	CY (p. 18)	height of plot
	MAXY (p. 18)	cut-off height
	Action (p. 19)	action to perform if cut-off height is reached: lift pen or draw straight line
	skip points (p. 19)	number of points to skip or average
	pen (p. 19)	pen for plotting spectrum
	style (p. 19)	line type of drawing
	spacing (p. 19)	spacing if a non-solid line type is selected
	radius (p. 19)	radius of circle, if line type digit is selected
Axis	Plot axis (p. 20)	plot axis, and units to use
	axis offset (p. 20)	offset of axis from spectrum
	tick increment (p. 21)	distance between ticks
	divide by (p. 21)	divide labels by this number
	tick length (p. 20)	length of ticks to draw upwards or downwards
	label increment (p. 21)	put label at every this number of ticks
	major tick scaling (p. 21)	make major ticks longer by this factor

	decimal places (p. 21)	use this number of decimal places to print label
	char. height (p. 21)	size of label
	text (p. 21)	text to put under axis
	pen (p. 21)	pen for plotting axis
HPGL	IW (p. 21)	put IW statement in HPGL file
Buttons	Load (p. 20)	load a layout
	Save (p. 20)	save the current layout
	as Default (p. 20)	save the current layout as default
	OK (p. 20)	plot the spectrum
	Cancel (p. 20)	cancel plotting
	Help (p. 20)	open the documentation



2.3 Plot Parameters

2.3.1 Dialog Title

The dialog title displays location and name of the currently active layout file. By default, this is the SPECPLOT.INI file. It is possible to change this via the Load (p. 20) button. (Using the Save (p. 20) and as Default (p. 20) buttons, the current settings can be saved to a specific file or the SPECPLOT.INI file.)

2.3.2 Spectrum

This entry specifies the NMR spectrum that is to be plotted. Its name can be entered directly into the edit box, or be selected interactively using the **Select** button.

SpecPlot can read all file formats supported by WSolids1, please refer to the WSolids1 manual for detailed information.

2.3.3 Update F1, F2

If this option is checked, the current settings for F1 (p. 18) and F2 (p. 18) will be neglected. After reading the selected spectrum (p. 17), its full width will be used to produce the plot.

2.3.4 Output

This entry specifies the name and location of the output file resulting from plotting the selected spectrum (p. 17). Its name can be entered directly into the edit box, or be selected interactively using the **Select** button. The file will be written in the selected output format (p. 17).

2.3.5 Append to data, if file exists

If this option is checked, the output resulting from plotting the selected spectrum will be appended to the output file, it it exists already. If this option is not checked, the new output will overwrite any existing data.

2.3.6 Absolute Intensity Mode

If this option is checked, the intensity of the currently selected file will be remembered and the following spectra will be scaled accordingly, until this option is deactivated again.

2.3.7 Output Format

Currently, the output format can be either HPGL (Hewlett Packard Graphics Language) or Adobe Postscript.

2.3.8 Rotate Plot

If this option is checked, the plot will be rotated by 90 deg.

Usually, this option is of interest only to people that are using a real plotter or the HPGL emulation mode of their printer.

2.3.9 Plot Speed

This parameter sets the plotter speed in cm/s. Valid values are in the range 0-38. This option is of interest only to people that are using a real plotter.

However, if the output format is a post script file, plot speed determines the line width (in multiples of 0.5 points), in this case at least 2 is recommended.

2.3.10 F1

F1 is the left extreme value of the axis, in units depending on the selection made under axis units (p. 20). The combination of the parameters **F1**, F2 (p. 18) and CX (p. 18) (length of X axis) determines the plot window in x direction. If the high-frequency limit of the spectrum is greater than F1, the spectrum will be clipped to F1. If the high-frequency limit of the spectrum is smaller than F1, the spectrum plot will start at the appropriate position on the x axis.

If the option Update F1,F2 (p. 17) is checked, the current settings for **F1** and F2 (p. 18) will be neglected. After reading the selected spectrum (p. 17), its full width will be used to produce the plot.

2.3.11 F2

F2 is the right extreme value of the axis, in units depending on the selection made under axis units (p. 20). The combination of the parameters F1 (p. 18), **F2** and CX (p. 18) (length of X axis) determines the plot window in x direction. If the low-frequency limit of the spectrum is smaller than F2, the spectrum will be clipped to F2. If the low-frequency limit of the spectrum is greater than F2, the spectrum plot will end at the appropriate position on the x axis.

If the option Update F1,F2 (p. 17) is checked, the current settings for F1 (p. 18) and **F2** will be neglected. After reading the selected spectrum (p. 17), its full width will be used to produce the plot.

2.3.12 X Offset

X offset is the distance, in centimeters, of the location of F1 (p. 18) measured from the origin of the page (usually the lower left corner).

2.3.13 Y Offset

Y offset is the distance, in centimeters, of the spectrum zero line measured from the origin of the page (usually the lower left corner).

2.3.14 CX, Spectrum Length

CX is actually the length of the X axis, i.e., the distance between F1 (p. 18) and F2 (p. 18) measured in centimeters.

2.3.15 CY, Spectrum Height

CY is the height, in centimeters, of the highest peak in the spectrum. If modified, the value of MAXY (p. 18), the clipping height, will be updated to this height also. This default behavior ensures that the spectrum is plotted to full height.

Actually, this defines the height of the plotting window. For a normal absorption mode spectrum, this will approximately correspond to the height of the highest peak. However, for a spectrum available as the first derivative the spectrum will be fitted within a window that is CY centimeters high.

The selection of the scaling mode will also influence the outcome. CY is either applied to the highest peak in the spectrum or to the highest peak within the specified region.

2.3.16 MAXY, Clipping Height

If the clipping height is smaller than the height of the spectrum, CY (p. 18), the spectrum will be clipped at this height. The course of action, if this condition is reached, depends on the setting of

the action (p. 19) parameter: either the pen is lifted until the spectrum points fall below the clipping height, or a straight line is drawn.

2.3.17 Action

This parameter customizes the behavior of the plot if the spectrum exceeds the clipping height, MAXY (p. 18). The course of action, if this condition is reached, is to either lift the pen until the spectrum points fall below the clipping height, or to draw a straight line.

2.3.18 Points to Skip

The value of this parameter determines the step width of the spectrum, i.e., how many points are plotted. A value of zero means that no points are skipped and all points of the spectrum within the limits F1 (p. 18) and F2 (p. 18) are plotted. A value of one means, that every second point is plotted; in general, every (1 + skip_points)-th is plotted.

The points are skipped, averaged, or the absolute maximum determined, depending on the selection.

2.3.19 Pen Spectrum

This parameter sets the number of the pen that is to be used to plot the spectrum. In general, the graphics programs that are able to import HPGL files employ different colors for different pen numbers. Valid numbers are 1 through 6.

2.3.20 Style of Line

Various line styles (combinations of dashes, dots and spaces) can be selected for plotting the spectrum (and the axis). If the line style contains spaces, the setting of the Spacing (p. 19) parameter affects the repeat-length of the pattern. Two line styles have a different behavior:

- The first available line style draws a solid line and requires no further parameters.
- The *digits* line style draws a small circle about the position of the spectrum point, the size of the circle is determined by the value of radius (p. 19).

If the resulting HPGL file is imported into a drawing program, it will depend very much on that program whether and how this parameter is honored.

2.3.21 Spacing

The spacing in percent determines the pattern length for line styles (p. 19) other than solid lines or digits. Valid values are between 0 to 127%, whereby 100% corresponds to 1 cm.

If the resulting HPGL file is imported into a drawing program, it will depend very much on that program whether and how this parameter is honored.

2.3.22 Radius

If the selected line style (p. 19) is digits, a circle of the selected radius is drawn about the position of each spectrum point (taking into account the number of points to skip (p. 19) in between).

If the resulting HPGL file is imported into a drawing program, it will depend very much on that program whether and how this parameter is honored.

2.3.23 Load

This button opens a file selection dialog box so that a file with layout information can be retrieved, overwriting the current settings if the layout. Usually, this file will be created using the Save (p. 20) button.

2.3.24 Save

This button opens a file selection dialog box, asking for a file name and location. Afterwards, the current settings of the layout parameters are written to that file and can be retrieved with the Load (p. 20) button.

2.3.25 As Default

This button causes the current settings for the layout to be written as default values into the SPECPLOT.INI file.

2.3.26 OK

After this button is pressed, the creation of the HPGL file is initiated.

2.3.27 Cancel

This button leaves the current dialog box, no HPGL file is created, and parameter changes are not ”memorized”.

2.3.28 Help

This button calls up the current help file.

2.3.29 Plot Axis

If this option is checked, an axis is drawn underneath the spectrum.

2.3.30 Axis Units

The axis units determine how the values of F1 (p. 18), F2 (p. 18), and tick increment (p. 21) are interpreted.

2.3.31 Axis Offset

This parameter determines where the axis is drawn relative to the zero line (base line) of the spectrum. A negative value puts the axis underneath the spectrum, a positive value puts it above the base line.

2.3.32 Tick Length

The tick length determines the length, in centimeters, of regular tick marks. Major ticks have a length determined by the product of this length and the major tick scaling (p. 21) factor.

A negative value indicates that the ticks are below the horizontal line of the axis, a positive value draws them above the horizontal line.

The horizontal spacing of ticks from each other depends on the Tick Increment (p. 21). The label increment (p. 21), an integer, determines the spacing between major tick marks. Major tick marks also carry a label.

2.3.33 Tick Increment

The horizontal spacing of ticks from each other depends on the tick increment. The label increment (p. 21), an integer, determines the spacing between major tick marks. Major tick marks also carry a label.

2.3.34 Divide By

Divide labels by this number, e.g. divide by 1000 to have kHz instead of Hz.

2.3.35 Major Tick Scaling

Major ticks have a length determined by the product of the tick length (p. 20) and this major tick scaling factor.

2.3.36 Label Increment

The label increment, an integer, determines the spacing between major tick marks. Major tick marks also carry a label.

2.3.37 Decimal Places

This integer determines how many decimal places are to be printed in labelling major (p. 21) ticks.

2.3.38 Character Height

This parameter, in centimeters, determines the character height of the major tick labels (p. 21).

2.3.39 Pen Axis

This parameter sets the number of the pen that is to be used to plot the axis. In general, the graphics programs that are able to import HPGL files employ different colors for different pen numbers. Valid numbers are 1 through 6.

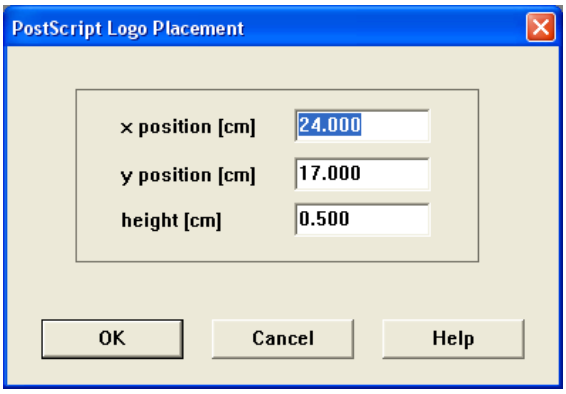
2.3.40 Axis Text

The entry of this box is plotted as axis text underneath the axis.

2.3.41 IW

If activated and the output format is HPGL, this inserts an input window command. This option, however, may cause problems with some HPGL import filters.

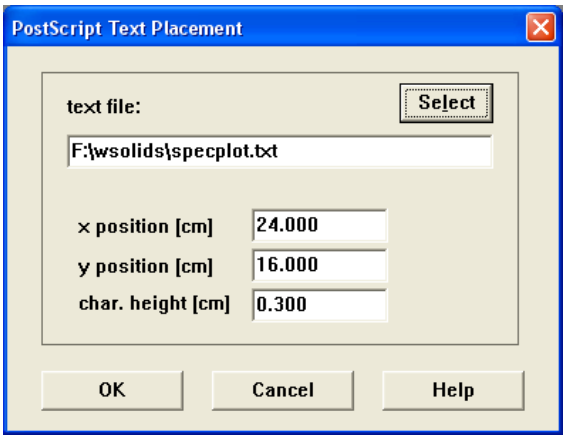
2.4 Add logo to postscript file



Purpose

This action adds the WSolids logo to the postscript file:

2.5 Add text to postscript file



Purpose

This action adds the content of a text file to the postscript file.

2.6 Exit

To exit the program, simply use:

- the menu item **File**|**Exit**
- the keyboard keys **ALT**−**F4**.

Purpose

This action exits the program.

2.7 Content

The contents of the help file can be displayed by using:

- the menu item **Help**|**Contents**
- the keyboard accelerator key **F1**.

Purpose

This action displays the contents for the help file as one of the possible entry points to obtain the desired information.

2.8 Search for Help on

To start WinHelp with a specific topic, on can search for a particular keyword by using:

- the menu item **Help**|**Search for help on**.

Purpose

Before starting the help file in WinHelp, this options lets the user search for help on a specific keyword first. The selected topic is then displayed. Once the help file is displayed, one can also use the **Search++** button to perform a full−text search.

2.9 About

To display version information on the program, use:

- the menu item **Help**|**About**

Purpose

The purpose of the About box is to give the user easy access to the current version number of the program. This could be important information to obtain support.

2.10 Known Problems

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