SpecMake — NMR Spectrum Generator

Contents

1 Getting Started

This chapter covers the following topics:
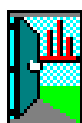
1.1 Introduction

This section covers the following topics:

- **Purpose of the program** Why I wrote this program

- **Features** What this program does (and what it doesn't do)

- **License** Who can use this program

- **Troubleshooting** What to do in case there is a problem

1.1.1 Purpose of the Program

Ever lost an NMR data file? Whether due to bad sectors on a storage medium, inadvertent deletion, or the rapid progress in technology that makes old data formats unreadable, there are many reasons for data loss. However, if there is still a decent printout available, don't despair, the situation is not hopeless. Scan the image and let **SpecMake** convert the picture into a Bruker WinNMR or TopSpin readable spectrum file.

Another potential application arises when you try to reproduce, i.e., simulate, published spectra, whether to check the interpretation of the authors or to check your simulation program. In such cases **SpecMake** helps you to generate an "'experimental"' spectrum from the published images. You may need to consider copyright issues in such cases.

Initially, SpecMake 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. The current version has been produced using Microsoft Visual C++ 2008 Express Edition.

1.1.2 Features

- Reads either raster picture data in Windows bitmap format or vector data in WordPerfect 5.0 graphics file format

- Converts the picture into a WinNMR or TopSpin readable NMR format

1.1.3 License

This program package can be used by any individual or organization without any fee, as detailed in the Copyright (p. 10) statement.

1.1.4 Troubleshooting

Although **SpecMake** 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. Especially the intricacies of the bitmap file formats could be sources of error. It is the responsibility of the user to determine the correctness of the results. As stated in the Disclaimer (p. 10), 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 SpecMake. Experienced users may use this information as a quick update on new program features.

1.2.1 New in Version 1.1.13 (30.07.2021)

- Bug fix: a change made to fix a signed / unsigned conflict broke the logic of bitmap conversion. Fixed the conflict and changed the logic.

1.2.2 New in Version 1.1.12 (20.05.2021)

- Bug fix: newer versions of Adobe Acrobat (Reader) should be supported for context sensitive help. (I am installing Acrobat only occasionally, hence I am not always able to check.)

1.2.3 New in Version 1.1.9 (17.04.2015)

- New feature: the location of the INI file (p. **??**) has changed: in the pograms directory for the portable version, or in the user's documents directory.
- New feature: added support for PDF-XChange Editor (by Tracker Software Products, Ltd., `http://www.tracker-software.com`) as PDF viewer to display context sensitive help.

1.2.4 New in Version 1.1.8 (11.03.2011)

- switched to Microsoft Visual C++ Express 2008

- new feature: there is an ini file parameter OutFile (p. 15) to set the spectrum output default format

- new feature: there is an ini file parameter Digits (p. 15) to fine tune the number of digits displayed in dialog boxes for floating point numbers

- new feature: the documentation is now in PDF format, added support for other PDF viewers to display context sensitive help (p. 14): added handling of PDF XChange Viewer (by Tracker Software Products, Ltd., `http://www.tracker-software.com`), **currently my prefered PDF viewer**, and Sumatra PDF Viewer (`http://blog.kowalczyk.info/software/sumatrapdf`), also deal with the new Adobe Reader X (p. 14).

1.2.5 New in Version 1.1.3 (22.02.2005)

- This is the first 32 bit Windows release.

1.2.6 New in Version 1.0.19 (04.06.2001)

- Some internal variables have been changed from normal (two−byte) integers to long (four−byte) integers, allowing manipulation of larger bitmaps.

- Each time the main window of SpecMake receives the focus (for example when switching back from the image processing software), it checks if the file time of the displayed picture has changed and updates the display accordingly (for bitmaps only).

- There is now a menu item (and keyboard short−cut) to close the displayed bitmap without leaving SpecMake.

- After reading a bitmap, the value of SI is updated depending on the width of the bitmap. The default value is the next higher number of points that is a power of 2 (important for the Hilbert transformation, vide infra).

- Introduced a linewidth parameter in the conversion dialog box.

- After generation of the real part of the spectrum, the imaginary part is generated via a Hilbert transform. This transformation is done only when SI is a power of two. Otherwise, the imaginary part is faked by copying the real part.

1.2.7 New in Version 1.0.13 (09.05.2000)

- Worked on a better placement and scaling of bitmaps within the client area of the application window.

- Micrografx Picture Publisher 7 sets one parameter incorrectly in the bitmap file header, and thus reading in SpecMake worked unreliably. Replaced this parameter by my own calculations.

1.2.8 New in Version 1.0.9 (10.05.1998)

- This is the first documented and released version, hence there is nothing to report right now. Microsoft's DIBAPI library for handling bitmap files had problems to display several different bitmaps (although my spectrum conversion worked properly). Hence I scrapped all DIBAPI calls and substituted them by functions from Petzold's SHOWDIB example from "Programming Windows 3.1" (what a great book!).

1.3 Overview

The ordering in this list corresponds to the order of actions taken in a typical session. New users may want to follow each step, and use the **Back** button to return to this screen.

Action	How to achieve this action
Prepare the image	SpecMake includes no features to acquire scanned images of a spectrum. Use your favorite scanner software to achieve this. There are, however, a few points worth considering, as oulined in the section Preparing Images for Conversion (p. 15)
Read picture data	The next step will be to read the image into SpecMake: Retrieve WPG, BMP (p. 11)
Convert picture into spectrum	Once a picture has been retrieved, it can be converted into an NMR data file: Create Spectrum (p. 12)

1.4 Acknowledgements

This section covers the following topics:

1.4.1 Credits

- The WPG functions are adapted from the ShowWPG example program by **Michael Bertrand**, (c) 1994, (published in "Windows/DOS developer's journal")

- The DIB handling functions are adapted from the SHOWDIB example by **Charles Petzold**, (c) 1992, published in "Programming Windows 3.1", by Microsoft Press. (Initially, I used the functions in the DIBAPI.DLL provided by Microsoft with the WINCAP example program, but this didn't work very reliably).

- **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.

- My prefered PDF viewer is the free **PDF XChange Editor** (by Tracker Software Products, Ltd., `http://www.tracker-software.com`), more powerful and reliable than the Adobe Acrobat Reader.

1.4.2 Trademark Acknowledgements

- *Microsoft (MS)* is a registered trademark and *MS-DOS* and *MS-Windows* are trademarks of Microsoft Corporation.

- *WIN-NMR* and *TopSpin* are products of Bruker Biospin.

- *WordPerfect* and *WordPerfect Presentations* are product of WordPerfect Corporation.

- Other brand and/or product names are used for identification purposes only and are trademarks, registered trademarks or copyrights of their respective owners.

1.4.3 Copyright Information

1.4.4 Disclaimer of Warranty

2 Reference

This chapter contains information on the following topics:
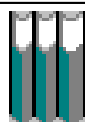
	Help on Menu Items (p. 11)	Explains the meaning of specific menu items
	Known Problems (p. 15)	Summarizes known problems

2.1 Help on Menu Items

Category	Menu Item	Action
File	Retrieve WPG, BMP (p. 11)	Read a WordPerfect 5.0 graphics file or a Windows bitmap
	Close bitmap	Closes the displayed bitmap file and clears the client area.
	Create Spectrum (p. 12)	Converts image into NMR data file.
	Exit (p. 14)	Exit SpecMake
Help	Content (p. 14)	Calls a PDF Reader and displays the contents page for this help file
	About (p. 14)	Displays version information for SpecMake

2.2 Retrieve WPG, BMP

Reads an image from the specified data file. Recognized are vector graphics in WordPerfect 5.0 format and Windows bitmap files.

If the image has been recognized properly, it is displayed on the screen. Depending on the sizes of the image and the client area of SpecMake, the image is squeezed or stretched. This does not affect the conversion process!

2.3 Create Spectrum
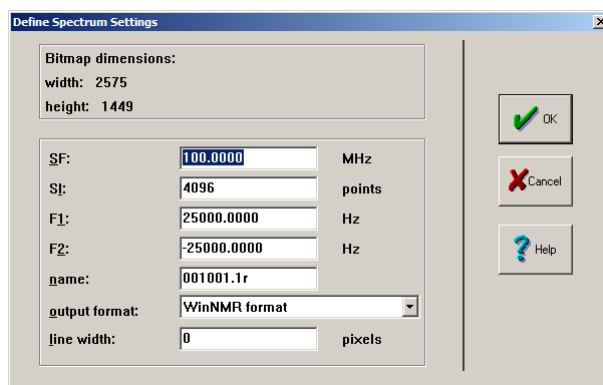
Converts the loaded image into an NMR spectrum. First, it queries for some spectral parameters and displays some information about the image:

parameter	meaning
SF	frequency of reference compound (standard), in MHz
SI	number of points for spectrum (real part); should be at least the width of the bitmap; use 1k, 2k, ... to obtain 1024, 2048... points. By default, this value is set based on the width of the bitmap to the next higher integer that is a power of 2 (required for the Hilbert transform)
F1	high−frequency limit of spectrum (relative to reference frequency), in Hz
F2	low−frequency limit of spectrum (relative to reference frequency), in Hz
name	name of resulting real data spectrum file; will be written to the same directory as the bitmap; by default **001001.1r**
output format	several different output formats, see text below
line width	width of the spectrum line in pixels (see below)

After that, conversion of the bitmap is initiated. Depending on the existing hardware, this may take a while. Starting on the left side of the image, SpecMake checks each column for the first and last occurence of a black point (pixel).

- If the line width parameter is zero, the average position is taken as intensity value for the spectrum. This procedure is suitable for wideline spectra (powder patterns) or for spectra where the peaks do not appear as sticks.

- If the line width parameter is greater than zero and the difference between the upper and lower limit is greater than the line width, the intensity is taken as the upper border minus the line width. If the difference is smaller than the line width, the average of upper and lower bounds is taken as intensity value. This procedure is suitable for MAS or other high resolution spectra where the peaks do not show a distinct line shape but rather appear as sticks. Obviously, this approach does not work for inverted spectra because it would simply trace the baseline (in such cases, flip the bitmap on a horizontal line, convert to a spectrum, and multiply by −1).

- In the future, more sophisticated algorithms using the line width are planned.

After generation of the real part of the spectrum, the imaginary part is generated via a Hilbert transform. This transformation is done only when SI is a power of two. Otherwise, the imaginary part is faked by copying the real part.

There are several output formats available:

1. a WinNMR file with UNIX-type ASCII parameter files;

2. in TopSpin/XWinNMR format;

3. in Solids format;

4. in ASCII format as rows of frequency, intensity data;

5. in JCAMP-DX format (only as uncompressed XYDATA in X++(Y..Y) format).

When writing WinNMR files, the file name should adhere to the `eeeppp.*` convention, where `eee` and `ppp` are zero padded integers representing experiment and processing number (e.g., `001`).

When writing Topspin files, please consider that the dialog was written initially for WinNMR. Therefore, if you want to create the file `d:\u\data\nmrguest\nmr\simulation\11\pdata\20\1r`, you should point the path to the `...\simulation` subdirectory and enter the file name `011020` (file type Topspin). SpecMake extracts from this file name the corresponding experiment and processing numbers.

2.4 Exit

To exit SpecMake, simply use:

- the menu item **File|Exit**
- the keyboard keys **ALT−F4**
- the accelerator key **X**

2.5 Content

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

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

Initially, SpecMake used for help and documentation the Windows Help program. Since version 1.1.8 I switched to the PDF format because it is suitable for both online viewing as well as printing. To view or print this documentation, any PDF viewer should work. Also, most viewers should be able to deal with the hyperlinks that cross-link topics in this help file. However, opening a PDF file at a specified position is more complicated. Therefore, not every PDF viewer will work with SpecMake to display context sensitive help. This matter is aggravated by the fact that every viewer has its own mechanism!

Currently, context sensitive help should work with the following PDF viewers:

- Adobe uses with its `Acrobat Reader` series of products a mechanism called Dynamic Data Exchange (DDE) to open a PDF file at a specific position. For ages, the name of the DDE server has been `acroview`. However, with the introduction of Acrobat Reader X this tradition has been broken on purpose, breaking many applications that rely on this mechanism. SpecMake should be able to work with older versions of the Acrobat Reader as well as with the `acroviewR10` DDE server of Adobe Reader X. Because I have been quite dissatisfied with the Adobe products from Reader 5 onwards, I am using a different PDF viewer and will not always check whether Acrobat is still working.

- My prefered PDF viewer is the free `PDF XChange Editor`, the successor of `PDF XChange Viewer` by Tracker Software Products, Ltd. (http://www.tracker-software.com), more powerful and reliable than the Acrobat Reader. The opening of a PDF file at a specific position is achieved via command line parameters.

- Another viewer used by people working with LATEX is the `Sumatra PDF Viewer` (http://blog.kowalczyk.info/software/sumatrapdf), also supported by SpecMake.

- Other PDF viewers such as FoxIt or NitroPDF do not support DDE or command line parameters, as far as I know.

2.6 About

To display version information on SpecMake, 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 SpecMake program.

2.7 Known Problems

None right now

2.8 Preparing Images for Conversion

During the preparation of images for conversion into NMR spectrum files, there are a few points worth considering:

- Conversion quality depends on the resolution of the scanned image. Therefore, use the highest scanner resolution and scale up the relevant area.
- White space does not provide much information but costs memory; select an area slightly larger than the area covered by the spectrum.
- Save the scanned image as monochrome bitmap in Windows bitmap format. At least the color of the spectrum should be black.
- Starting on the left side of the image, SpecMake checks each column for the first and last occurence of a black point (pixel), the average position is taken as intensity value for the spectrum (other methods are also implemented, see Create Spectrum (p. 12)). Hence, it is important that the image does not contain any other black spots such as due to scratches or dust. Use your favorite image processing software to clean up pictures.
- Missing points are interpolated linearily; hence it is ok if the scanned spectrum has a few faded spots. Otherwise, you may need to draw in the missing parts manually.

2.9 Default Output File Format: OutFile

```
[FILES]
OutFile=1
```

The parameter `OutFile` in the `FILES` section of the INI file preselects the standard output format of spectra. Currently, the value of `OutFile`, an integer, will correspond to the following file formats:

OutFile	Format
1	WinNMR
2	Topspin
3	Solids
4	ASCII file
5	JCAMP-DX format

2.10 Number of Decimal Digits: digits

```
[Document]
Digits=5
```

In order to fine tune the number of digits displayed in dialog boxes for floating point numbers, you can use the parameter `Digits` in the `DOCUMENT` section of the INI file. Note that `Digits` only affects the display, not the actual number of decimal digits evaluated when entering floating point numbers. I.e., the accuracy is not affected by `Digits`!

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