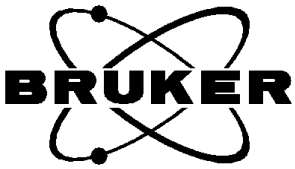
XWIN-PLOT



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1

Introduction

1.1 What is XWIN-PLOT?

XWIN-PLOT is a fully object-oriented, interactive and easy to use WYSIWYG[1)] plot editor for creating high quality printouts of NMR data obtained with the Bruker XWIN-NMR software package.

You will find a lot of parallels between the plot editor and other well-known drawing programs and because of this it will be very easy for you to work with XWIN-PLOT.

XWIN-PLOT is built on two basic concepts: Layouts and data set portfolios. A layout describes all the attributes of graphic objects, e. g. position, size and color, but does not contain any NMR related data. To get a relationship between such graphical objects and NMR data, a layout must be combined with a data set portfolio. A layout, once created, can easily be reused by combining it with different portfolios. You also may use one portfolio for several layouts to get different views of the same data sets.

If you are still reading at this point, fine. The main problem with most software products is that their manuals are never read. To be honest, we have to admit that

1) „**W**hat **Y**ou **S**ee **I**s **W**hat **Y**ou **G**et“

we do not like spending too much time leafing through books either. On the other hand, manuals are important because they provide a vital source of information. Most problems that arise when using a software product can be solved by carefully studying the software documentation.

In order to ensure that you can start using XWIN-PLOT as soon as possible, a special Quickstart chapter has been added to this manual. So if you do not want to wait any longer to get your first results, please take a look at that chapter.

1.2 AUTOPLOT

XWIN-PLOT provides a convenient means to create graphics interactively. Nevertheless there are situations which require layouts to be used without any user interaction. In these cases AUTOPLOT can control the printing. With AUTOPLOT you can print several data sets with only one command line.

1.3 The Bruker ftp server

A convenient way for obtaining add-ons or updates to the Bruker software packages is the Bruker ftp server, ftp.bruker.de. You can connect to this server from your local workstation or PC by issuing the following command:

```
ftp ftp.bruker.de
```

When the connection is established, you will be prompted for your login name and your password. Use the keyword `anonymous` as login name and your email address as a password. For further information about the `ftp` program consult your `ftp` manual.

1.4 The Bruker WWW server

Bruker also maintains a WWW server which can be reached via `http://www.bruker.de` using one of the several WWW clients that are available for various computer platforms, e. g. `Netscape`. On this server you can find information about the hardware and software products maintained by Bruker. You can also download files offered by the Bruker ftp server.

1.5 Notation

In this manual different font styles are used to represent various types of information:

Italics are used for:

• New terms when they are defined.

`Typewriter` font is used for:

• Pathnames, filenames and program names.

• Text on the screen.

Boldface is used for:

• Names of buttons, menus and menu options.

1.6 Bug reports

Did you ever find a software package that fulfilled your needs in every respect and which also did not have any bugs? Surely not. Nevertheless experience shows that most of the problems a user is confronted with can easily be solved by taking a look at the manual. So please make sure that you carefully read the manual passages referring to your particular problem. If any difficulties remain, try to formulate the problem into a formal, detailed description before contacting us.

We really appreciate constructive criticism, so if you think you have some useful comments concerning XWIN-PLOT, feel free to get in touch with us. If possible, please use this email address:

nmr-software-support@bruker.de

And now we wish you success and enjoyment using Bruker's XWIN-PLOT plot editor.

2

Starting XWIN-PLOT

Both XWIN-PLOT and AUTOPLOT are available as a stand-alone programs and as modules which can be started from XWIN-NMR.

2.1 The XWIN-NMR module versions of XWIN-PLOT and AUTOPLOT

If started from within XWIN-NMR, XWIN-PLOT and AUTOPLOT automatically load the current data set and a layout that is specified by setting the XWIN-NMR `LAYOUT` parameter. To set this layout parameter, you can use the XWIN-NMR command `edo`. Click on the **LAYOUT** entry in the *Output device parameters* dialog window and enter the layout filename for the current data set (Figure 2.1). If no layout is specified (i.e. `LAYOUT` contains an empty string), XWIN-PLOT starts with a new empty layout. AUTOPLOT cannot be started without a layout specification.

If XWIN-PLOT is started from XWIN-NMR and a layout is saved using **Save As** in the **File** menu, the specified file name will automatically be transferred to the `LAYOUT` parameter. (See chapter 5.7 on page 49.)

During start-up XWIN-PLOT first loads the default portfolio of the current user. If there is a file `portfolio.por` found in the current dataset that is loaded instead. Finally, the content of the portfolio is transferred to the dataset list and the first

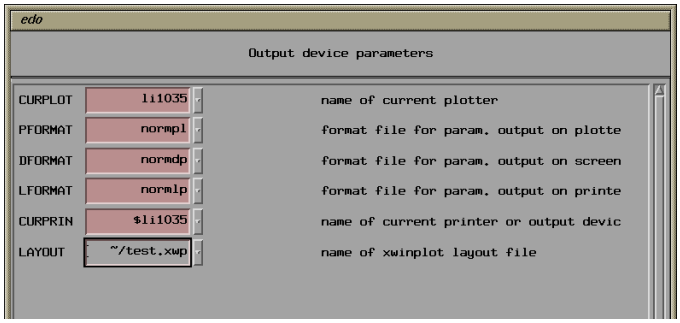


Figure 2.1 Choosing an XWIN-PLOT layout in XWIN-NMR

entry is replaced with the current dataset to ensure the user initially works on the same dataset as seen in XWIN-NMR before.

XWIN-NMR provides a familiy of three commands that can be used to start XWIN-PLOT:

2.1.1 The command `xwinplot`

Whenever you type `xwinplot` command within XWIN-NMR XWIN-PLOT will simply open the selected layout and display it exactly like you have saved it during your last session. No automatic changes are applied. Especially the axis limits will be those saved in the layout.

2.1.2 Using XWIN-NMR plot limits with the `xwp` command

The XWIN-NMR command `xwp` will start XWIN-PLOT with the current layout and set the plot limits of all data objects to those limits stored in the parameters `F1P/F2P` (for 1D objects), or `F1PLO/F1PHI/F2PLO/F2PHI` (for 2D objects), respectively. If you already adapted the display in XWIN-NMR to show the region of your interest you can simply press the **defplot** button to store them in the plot parameters and type `xwp` to have the same region displayed in XWIN-PLOT.

The **autoplot** button in Xwin-nmr will create the same plot but send it directly to the printer without any user interaction.

2.1.3 Starting XWIN-PLOT with automatically calculated plot limits

When started by the XWIN-NMR command `xwpr`, XWIN-PLOT will apply reset actions on all objects after loading the layout. This is similar to choosing **Reset all objects** from the menu **Edit**. The plot limits then will be recalculated based on the rules that are defined in the **Automation** dialog for each NMR object. See Chapter 7.1 on page 81 for further information about those reset actions.

This may be useful if you want to check your selected reset actions, or make use of more complex layouts (like e.g. the `1D_H+zoom.xwp` layout).

To create this plot and send it to the printer without further interaction you can type `autoplot` in XWIN-NMR.

2.2 The stand-alone versions of XWIN-PLOT and AUTOPLOT

The stand-alone versions of XWIN-PLOT and AUTOPLOT can be started by executing the command

```
xwinplot [options] layout1.xwp layout2.xwp ...
```

or

```
autoplot [options] layout1.xwp layout2.xwp ...
```

respectively.

2.2.1 Options for the stand-alone version of XWIN-PLOT

XWIN-PLOT can be started with the following options:

`-p portfolio.por` Loads the portfolio file `portfolio.por`

`-r` resets all objects after start-up

If no portfolio file is specified, XWIN-PLOT will automatically load the portfolio that was saved with **Save As Default** in the **File** menu of the *Portfolio Editor* dialog. (See chapter 5.6.2 on page 47.)

2.2.2 Options for the stand-alone version of AUTOPLOT

2.2.2.1 Portfolio related option

If you use these options on the command line, their order is important. AUTOPLOT evaluates all of its options from left to right.

`-p portfolio.por` Loads the portfolio file `portfolio.por`

`-a portfolio.por` Like `-p`, but appends to the portfolio instead of overwriting its contents

`-d /u/data/...` Adds data set `/u/data/...` to the portfolio

`-r /u/data/...` Removes data set `/u/data/...` from the portfolio

`-sa` Sorts portfolio inascending order

`-sd` Sorts portfolio in descending order

You can combine these options in any way you like. For example you can load a portfolio with the `-l` option, then you can sort it and afterwards you can append additional data sets to it with the `-d` option.

The `-d` and `-r` options expect a full data set path name, e. g.

```
-d /u/data/guest/nmr/demospect/1/pdata/1
```

2.2.2.2 Other options

`-s setup.prt` Use printer setup file `setup.prt` instead of the printer setup that was saved with the layout (not available for Windows NT/2000 version)

`-l N` Remove N data sets from the portfolio and print again

`-n` Don‘t reset before printing

-f Force all 1D and/or 2D objects in the layout to use axis limits as used in XWIN-NMR (uses the `F1P/F2P` parameter, or `F1PLO/F1PHI/F2PLO/F2PHI` parameter, respectively)

`-o`	Preview instead of printing
`-e output.ps`	Create Postscript file instead of printer output (Windows NT/2000: PostScript (.ps) or Metafile (.emf) format)
`-v`	Show AUTOPLOT version number
`-h`	Show help text
`-?`	Same as `-h`
`--`	Explicit end of options. Use this option before specifying a layout file that has a `-` as its first letter.

2.2.3 Layout file name syntax

To simplify the file name specification for layouts, it is possible to use the following abbreviations in layout filename paths:

- `~/` can be used as an abbreviation for the home directory. If, for example, the user guest has the home directory `/usr/people/guest`, the specification

  ```
  ~/my_layouts/layout1.xwp
  ```

  is expanded to

  ```
  /usr/people/guest/my_layouts/layout1.xwp
  ```

- `+/` is an abbreviation for the directory $XWINNMRHOME/plot/layouts. For example

  ```
  +/layout1.xwp
  ```

  could be expanded to

  ```
  /u/plot/layouts/layout1.xwp
  ```

2.2.4 Dataset-related file name syntax

For objects that reference external files (NMR text objects, and the objects for imported graphics EPSI and Meta) there also exist similar file name abbreviations:

- `~/` can be used as an abbreviation for the home directory. If, for example, the user guest has the home directory `/usr/people/guest`, the specification

  `~/my_nmr_texts/nmrtext.txt`

  is expanded to

  `/usr/people/guest/my_nmr_texts/nmrtxt.txt`

- `+/` means that the referenced file is located in a dataset directory. For example

  `+/nmr-text.txt`

  is expanded to

  `/<DU>/data/<USER>/nmr/<EXPNO>/pdata/<PROCNO>/nmr-text.txt`

- `$XWINNMRHOME` is expanded to the installation path of the current XWIN-NMR installation (e.g. `/u` for SGI/Linux, or `C:\Bruker\XWIN-NMR` for Windows NT/2000 versions)

3

XWIN-PLOT and XWIN-NMR

When working with XWIN-PLOT and XWIN-NMR always keep in mind that XWIN-PLOT is a software package for displaying existing data. These data must have been acquired or created with XWIN-NMR before it can be referred to in XWIN-PLOT. If data is missing, the plot editor will display a warning message.

To create missing data, you can either enter the commands described below directly in XWIN-NMR, or you can use the *XWIN-NMR Interface* dialog in XWIN-PLOT. (See chapter 3.9 on page 20.) If you have entered the commands manually in XWIN-NMR, you must use **Update Data from XWIN-NMR** in the **XWIN-NMR** menu to transfer the changes to XWIN-PLOT.

Some data can be generated without overwriting sensible parts of the dataset (peak lists and parameter lists). XWIN-PLOT and AUTOPLOT try to generate these files automatically when started from within XWIN-NMR to avoid unnecessary error messages.

3.1 Creating a title

In XWIN-NMR the plot title can be set by the command `setti`. With this command you can edit the contents of the file `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/title`[2)].

3.2 Creating a parameter listing

To create a parameter list, use the XWIN-NMR command `xwp_lp`. This command will store the parameter list in `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/parm.txt`.

XWIN-PLOT and AUTOPLOT will automatically execute this command as necessary when started from within XWIN-NMR.

3.3 Creating a peak list

Use the XWIN-NMR `xwp_pp` command to create peak label information. This command will store the peak list in the file `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/peak.txt`.

XWIN-PLOT and AUTOPLOT will automatically execute this command as necessary when started from within XWIN-NMR.

3.4 Creating an integral range file

Integral ranges in XWIN-NMR can be determined in two ways. The command `abs` starts an automatic baseline correction of the NMR spectrum and additionally determines the regions containing spectral information. These regions are stored in the file `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/intrng` and can be used to calculate the integrals. The integral ranges can also be determined manually. Click on the button **integrate** to switch to the **integral** menu. Place the mouse inside the spectrum with the left mouse button and select integral regions by clicking the middle mouse button. Open the **File** menu and click on **Save as intrng** in order to store the integral ranges.

2) `<DU>` stands for the disk unit (e.g. `u`), `<USER>` for the user id, `<NAME>` for the name of the data set, `<EXPNO>` for the experiment number and `<PROCNO>` for the processing number.

3.5 Creating a region file

It is possible to save the integral ranges in a special region file. This region file can be used to determine the reset behavior of spectra (See chapter 6.1.7 on page 66.). Simply use **Save as reg** instead of **Save as intrng** to create the region file `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/reg`.

3.6 Creating a levels file

The number of contour levels used for the display of 2D data in XWIN-NMR can be set with the command `defplot`. To specify the value of each level, the command `edlev` can be used. The levels are stored in the file `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/level`. If you select a 2D data set in XWIN-NMR and a level file does not already exist, XWIN-NMR uses the default levels.

3.7 Creating projections

In case positive or negative projections were defined by the XWIN-NMR commands `rhpp`, `rhnp`, `rvpp` or `rvnp`, XWIN-PLOT will automatically add the corresponding data to the *Data Set Selector* when started from within XWIN-NMR. Note that XWIN-PLOT will not accept a projection that is based on a data set file that is older than the 2D data set file.

3.8 Creating T1/T2 curve data

XWIN-PLOT can plot T1/T2 and all other relaxation type curves generated by XWIN-NMR. The point picking for these curves and the curve calculation are done in the **T1/T2 Relaxation** submenu of XWIN-NMR.

All XWIN-NMR commands which create or update the points shown on the XWIN-NMR display[3)] create a file `/<DU>/data/<USER>/nmr/<NAME>/<EXPNO>/pdata/<PROCNO>/t1t2.jdx` containing these points. Only the points of one peak are written to the `t1t2.jdx` file at this time.

3) `pd, pd0, pft2, prxy, lstp, nxtp, elim, rstp`

All fitting commands write out the list of fitted points, the function used for the fit and the resulting fit parameters.

If a command which only fits the currently displayed points is used[4], only these points and the fitting results are written to the `t1t2.jdx` file.

If a command which fits all points of all picked peaks is used[5], all points with all fitting results will be written to the `t1t2.jdx` file.

3.9 The XWIN-NMR Interface

If XWIN-PLOT was started from XWIN-NMR, you may additionally make use of the **XWIN-NMR Interface** dialog (see Figure 3.1).

With the help of this dialog, you can easily run XWIN-NMR commands on several data sets. First select the data sets which you wish to work on. You now have the choice of either running arbitrary commands on these data sets by entering the commands into the text field, or of running predefined commands by using the command buttons. These buttons include commands to edit the title, create a parameter list, create a peak list, create integrals and to change levels.

4) `ct1, ct2, simfit, simfit asc`
5) `dat1, dat2, simfit all, simfit asc all`

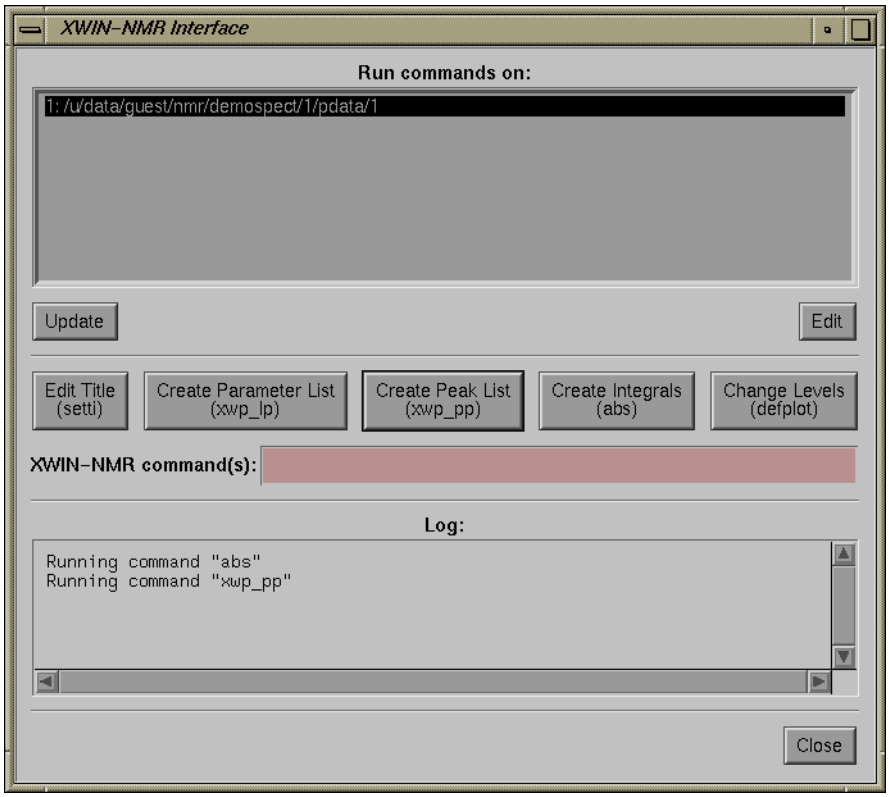


Figure 3.1 The *XWIN-NMR Interface*

4

Quickstart guide

To get your first printouts with the XWIN-PLOT plot editor as quickly as possible, this guide presents an example of how to create a simple layout.

4.1 Starting XWIN-PLOT from XWIN-NMR

Since the sample layout described in this quickstart guide contains a title and parameter list, you have to use the commands `setti` (to edit the title) and `xwp_pp` (to create a parameter list) in XWIN-NMR on the current data set before starting XWIN-PLOT. (See Chapter 3.) As an alternative you can request this data with the plot editor's XWIN-NMR interface after starting XWIN-PLOT.

After processing your NMR data with XWIN-NMR, you can start XWIN-PLOT by typing `xwinplot` on the XWIN-NMR command line or by clicking on the **Plot-editor** menu entry in the **Windows** menu. When started this way, XWIN-PLOT automatically loads the current data set. (See Chapter 5.6 for more information about which datasets are loaded at start-up).

4.2 Setting up the printer under Unix

Before you can create your first layouts with XWIN-PLOT, you have to set up your printer configuration. After selecting the *Printer Setup* entry in the **Options** menu,

the dialog window shown in Figure 4.2 will be displayed. Don‘t be confused by

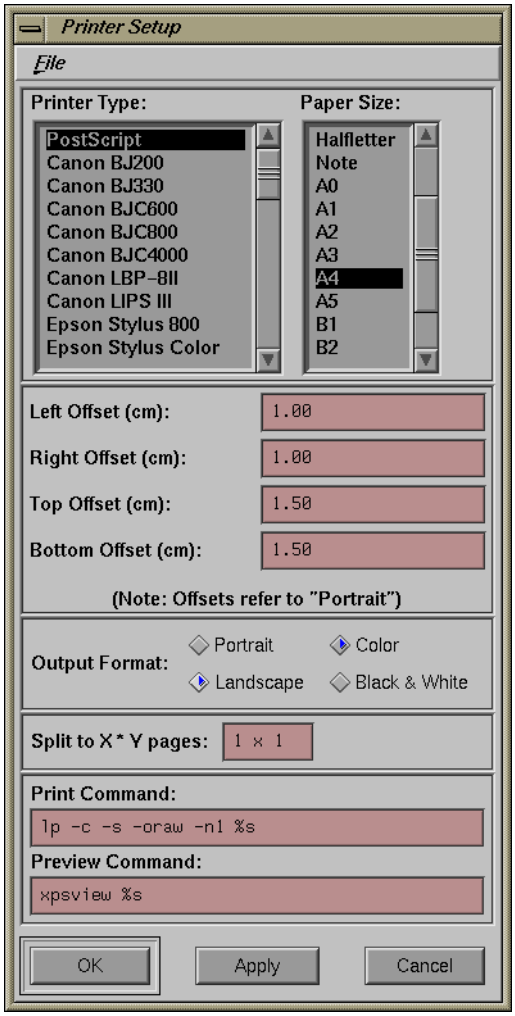


Figure 4.1 The *Printer Setup*

the variety of options available. Most of them are not important for this example. Simply choose your printer from the **Printer Type** list and select the paper format from the **Paper Size** list.

The **Print Command** text field defines the command that will be used by XWIN-PLOT when sending data to the printer. Your print command should look like this:

```
lp -c -s -oraw -n1 %s
```

`lp` is the standard Unix print command for a System V Unix environment. The options `-c` and `-oraw` as well as the `%s` are required. XWIN-PLOT will not print without these options. See Chapter 5.11.3 on page 54 for more information about the printing options.

For Linux system you should use the command

```
lpr %s
```

to use the standard Linux print system.

You can save the current settings as the default configuration with **Save As Default** in the **File** menu. You must exit the *Printer Setup* dialog window with the **OK** button in order for your changes to be accepted.

4.3 Setting up the printer under Windows

For your first layout you do not need to change the printer setup. XWIN-PLOT automatically chooses your default printer and the paper size is set to the default format that is selected for that printer in your system (which will be typically *Letter* or *A4*).

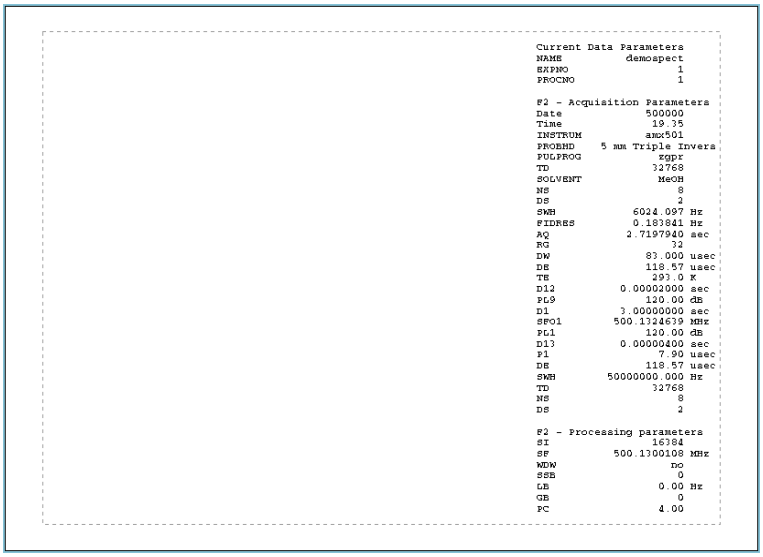
It is absolutely necessary to have at least one printer driver installed on your Windows NT/2000 system to give XWIN-PLOT a chance to calculate correct page sizes.

4.4 Creating a layout

Now you are ready to draw a simple layout containing a one dimensional NMR spectrum with an expanded region, the spectrum parameters and a title.

The first object in the layout will be the spectrum parameters. You enter the parameter mode by clicking on the corresponding icon (Figure 4.2). Now you can place the rectangular area containing the parameters inside the layout window. Your layout should look similar to the one in Figure 4.3 now. In case you make a mistake

Figure 4.2 The parameter mode icon



```
Current Data Parameters
NAME            demospect
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date                500000
Time                 19.35
INSTRUM           amx501
PROBHD     5 mm Triple Invers
PULPROG              zgpr
TD                  32768
SOLVENT              MeOH
NS                      8
DS                      2
SWH              6024.097 Hz
FIDRES           0.183841 Hz
AQ               2.7197940 sec
RG                     32
DW                 83.000 usec
DE                 118.57 usec
TE                  293.0 K
D12           0.00002000 sec
PL9                120.00 dB
D1            3.00000000 sec
SFO1         500.1324639 MHz
PL1                120.00 dB
D13           0.00000400 sec
P1                   7.90 usec
DE                 118.57 usec
SWH        50000000.000 Hz
TD                  32768
NS                      8
DS                      2

F2 - Processing parameters
SI                  16384
SF           500.1300108 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   4.00
```

Figure 4.3 A layout containing a parameter list

when creating or changing an object, simply click on the **Undo** button to reverse an operation.

In the next step you are going to add the NMR spectrum object. Switch to the spectrum creation mode by clicking on the 1D spectrum icon (Figure 4.4).

Figure 4.4 The 1D spectrum mode icon

Now you can create an object containing the one dimensional spectrum of the current XWIN-NMR data set. Place the mouse cursor at the upper left edge of the layout window and press the left mouse button to place the spectrum object on the drawing area. As long as you keep the mouse button pressed, you can change the objects dimensions by moving the mouse. XWIN-PLOT displays the part of the spectrum that is visible in the XWIN-NMR processing window (See Figure 4.5).

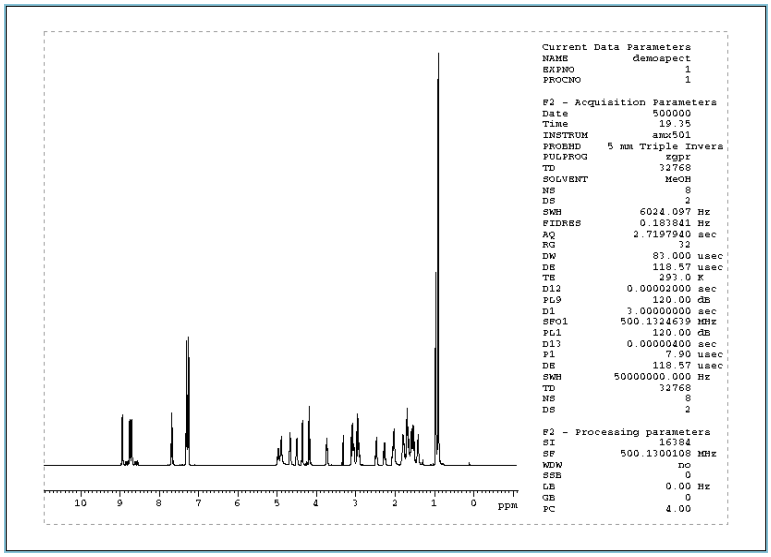


Figure 4.5 Adding a spectrum to the layout

When you are satisfied with the spectrum‘s position and size, release the mouse button.

The next object in this example is an expanded view of a particular spectral region which is to be added above the spectrum. Create an additional, smaller spectrum object as already described and place it above the first. Enter the **Expand** mode by clicking on the corresponding icon (Figure 4.6). Now you can define a rectangular region inside the spectrum with the mouse. Press the left mouse button when you are on the spectrum object and mark the region to be expanded. After releasing the mouse button XWIN-PLOT will expand this region. This will result in a layout similar to Figure 4.7.

Figure 4.6 The expand mode icon

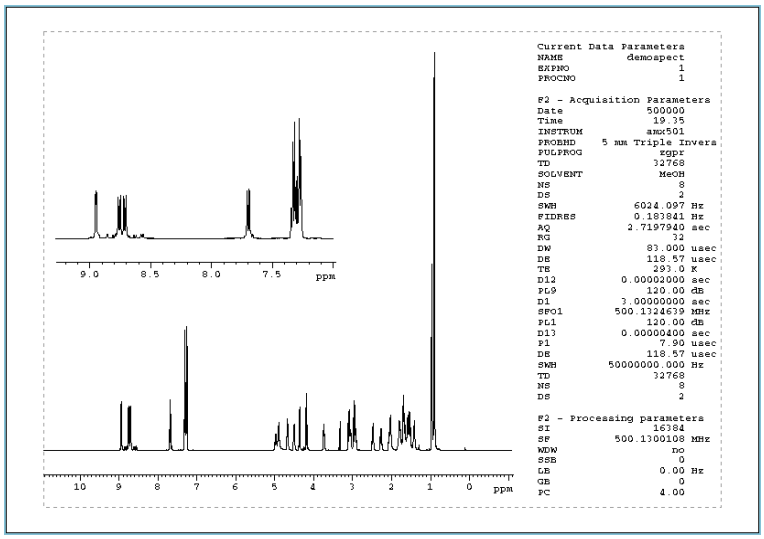


Figure 4.7 The sample spectrum with an expanded region above

Now it‘s time to create a title for the spectrum. To select the font type and size for the title object, click on the **Attributes** button. While in the *Attributes* editor (Figure 5.12), you will not only be able to change the font settings, but other attributes as well. The settings chosen in this dialog window will be valid for all the objects created after selecting **Apply** or after leaving the window with **OK**.

Activate the title mode by clicking on the icon shown in Figure 4.8. The title object can be placed inside the drawing area as already described for the other objects. Figure 4.9 shows the drawing area after this operation.

Figure 4.8 The title mode icon

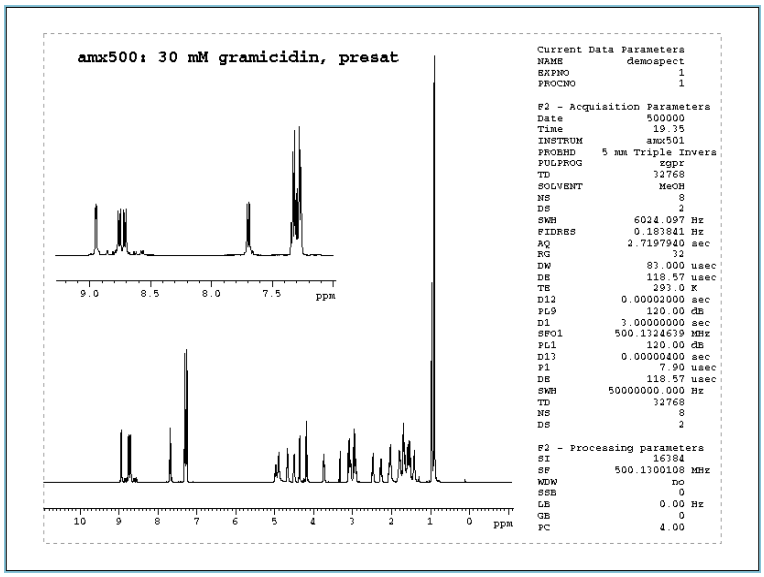


Figure 4.9 A layout with spectrum, parameters and title

In the last step you will add an annotation to the spectrum. If you want to change the annotations font you can do this as described above in the *Attributes* dialog window. Once you have adjusted the font, enter the text mode by activating the text mode icon, visible in the **Basic** major editing mode (Figure 4.10). After click-

Figure 4.10 The text mode icon

ing at the desired location on the layout window, you can enter a text, such like „Annotation“ in this example. The final text position can be set by pressing the left mouse button. For our example we will place the text near one of the prominent peaks in the lower spectrum. This will result in a layout similar to the one shown in Figure 4.11.

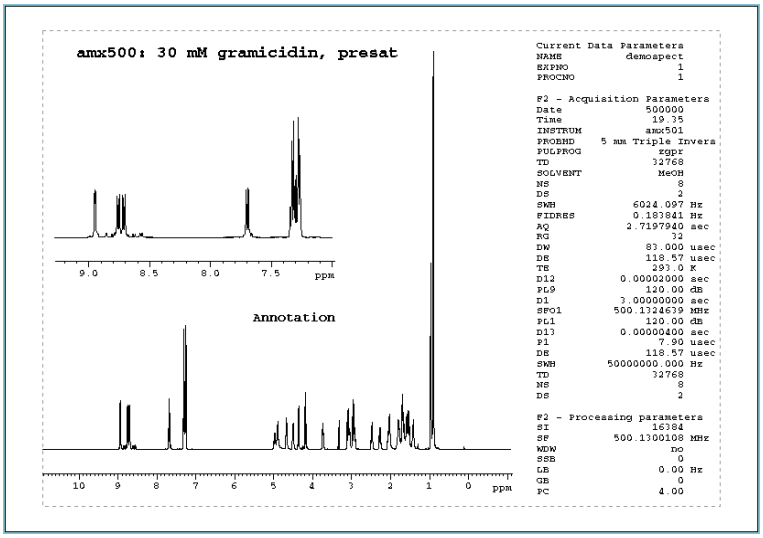


Figure 4.11 Placing an annotation above the spectrum

The annotation may be a reference to one of the spectrum‘s peaks. You can emphasize fact by drawing an arrow from the annotation to the peak on the left. Before you draw an arrow, go to the *Layout Setup* (Figure 4.12) and select the „Snap-In“ mode **None**, which allows objects to be positioned at arbitrary points. To create an arrow object, you go into the **Basic** editing mode and to enter the line mode by selecting the corresponding icon (Figure 4.13). Now draw a line with the mouse, starting near the annotation and ending near the peak. The line‘s starting point is set by pressing the left mouse button. Releasing the mouse button marks the end of the line.

Finally, add an arrow tip to the end of the line. After entering one of the marking modes (Figure 4.14) you can mark the line object by clicking on it with the left mouse button. To edit the object select the **Edit** command button. The line objects

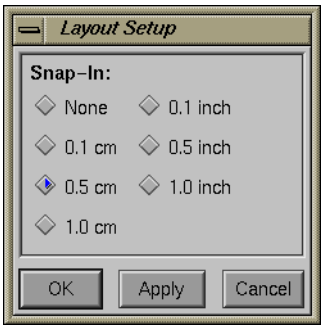


Figure 4.12 The *Layout Setup*

Figure 4.13 The line creation mode icon

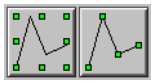


Figure 4.14 The marking mode icons

edit dialog window will pop up as shown in Figure 4.15. In this editor you can select various line attributes and you can convert a line into an arrow by selecting the corresponding buttons. The arrow tips width can be changed with a slider.

After accepting your changes with **OK** or **Apply** the sample layout is complete. It should look similar to the layout in Figure 4.16.

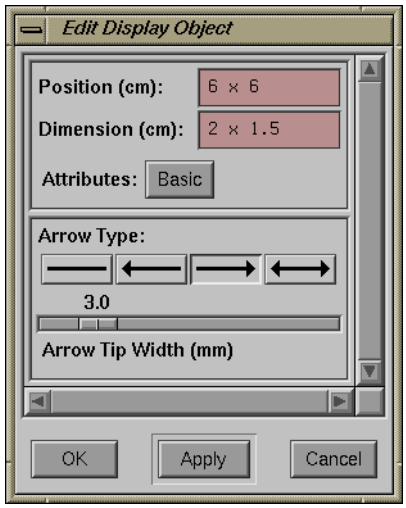


Figure 4.15 The line object editor

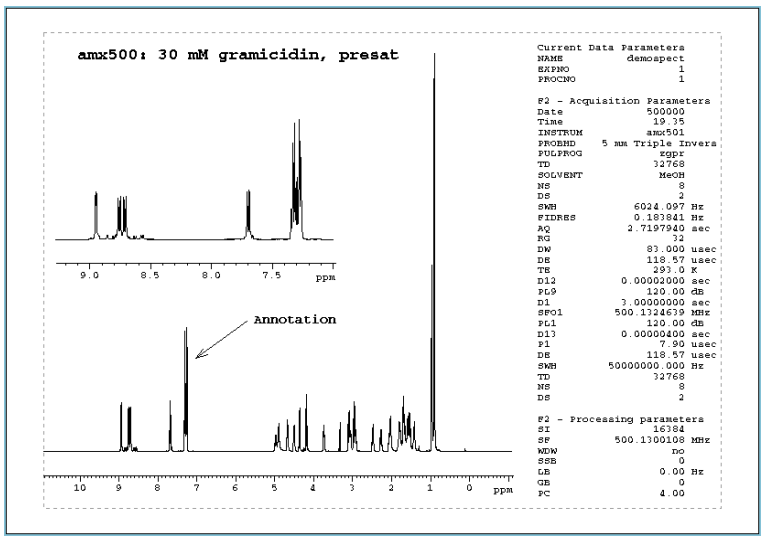


Figure 4.16 The final sample layout

4.5 Printing the layout

To print your layout, choose the **Print** option in the **File** menu. Printing will commence after clicking on the **Print** button in the *Print* dialog window (Figure 4.17).

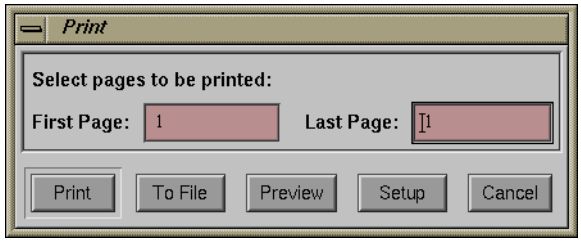


Figure 4.17 The *Print* dialog window

Depending on your printer it will take a while for a document to print, so be patient. You can continue to work with XWIN-PLOT or XWIN-NMR while printing is in progress.

4.6 Saving the layout

If you want to save the layout for use with other data sets later on, choose **Save As** in the **File** menu. A file selector will appear where you can enter the name of your layout[6)]. In case XWIN-PLOT was started from within XWIN-NMR, information about the layouts filename will be saved in the current data set parameters.

6) By convention XWIN-PLOT layout filenames have the extension `.xwp`.

5

The layout window

A key concept of XWIN-PLOT are its layouts. After starting the plot editor, an empty layout window will be displayed.

5.1 The structure of a layout window

XWIN-PLOT can maintain a virtually unlimited number of layout windows. Each layout window may contain simple graphic objects like lines or rectangles as well as complex NMR related objects like FIDs and NMR spectra. Most of the interaction between the user and the plot editor is mouse based and takes place within the layout windows. Additional layout windows can be opened by selecting **New** in the **File** menu or, if the layout to be used is already available on disk, with the **Open** command.

A layout window consists of five main areas. (See Figure 5.1.) At the top of each window a menu bar is displayed. Most entries in the menu can be reached using keyboard shortcuts.

Below the menu there is a button bar with some frequently used commands. With the icons located on the left side of the window, the user can choose the plot editors drawing mode. The active mode is displayed in the **Mode** field at the top left-hand side of the window and can be changed by clicking on one of the drawing mode

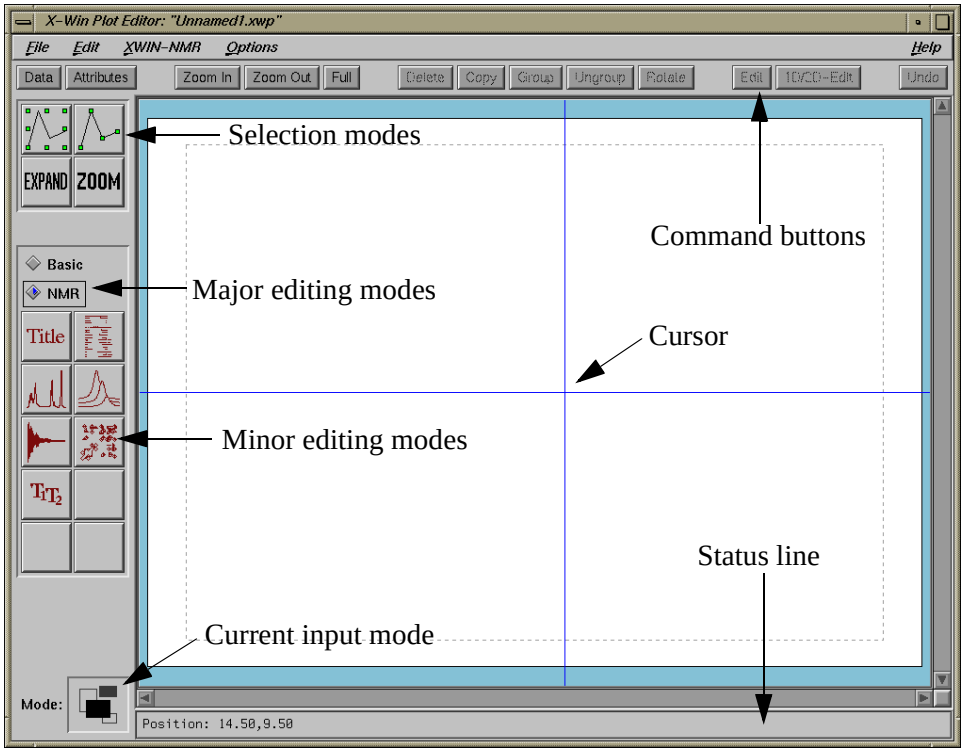


Figure 5.1 An empty layout window

icons. There are two major editing modes: **Basic** mode for drawing simple, not NMR-related objects, and **NMR** mode.

The main part of the layout window consists of the layout area which represents a sheet of paper including its borders. An object that is on or outside the border lines will not be printed.[7)]. The paper size and format can be defined in the *Printer Setup* dialog. (See “Printing a layout” on page 50.) By moving the scroll areas at the right and bottom of the graphics area the visible part of the drawing area can be moved. Scrollbars are only present if the size of the current graphics area exceeds the size of the visible drawing area.

7) If a graphics object is placed on the border it will be clipped when it is printed.

5.2 Input Modes

5.2.1 Creation modes

The object types that can be created by XWIN-PLOT include simple objects like lines or rectangles in **Basic** editing mode as well as complex NMR related objects in **NMR** editing mode, e. g. FIDs or spectra. An object is drawn by first choosing the editing mode and then selecting the corresponding drawing mode. This mode is selected by clicking on one of the icons at the left edge of the graphics window. The current drawing mode is indicated by the icon inside the **Mode** field at the lower left. (Figure 5.2) A new object is placed on the screen by pressing the left

Figure 5.2 The mode field reflects the current drawing mode

mouse button and simultaneously moving the mouse pointer. If an object is defined by several points, e. g. a polyline or a bezier curve, the last point is set with the middle mouse button.

The graphic attributes (e.g. color, line and fill style, font type) of new objects is taken from the *Attributes Selector* (see Chapter 5.5 on page 44). For new objects that require an NMR data set, the data set is taken from the *Data Set Selector* (see Chapter 5.6 on page 46).

5.2.1.1 Basic objects

XWIN-PLOT supports the following basic graphical object types which are accessible in the **Basic** major editing mode:

- Lines
- Polylines
- Polygons
- Rectangles

- Circles
- Open and closed bezier curves
- Standard text objects
- EPSI[8)] objects (Unix version) / Metafile objects (Windows version)

For each of these objects there is a corresponding drawing mode which can be selected by clicking on one of the drawing mode icons shown in Figure 5.3. The

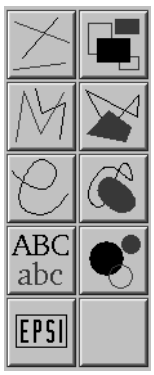


Figure 5.3 The icons for creating basic objects

editing of basic objects will be described in detail later. (Refer to page 59 in Chapter .)

5.2.1.2 NMR objects

The following NMR objects are supported by XWIN-PLOT when the **NMR** major editing mode is selected:

- Spectral parameters
- Spectra titles
- FIDs
- 1D spectra

8) Encapsulated PostScript Interchange

- Stacked 1D spectra
- 2D spectra
- T1/T2 curves
- NMR dataset-related text objects

The NMR objects are handled the same way as the basic objects.

For each object there is a corresponding drawing mode which is activated by selecting one of the icons on the left side of the graphics window. The editing of

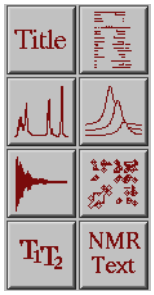


Figure 5.4 The icons for creating NMR related objects

NMR related objects will be described in detail in Chapter .

5.2.2 Expand and zoom mode

With the expand and zoom modes (Figure 5.5) a part of the layout or of an individual object can be enlarged. Expansion applies to the individual objects of a layout.

While the expansion of objects only applies to NMR objects like FIDs and spectra, zooming affects the layout as a whole.

Figure 5.5 The icons for expanding and zooming

After entering the zoom mode you can mark the area to be zoomed by moving the mouse while the left mouse button is being pressed. The area on which the zooming will have an effect is indicated by a rectangle. After releasing the mouse button, XWIN-PLOT will display an enlarged view of this area.

The buttons **Zoom In** and **Zoom Out** in the upper part of the layout window (Figure 5.6) can be used to zoom the currently visible region. Click on **Full** if you want

Figure 5.6 Buttons for zooming in or out of a graphic

the whole layout to be displayed.

The expand operation is similar to zooming but only applies to a single object. In expand mode the part of an object that was marked with the mouse is enlarged and replaces the original object. When expanding an object with the **Shift** modifier key pressed, the objects height remains unchanged. If the **Control** modifier key is pressed, the width is not changed. Pressing the **Alt** modifier key will „blow-up“ a portion of the spectrum according to the settings in the *Global Setup* dialog (See chapter 5.11.1 on page 52.). Figure 5.7 shows an example.

5.3 Working with objects

5.3.1 Moving objects

An object can be moved any time, i. e. independent from the input mode. To move an object, place the cursor within the object‘s bounding box, keep the middle mouse button pressed and move the mouse. The bounding box is indicated by a dotted rectangle as soon as the cursor enters the box. It is not necessary to mark an object in order to move it.

5.3.2 Marking objects

Within XWIN-PLOT there are two different modes for marking objects. Objects can be selected either by their individual points (Figure 5.9) or as a whole (Figure

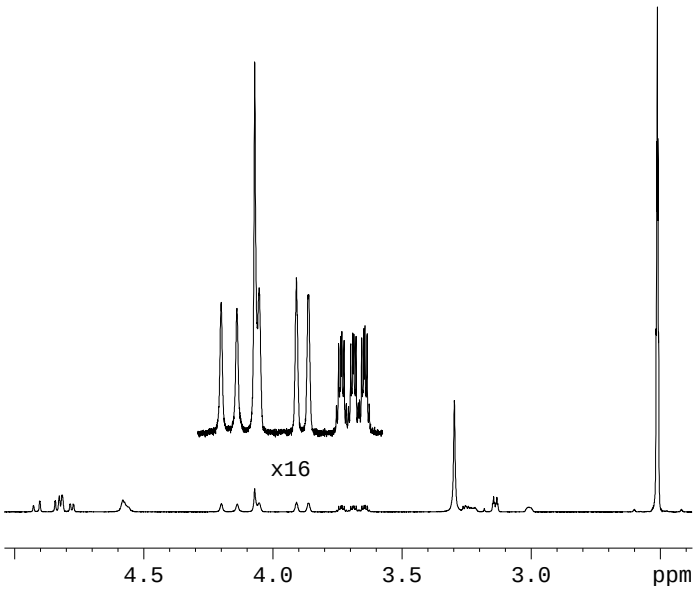


Figure 5.7 Spectrum „blow-up“

5.10), depending on the marking mode. (See Figure 5.8.) Objects that have been marked can be identified by the markers that have been placed around them[9)].

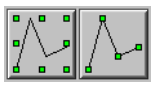


Figure 5.8 The icons for the marking modes

With most objects there is no difference between the two marking modes. For objects like polygons, however, which are defined by several base points, the two modes have a different meaning. When marking such an object by its individual points, the position of each base point can be changed individually using the mouse. This results in the object changing its form, i. e. the form of its bounding

9) The marker size can be changed in the *Global Setup*.

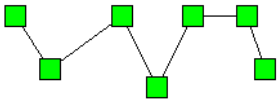


Figure 5.9 A polyline object marked by its points

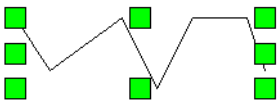


Figure 5.10 The same object as in Figure 5.9, this time marked as a whole

box. When an object is marked as a whole (Figure 5.10), only the objects dimensions can be changed, but not its individual point positions.

To mark more than one object you have to select each item with the left mouse button while holding down the **Shift** modifier key. Several objects can be marked simultaneously with the mouse by putting a frame around them. Place the mouse cursor outside the layout region to be marked, press the left mouse button and move the mouse over the objects. A frame appears and all objects inside this frame are marked after releasing the mouse button.

Use the **Mark All** command from the **Edit** menu if you want to mark all objects simultaneously. **Mark All** implicitly activates marking mode.

5.3.3 Using a spectrum or FID as a clipping window

If modifier keys are pressed while scaling or moving a FID or spectrum, the FID or spectrum will not change its x position (provided **Shift** or **Alt** is pressed) or y position (provided **Control** or **Alt** is pressed). The FID or spectrum object may thus be used as a a clipping window.

5.3.4 Deleting marked objects

Delete removes all marked objects.

5.3.5 Copying marked objects

The **Copy** command duplicates all marked objects. After copying an object the copy is independent from the original object.

5.3.6 Rotating marked objects

Use **Rotate** to rotate all marked objects by 90, 180 and 270 degrees, respectively.

5.3.7 Creating object groups

Sometimes operations like moving or scaling have to be applied to a number of objects. In this case it may be convenient to combine all of these objects into a group. Before a group can be created at least two objects have to be marked. Click on the **Group** button or use the **Group** menu entry to combine the objects.

If all the objects within a layout are intended to be part of a group, the menu command **Mark All** can be used as a shortcut for selecting all the objects at once.

To split a marked group into its individual parts, use the **Ungroup** button in the layout window or the menu bar.

5.3.8 The stacking order

If a layout contains overlapping objects, you may want to move an object to the foreground or background. The commands **Raise** and **Lower** in the **Edit** menu are provided for this purpose. The command **Raise** places the marked objects in the foreground, while the command **Lower** places them in the background.

5.4 The Popup Menu

Pressing the right mouse button or the **[F4]** function key[10)] will automatically mark the object under the cursor and display a popup menu that contains the most frequently used commands (Figure 5.11). This is especially useful if you want to edit an object.

10) On many Unix type systems the popup menu will not work as long as the NUMLOCK state is activated on your keyboard. Press the NUMLOCK key again to deactivate it. This behavior cannot be influenced by XWIN-PLOT

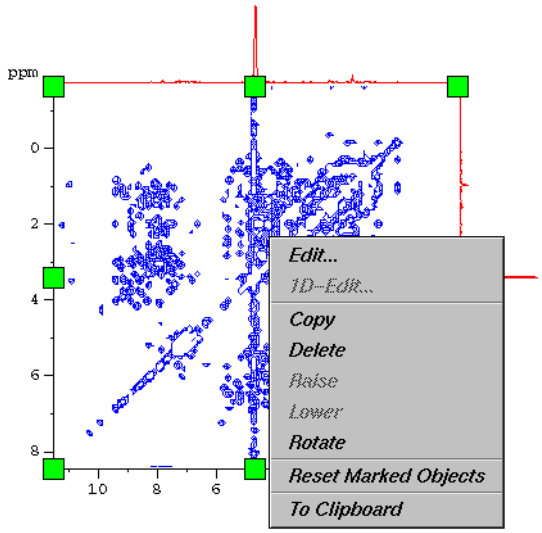


Figure 5.11 The popup menu

5.5 Attributes

The *Attributes Selector* (Figure 5.12) is displayed by clicking on the **Attributes** button. If one of the creation modes (Chapter 5.2.1) is active, after clicking **Apply** or **OK** all changes made in the *Attributes Selector* will affect objects created subsequently. If one of the marking modes (Chapter 5.3.2) is active, the attributes of the marked objects can be changed by pressing the **Set** button. The **Reset** button will set all attributes to their default values.

XWIN-PLOT supports two different color models, namely a set of 16 fixed colors and arbitrary color settings depending on RGB values. The active color is selected with either the 16 buttons for the standard colors or by activating the RGB color button. The settings for line and fill colors can be changed independently. You can switch between the line and fill color settings by selecting the corresponding radio button.

After clicking on the button **RGB Settings**, the *RGB Settings* dialog window will be displayed (Figure 5.13). RGB colors can be changed by entering red, green and

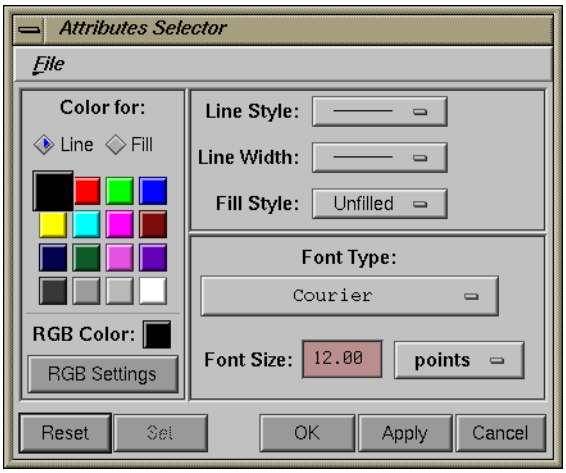


Figure 5.12 The *Attributes Selector*

Figure 5.13 Changing the RGB settings

blue values in textfields or by moving sliders. The current RGB values and the resulting color are displayed while you are editing. If the number of available col-

ors is exhausted, the color shades shown in the **Color** field may not reflect the true values indicated by the contents of the textfields or by the slider positions[11)]. However, this does not affect the colors as they appear on a printout.

To change the font size, choose one of the font units in the option menu and enter a value in the **Font Size** input field.

All the settings of the *Attributes Selector* can be loaded and saved with the commands available in the **File** menu.

5.6 Data set handling

5.6.1 The Data Set Selector

The *Data Set Selector* (Figure 5.14) contains all the data sets available for XWINPLOT. All data sets that are to be displayed as parts of NMR related objects have to be chosen in this selector first.

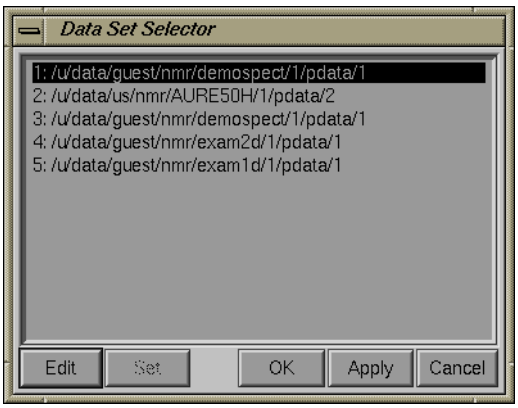


Figure 5.14 The *Data Set Selector*

The data set that is selected in the *Data Set Selector* is the one that will be used if new NMR objects are created. For stacked plot objects, which usually contain

11) The maximum number of different colors depends on the display hardware.

more than one spectrum, the first of these spectra has to be selected in the selector. All stacked plot spectra are taken from the *Data Set Selector* in ascending order, beginning with the active data set.

To select a data set, mark it with the left mouse button and press **Apply** or **OK**. Press **Set** to change the data set for the currently marked objects. Double clicking on a data set name selects this data set and closes the selector.

After clicking on the **Edit** button, the *Portfolio Editor* will pop up.

5.6.2 The Portfolio Editor

In XWIN-PLOT all actions related to loading NMR data sets are handled by the *Portfolio Editor* (Figure 5.15) in combination with the *Data Set Selector.*

Figure 5.15 The *Portfolio Editor*

In the *Portfolio Editor* NMR data sets can be selected by name. These names are composed of the data directory the data sets reside in, the user and data set names and the experiment and processing numbers. Before an NMR data set can be used in the plot editor, it must be added to the portfolio editors selection list. This is done by double clicking on the data set entry or by selecting it and clicking on the **Append** button. All active data sets are listed at the bottom of the *Portfolio Editor* form. With **Insert** a data set can be inserted into the list of active data sets at an arbitrary position. The new entry is placed before the active one. **Remove** deletes a data set from the portfolio list. **Apply** finally accepts all selections and updates the *Data Set Selector*. The data sets to be displayed in NMR related objects can be selected from the *Data Set Selector*, as described in 5.6.1.

The *Portfolio Editor*'s **File** menu provides commands for saving, loading and appending portfolio contents. By convention portfolio file names end with `.por`. If a portfolio is saved as default, it is loaded automatically each time XWIN-PLOT is started. If the plot editor is started within XWIN-NMR, it additionally searches for a portfolio named `portfolio.por` in the processing directory of the current dataset and loads that if present. Otherwise the default portfolio remains loaded. Content of the portfolio is transferred to the data set list. Finally the first entry in the list is replaced by the current data set, and if there are projections these are placed on positions 2 to 5. The rest of the portfolio remains unchanged. The default portfolio data is also used by the XWIN-NMR `search` command. The **Edit** menu offers options to sort the portfolio data in ascending or descending order and a **Clear** command to remove all selections.

With **Edit Directory List** in the **Edit** menu you can specify the directories (formerly called *disk units*) that contain XWIN-NMR data files. Directories are valid data directories if they contain a folder `data` with XWIN-NMR data. The directory list dialog window displays all currently valid directories in a list box (Figure 5.16). Data directories can be added to this list by specifying their name in the **Directory** text field and pressing the **Return** key or the **Add** button. Select one or more directories and click on **Remove** to delete them from the directory list. The current directory list will be accepted by the *Portfolio Editor* after clicking on **Apply**.

Figure 5.16 Editing the data directory list

5.7 File handling

All file related functions are found in the plot editor‘s **File** menu. Select **New** to open a new, empty layout window. With **Open,** a previously existing layout can be loaded. With **Save** you can save a layout under its current name. Use **Save As** if the layout is to be saved under a new name. Select **Abandon** to reload the current layout and discard all changes.

Save Layout/Portfolio to Dataset saves the layout in the processing directory of the current dataset. Additionally the contents of the current portfolio is saved under the predefined name `portfolio.por`. Select **Open Layout/Portfolio from Dataset** to open them againt. See also Chapter 5.6 on how the file `portfolio.por` is using during startup of XWIN-PLOT.

To close a layout window select the **Close** menu entry. As soon as the last layout window is closed, XWIN-PLOT will terminate. XWIN-PLOT also terminates if the **Close All** menu option is selected.

5.7.1 Archive functionality

AUTOPLOT will always store a backup copy of the currently used layout to the first data set on the list. The backup copy gets the fixed name `last_plot.xwp`.

This ensures that you always could exactly reproduce the last plot of this dataset even when your standard layouts have been changed in the meantime. In that case use the **Open Layout/Portfolio from DataSet** command to load `last_plot.xwp` into XWIN-PLOT again.

5.8 Printing a layout

The graphics created by the XWIN-PLOT editor can be printed in high quality on most printer types, including dot matrix printers as well as ink jet or laser printers. Additionally a graphic can be saved as a file which can be imported into a text document.

To print or preview a layout select the **Print** menu entry in the **File** menu.

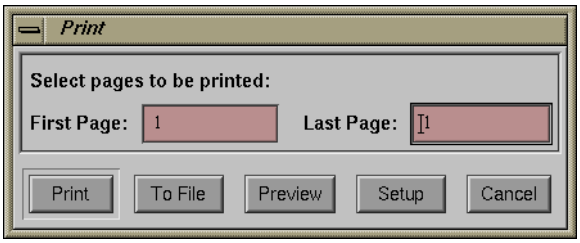


Figure 5.17 The Print form

The *Print* form (Figure 5.17) allows you to print, save or preview the graphics according to the settings chosen in the *Printer Setup* (See chapter 5.11.3 on page 54.). The *Printer Setup* may be selected from the *Print* form or from the **Options** menu. You can also select the range of pages to be printed.

Select **To File** to save the graphic in the natural printer format according to the printer setup. A graphic that is saved to a file can be imported into a text document.

After clicking on **Preview** a new window is opened and a preview of the current graphic will be displayed.

5.9 Undo

Any operation on a layout can be reversed by clicking on the **Undo** button or choosing the **Undo** command in the **Edit** menu.

5.10 The XWIN-PLOT clipboard

Note: For differences in the Windows version of XWIN-PLOT please refer to Chapter 11.

For copying objects between different layout windows a clipboard mechanism is available. To display the clipboard window (Figure 5.18) select the **Show Clipboard** option in the **Edit** menu. After marking your objects, they can be copied to the clipboard by selecting **Put to Clipboard** in the **File** menu.

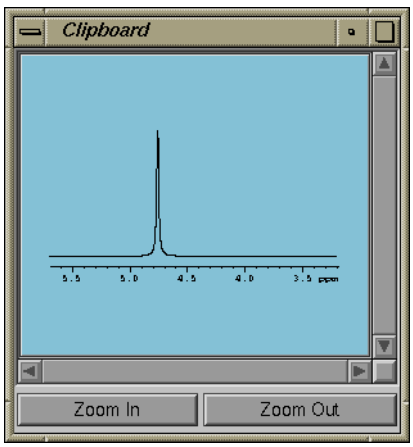


Figure 5.18 The clipboard with an object in it

The clipboard contents can be zoomed using the **Zoom In** and **Zoom Out** buttons. With **Get from Clipboard** the clipboard data is copied to the active layout window. **Clear Clipboard** removes the clipboard contents[12)].

5.11 Setting up XWIN-PLOT

All setup-related options are found in the **Options** menu and will be described in the following sections.

5.11.1 The Global Setup

Within the *Global Setup* shown in Figure 5.19 you can change some general parameters. The *Global Setup* dialog window is displayed after selecting the corresponding menu entry.

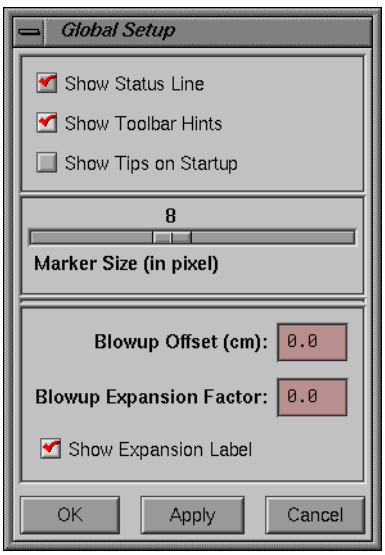


Figure 5.19 The *Global Setup* dialog window

12) This operation cannot be reversed by *Undo*.

Each layout window has a status line below its drawing area which contains information about the current mouse cursor position, the size of the active object or a data set name. Deselect the button **Show Status Lines** if you do not want this information to be displayed. Removing the status line will provide additional space for the graphics. If **Show Toolbar Hints** is enabled, small popups providing a short help text are displayed when the mouse stays a certain time over a particular button in the layout window. XWIN-PLOT displays a dialog window with helpful tips about certain program features each time the program is started, if the option **Show Startup Hints** is selected (Figure 5.20).

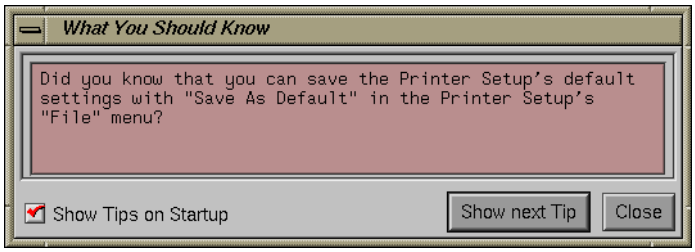


Figure 5.20 A startup tip

Depending on your screen resolution it may be necessary to change the size of the markers XWIN-PLOT displays around marked objects. The marker size can be changed with the slider **Marker Size (in pixel)**.

In the *Global Setup* dialog you can also set the parameters for the „blow-up“ function that is available in expand mode (See chapter 5.2.2 on page 39.).

The settings made in the *Global Setup* are automatically saved when leaving XWIN-PLOT.

5.11.2 The Layout Setup

In addition to the global settings made in the *Global Setup*, for each layout window there is a *Layout Setup* with options that affect only the current layout window. (See Figure 5.21.)

Usually objects are not placed arbitrarily on the screen but their positions are aligned horizontally or vertically. XWIN-PLOT provides an invisible grid which

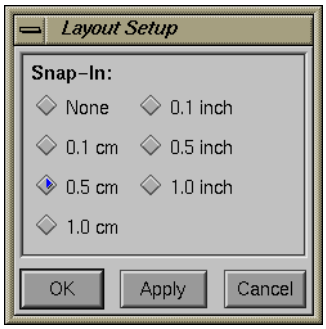


Figure 5.21 The *Layout Setup*

helps in aligning objects. The grid distance is selected by the radio buttons under **Snap-In**. When placing an object on the screen the mouse cursor will automatically jump to the locations marked by the grid[13)].

5.11.3 The Printer Setup

Note: For differences in the Windows version of XWIN-PLOT please refer to Chapter 11.

The *Printer Setup* dialog window (Figure 5.22) contains all printer related options. The setup data is saved automatically, together with the layout information, if you choose **Save** or **Save As** from the layout window‘s **File** menu.

The XWIN-PLOT plot editor comes ready for use with a variety of printers. Select your printer from the **Printer Type** list at the top of the *Printer Setup* dialog window. If you have a printer with built-in PostScript support choose the **PostScript** entry. Otherwise select the entry corresponding to your printer name. If your printer is not listed, you will have to choose an entry that is compatible with your printer, i. e. a printer which offers the same printer emulation as yours. Please consult the printer manual if you are in doubt about the emulation mode needed for your printer. Most dot matrix printers have built-in Epson emulation, a lot of laser printers are compatible with the HP LaserJet series. Ink jet printers usually are compatible with the HP DeskJet or the Canon BubbleJet. If no information about

13) The Snap-In settings have no effect in expand and zoom mode.

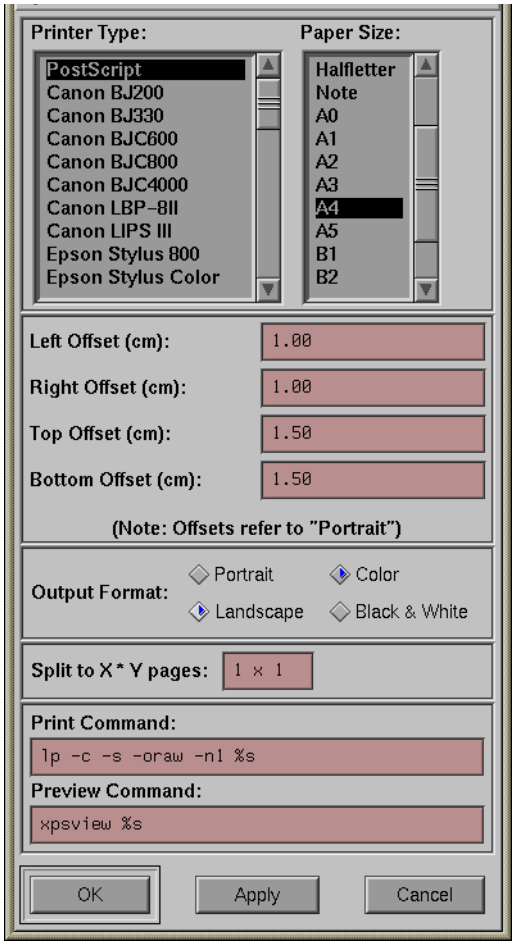


Figure 5.22 The *Printer Setup* dialog window

the printer emulation is available it is a good idea to try some of the predefined printer types. Choosing the wrong emulation will not harm a printer, but it will give bad or no results. On the other hand, if the printer output is identical to the graphics on the computer screen, you can be quite sure that you have found an emulation compatible with your printer type.

The **Printer Type** list also contains entries for creating graphic export files. An important entry of this type is EPSI[14]. Choose this entry if you want to import your graphic into programs that support Encapsulated PostScript import, e. g. `FrameMaker` or *Corel Draw.*

XWIN-PLOT recognizes most common paper formats which can be selected in the **Paper Size** list. Because of their mechanics most printers do not utilize the full area of a sheet of paper. To ensure that parts of a layout do not exceed the printable paper size, printer offsets have to be specified for each edge of the page. Usually these values need not to be changed since the default values work with most printer types.

The **Paper Size** settings have an effect on the printer output as well as on the screen layout of the plot editor‘s layout windows. If the paper size or offsets are changed, the dimensions of the screen layout are adjusted accordingly after pressing **Apply** or **OK**.

The XWIN-PLOT editor supports both the *Portrait* and the *Landscape* output format. Choose one of these formats from the **Output Format** options. Switching between the Portrait and the Landscape format will also affect the current layout. If a color printer is available you can choose between monochrome or color printings. It is recommended that the color option is used with color printers only and not with black and white ones. Otherwise the graphics might be modified by the printer or the printer driver in order to visualize different color shades. In this case the **Color** option does not give satisfying results on most black and white printers.

If the desired size of a printing job is larger than the physical paper size, e. g. for a poster, it can be split and distributed over several sheets of paper. To print the graphics on several pages, select the number of pages for each dimension using **Split to X*Y Pages**. These pages can be fit together at their edges later on. The screen layout will display the splitting settings after pressing **Apply** or **OK**.

As XWIN-PLOT was preconfigured to directly work with a standard SVR4 Unix environment, the **Print Command** and **Preview Command** options at the bottom of the *Printer Setup* form in most cases will only have to be changed in a non-standard environment. With **Print Command** you can define the command string the plot editor uses when transferring the plot data file to the printer spooler. A valid command string might look like this:

14) Encapsulated Postscript Interchange

```
lp -c -s -oraw -n1 -dMyPrinter %s
```

`lp` is the name of the standard Unix printer spooler program to be used, followed by several options:

- The `-c` option tells `lp` to copy the print code file and print the copy instead of the original file. *This option must not be omitted since the print code file will be deleted immediately after executing the `lp` command.*
- The `-s` option prevents `lp` from reporting status messages about the print job.
- The `-oraw` option tells `lp` to work in raw mode, i. e. data is not interpreted. *This option must not be omitted.*
- The `-n` option specifies the number of copies to be printed, e.g. `-n2` for two copies. If you just want to have one copy, this option can be omitted.
- The `-d` options tells `lp` which printer to use, e.g. use `-dMyPrinter` to print on the printer with the name `MyPrinter`. If you want to use the default printer, this option can be omitted.
- The option `%s` stands for the name of the file to be printed and is automatically replaced by an appropriate filename during runtime. The `%s` must not be omitted.

If the BSD printer spooler is running on your machine, the command for printing with XWIN-PLOT will probably be (use this on Linux systems):

```
lpr -h -#1 %s
```

The option `-h` will suppress the printing of the burst page. With `-#` the number of copies can be specified.

The **Preview Command** textfield defines the command which runs the PostScript previewer. On an *SGI* platform the *xpsview* software package is used as default previewer.

Once you have selected printer settings reflecting your configuration and your needs, the new setup can be activated by clicking on **Apply** or **OK**. If you want to exit without the changes taking effect, choose **Cancel**.

To select the current printer configuration as the default setup, use the **Save As Default** option in the *Printer Setup*'s **File** menu. Use **Save As** for saving the current printer setup with a specific name. The setup can be retrieved later using the **Load** command.

5.12 On-line help

The complete XWIN-PLOT manual is available in a Hypertext help format. Help texts are displayed after selecting the corresponding entries in the **Help** menu.

6

Object editors

XWIN-PLOT supports a variety of object editors:

- There are several standard object editors which allow for the setting of all relevant parameters for all graphic objects.
- There is a special 1D object editor for FIDs, T1/T2 curves and 1D spectra and a special 2D object editor for 2D spectra.
- The *Attributes Selector* (see Chapter 5.5 on page 44) can be used to modify an object‘s graphic attributes.
- The *Data Set Selector* (see Chapter 5.6 on page 46) can be used to change an object‘s data set.

6.1 Standard object editors

After marking an object and clicking on the **Edit** button one or more standard object editors will be displayed. The number and types of these editors depend on the type of the object for which the edit command was called. For simple objects like rectangles only the basic object editor will be displayed. For more complex objects there are additional object editors.

As long as an object is being edited it cannot be modified in the layout window.

6.1.1 The basic object editor

With the basic object editor the position and dimension of an object can be set.

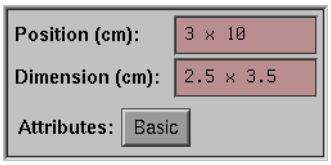


Figure 6.1 The basic editor

Note that the position and dimension are the logical position and dimension, not the position and dimension of the bounding box. The markers placed around objects (see Chapter 5.3.2 on page 40) show the logical position and dimension, while the dotted rectangle that appears as soon as the mouse cursor enters an object, shows the position and dimension of the bounding box.

The logical position and dimension and the position and dimension of the bounding box only differ for a few objects, e.g. for a line object with arrow tips or for a spectrum or FID object with axes and the option **Scale Bounding Box** set to false.

After clicking on the **Basic** button an attribute editor will pop up. This editor allows you to change the marked objects attributes. The **Basic** button can only be used to select objects that support basic editing functions.

6.1.2 The arrow object editor

Arrows tips can be added to lines and bezier curves. When editing these objects the arrow style and tip width can be selected as shown in Figure 6.2. If you want a filled arrow tip, use the basic attributes to set the fill style and the fill color accordingly.

6.1.3 The EPSI object editor

Note: For differences in the Windows version of XWIN-PLOT please refer to Chapter 11

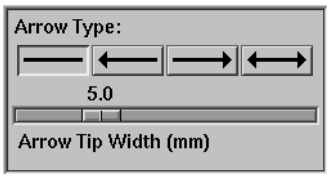


Figure 6.2 The arrow object editor

For EPSI objects the EPSI object editor (Figure 6.3) provides the means to select

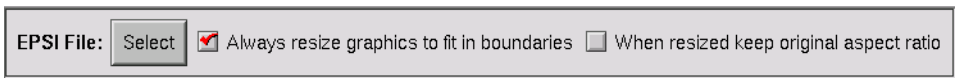


Figure 6.3 The EPSI object editor

an EPSI file which is to be displayed inside an EPSI object. After clicking on **Select** the EPSI file can be specified in the file selector. EPSI objects can use EPSI files relative to the current data set. Then the same layout will include different graphics for different data sets. When entering the filename you can specify the path as specified on page 15. You can also use absolute paths to use always the same graphics file.

By default, XWIN-PLOT will resize the graphics so it will never exceed the boundaries of the EPSI object. This may result in distortion of the graphics. Checking the option **Always maintain aspect ratio** ensures the graphics will not be distorted if the aspect ratio of the EPSI graphics differs from that of the object while still resizing it. When **Always resize graphics to fit in boundaries** is unchecked the graphics will not be resized at all and possibly clipped off by the boundaries of the EPSI object.

It is possible to set up the EPSI object editor to recalculate the position and dimension of the EPSI object according to the aspect ratio provided by the postscript file when pressing **OK** or **Apply** (Figure 6.4).

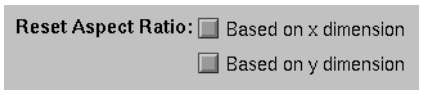


Figure 6.4 Resetting the aspect ratio of EPSI objects

6.1.4 The text object editor

Text objects can be aligned vertically and horizontally by selecting vertical or horizontal alignments. (See Figure 6.5.) You can also edit the text by selecting **Edit**

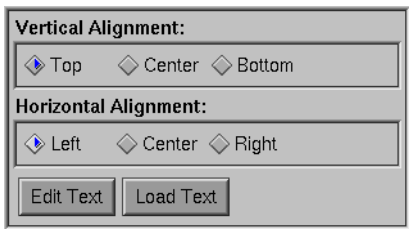


Figure 6.5 The text object editor

Text. A dialog window with a simple text editor will be displayed. The button **Character Chart** displays a chart showing all available characters of the current character set, including those that cannot be typed on the keyboard. To select one of these characters click on the corresponding button. The character will be inserted in the current text at the text cursor position.

With **Load Text** the text to be displayed can be loaded from a text file. After loading the text you can edit it with **Edit Text**. Note that the contents of this kind of text object can only be changed manually. Sometimes it is desirable that the actual text is read from a file and that there is a unique text file for each NMR dataset. The NMR text object has to be used in this case. “The NMR text object editor” on page 78 provides more information.

When making changes to the text alignment, it may be necessary that the *hot point* remains unchanged[15)]. For this purpose an additional option should be used (Figure 6.8). When changing a text objects contents, the object dimensions often

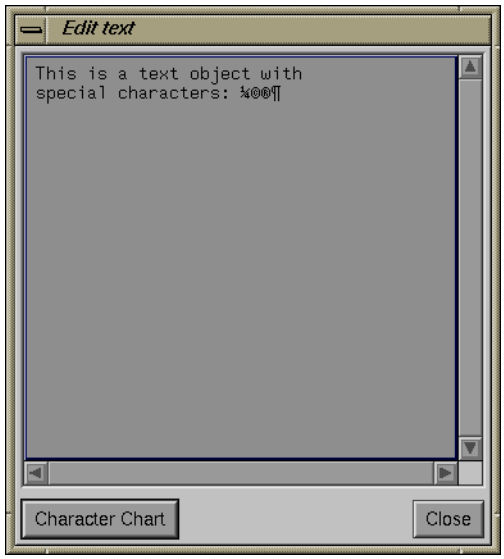


Figure 6.6 Editing a text object

change, too. If the switch **Recalculate Object Dimensions** is activated, XWINPLOT will adjust the objects edges to fit the new size text object exactly. With some objects, especially those with centered text, this may give undesired results. If you don‘t want the text object‘s size to be affected after changing the text, deselect this option. The hot point option and the recalculation option do not change the object directly but only the way **OK** or **Apply** work on this object.

6.1.5 The resizable text object editor

Text objects can be set up to change or not to change the font size automatically after scaling. This can be done by enabling or disabling the button **Allow automatic font resize** (Figure 6.9).

15) The *hot point* is the text‘s anchor point.

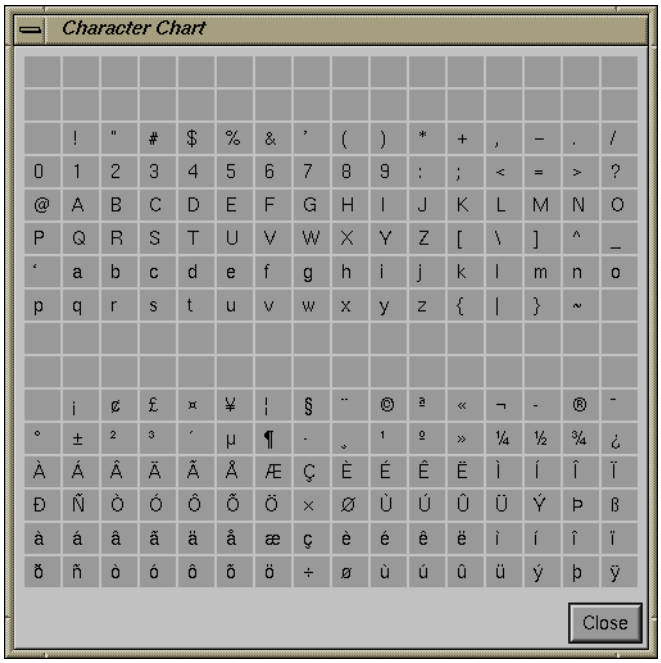


Figure 6.7 The character chart

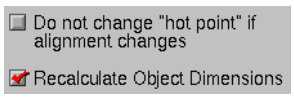


Figure 6.8 Options for editing text objects

Figure 6.9 The resizable text object editor

6.1.6 The graph object editor

The graph editor (Figure 6.10) provides basic operations that can be applied to all objects which support axes and grids. The horizontally and vertically visible parts

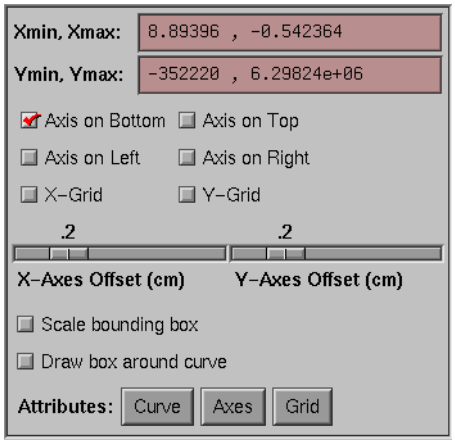


Figure 6.10 The graph editor

of a spectrum are affected by the data in the **Xmin**, **Xmax**, **Ymin** and **Ymax** text-fields. Horizontal and vertical axes or grids can be switched on and off with the corresponding toggle buttons. The **X-Axes Offset** and the **Y-Axes Offset**, resp., change the distance between the spectrum and its axes.

By default, the logical position and dimension of a graph object is the position and dimension of the curve that is displayed within this object. If you want the logical position and dimension of the graph object to be the same as the position and dimension of the graph object‘s bounding box, activate the button **Scale Bounding Box**. This is useful if you intend to group a graph object with a frame and want to scale this group. You should not activate **Scale Bounding Box** in order to group a graph object with text and line objects that serve as annotations. Scaling such a group with **Scale Bounding Box** activated will change the relative positions of the annotations to the curve of the graph object.

When **Draw Box around Curve** is selected, XWIN-NMR places a box around the curve object. For 2D spectra this is the default behavior.

For each part of a graph object the basic attributes may be set independently. This enables you, for example, to assign a spectrum‘s axes a color different from the spectrum itself. To change the attributes of the spectrum‘s curve, the axes or the grids, click on one of the corresponding buttons **Curve**, **Axes** or **Grid**. This will pop up the attribute editor.

6.1.7 The 1D spectrum object editor

The 1D spectrum object editor provides additional functions for 1D spectrum objects (Figure 6.11).

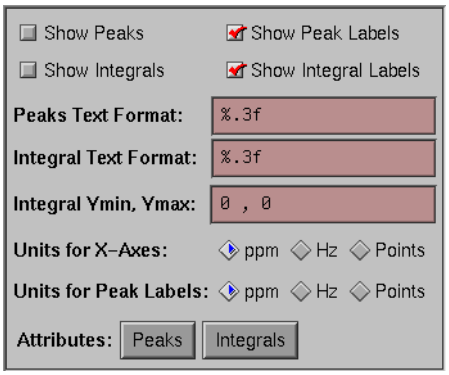


Figure 6.11 The 1D object editor

XWIN-PLOT can add peak labels and integral data to a spectrum, depending on the way a data set was processed in XWIN-NMR. If present, the additional information will be displayed after selecting the appropriate toggle buttons. The format for displaying numerical peak and integral data can be configured in the corresponding text fields. The notation for specifying the display format, in particular the number of digits to be displayed, is identical to the one used in the C programming language[16)]. The default format is

```
%.3f
```

16) See the on-line manual page for more information by executing the command `man printf` in a Unix shell.

which denotes that the data is to be displayed in a floating point format with three decimal places.

The units for axes and peak labels can be chosen independently. The graphic attributes of peaks and integrals may be changed as well as the attributes for curves, axes and grids.

6.1.8 The 1D stacked spectrum object editor

With the stacked plot editor you can change the look of stacked plot objects. (See Figure 6.12.) The horizontal and vertical distance between the individual spectra of

Figure 6.12 The stacked plot parameters

a stacked plot can be selected within the **Spectra Offset** text field.

Figure 6.13 gives an example of a white washed stacked plot that was created with XWIN-PLOT. As you will notice, only the lines in the foreground are visible. This is the result of setting the fill color in the stacked plots curve attributes to white and the fill style to „filled“. If **Set Curve Attributes to White Wash** is active when pressing **OK** or **Apply**, XWIN-PLOT will automatically set the curve attributes this way. Change the curve attributes to the standard values if you want to remove the white wash look.

Before spectra can be combined to a stacked plot, they have to be added to the *Data Set Selector*. The active spectrum in the selector is the first to be displayed in the plot. The additional spectra for the stacked plot are those listed in ascending order behind the selected spectrum.

When creating the spectra list for the *Data Set Selector* in the *Portfolio Editor*, it is often beneficial to use the sorting options in the portfolio‘s **Edit** menu to ensure the correct order of spectra. Usually either an ascending or a descending order is preferable. It is recommended that the data set names for spectra that are intended to be used in a stacked plot are selected in such a way as to allow efficient sorting for the order needed for the plot. For temperature dependent spectra, for example,

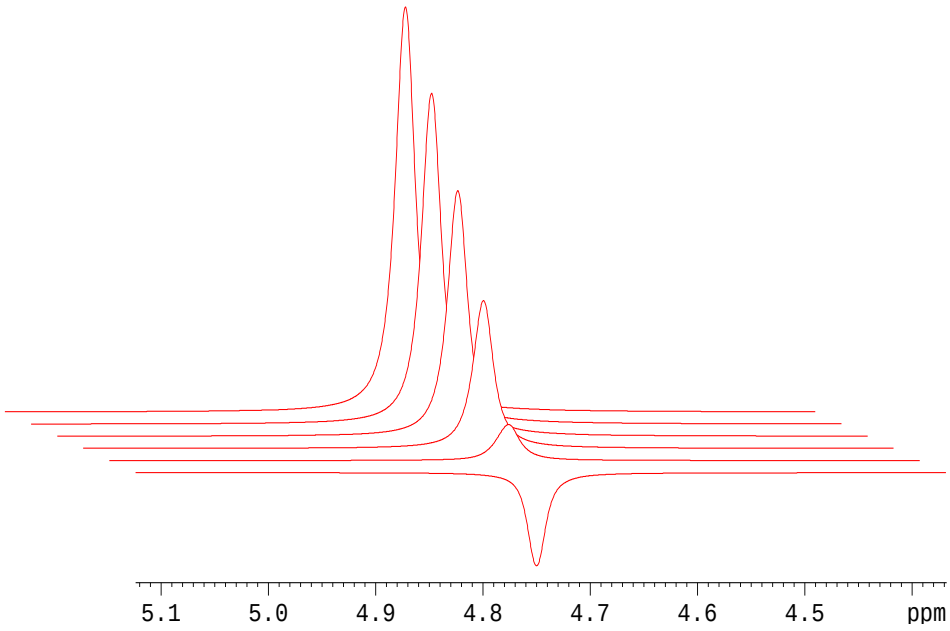


Figure 6.13 A white washed stacked plot

Figure 6.14 Setting white wash attributes

this means that the data set names should contain information about the acquisition temperature. In stacked plots such spectra usually are displayed according to rising or falling temperatures, so data set names with the temperature as one of their components will guarantee that a particular order can easily be achieved.

6.1.9 The 2D spectrum object editor

When editing 2D spectra, the units may be chosen separately for each of the two axes. The graphic attributes for negative and positive levels can be selected glo-

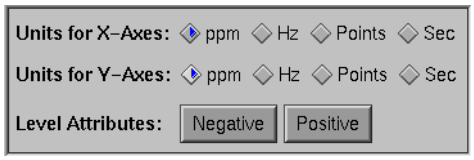


Figure 6.15 The 2D object editor

bally. Use the interactive 1D/2D editor to change the color settings for a particular level.

6.1.10 The 2D projection object editor

This editor allows to select 1D spectra that will be displayed as projections at the axes of a 2D NMR spectrum. Each axis has a toggle button which allows to display

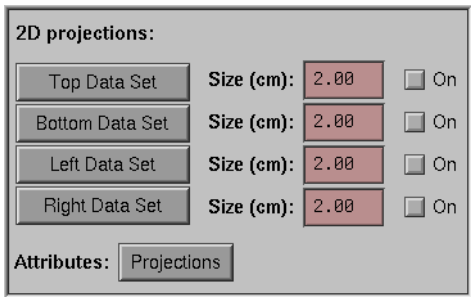


Figure 6.16 The 2D projection editor

the corresponding projection (Figure 6.16). To select a projection data set, click on the buttons **Top Data Set**, **Bottom Data Set**, **Left Data Set** and **Right Data Set**, respectively. The *Data Set Selector* will pop up and you can select the data set to be displayed. The projection size can be changed in the corresponding text fields. All projections have identical graphic attributes which can be edited by clicking on the **Attributes** button.

6.1.11 The T1/T2 object editor

XWIN-PLOT is capable of displaying T1/T2 curves created by the XWIN-NMR relaxation (T1/T2) routine. In the T1/T2 object editor the curve attributes can be changed (see Figure 6.17). For each of the T1/T2 relaxation point lists you can edit

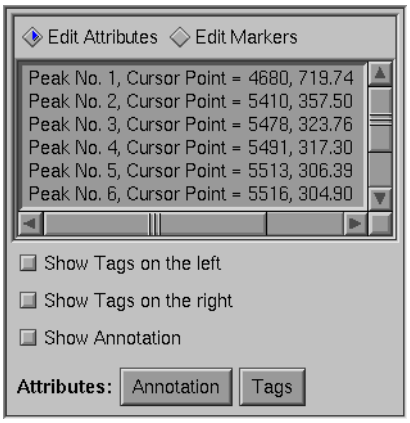


Figure 6.17 The T1/T2 object editor

the graphic attributes by clicking on a list entry while the button **Edit Attributes** is active. Click on **Edit Markers** and select a list entry afterwards in order to change the marker type and size in the *Marker Selector* (Figure 6.18). Optionally tags

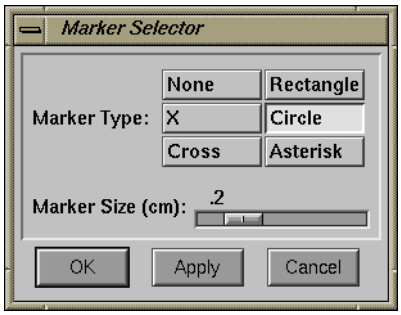


Figure 6.18 The *Marker Selector*

identifying a curve can be displayed on the left or right of each curve. **Show Annotation** will display an annotation below the T1/T2 object. The graphic attributes for the tags and the annotation can be chosen independently. Figure 6.19 demonstrates how a T1/T2 plot can look like. Note that the start and end points of the hor-

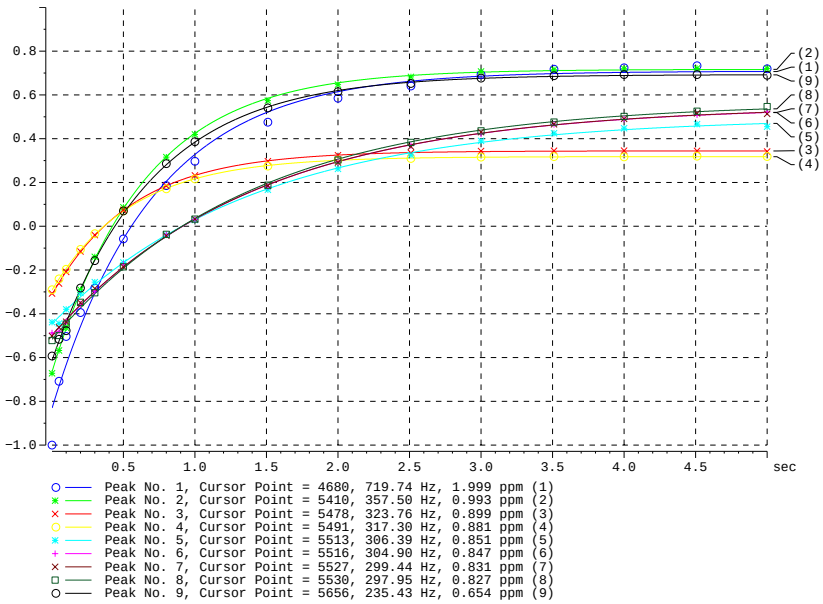


Figure 6.19 An example of a T1/T2 plot

izontal scale are taken from the minimum and maximum information provided by the corresponding JCAMP file containing the T1/T2 data. The range of the scale can be changed in the graph object editor.

6.1.12 The NMR object editor

When editing NMR-related objects, you can choose a new data set for the current object in the NMR object editor (see Figure 6.20). After clicking on **Select from Portfolio** the *Data Set Selector* will pop up and another data set can be selected as already described in Chapter 5.6.

Figure 6.20 The NMR object editor

6.2 The 1D/2D object editor

The way how a 1D object, e. g. a spectrum or a FID, is displayed can be changed by using the interactive editing facilities available after clicking on the **1D/2D-Edit** button while a 1D object is selected. 1D and 2D objects can also be edited by using the extended editing mode which can be entered by selecting the **Edit** button. The interactive editing mode provides tools for changing the dimensions of a 1D or 2D object as well as adding or removing axes and grids.

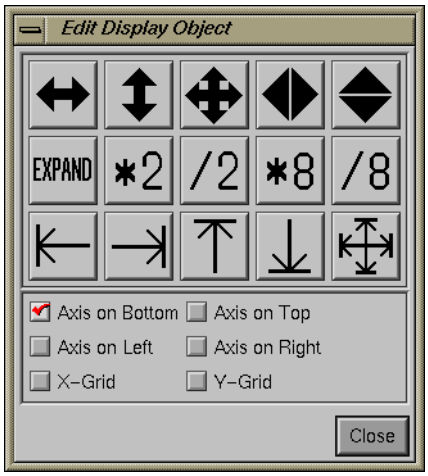


Figure 6.21 Interactive 1D/2D editing

The 1D/2D object can be moved vertically or horizontally with the tools on the left of the toolbar‘s upper row. When clicking on one of the icons with the left mouse button and keeping the button pressed, you can change the spectrum‘s position by moving the mouse in the directions indicated by the arrows inside the icons.

By using the two icons on the right of the upper row the graphic can be expanded horizontally or vertically. As long as the mouse button remains pressed and the mouse is being moved the spectrum or FID will change.

Use the **EXPAND** button to expand the spectrum in all directions simultaneously. Moving the mouse pointer upwards results in the object being magnified. Moving the pointer downwards reduces the object size.

If a 1D graphic is to be stretched vertically by well defined values you can multiply or divide its height by 2 or 8. Applied to a 2D object the level values of the object will be affected by the multiplication or division.

With the next group of editing tools the object‘s edges can be adjusted to exactly fit the object‘s dimensions. Each edge can be adjusted separately. When clicking on the icon on the right the spectrum‘s edges are reset to their original values.

XWIN-PLOT provides axes that can be displayed outside the 1D/2D object. A horizontal or vertical grid inside the spectrum area is also provided. (See Figure 6.22.)

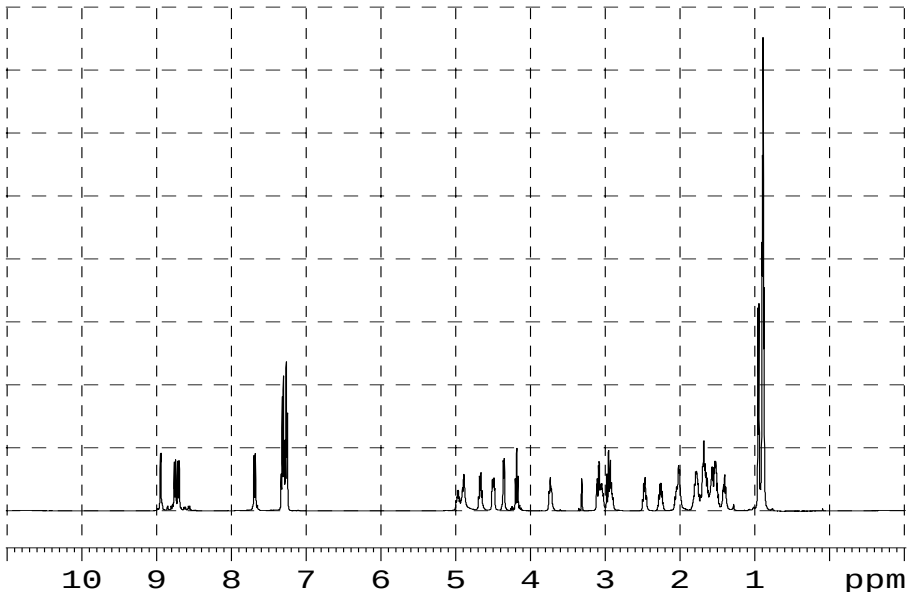


Figure 6.22 A spectrum with a horizontal and a vertical grid

The type of axes or grids can be selected using the corresponding toggle buttons.

6.2.1 Additional functions for 1D spectrum objects

When editing 1D spectrum objects the 1D/2D editor will display additional features. On top of the edit dialog window you can choose if interactive editing operations affect spectra or integrals or both (Figure 6.23).

Figure 6.23 Selecting the editing scope

Peak labels and integral curves can be added to 1D spectra objects by activating the **Show Peaks** and **Show Integrals** options, respectively. (See Figure 6.24.)

Figure 6.24 The options for adding peak labels and integral curves

It is often necessary to have a well defined relationship between the frequency scale and a spectrum‘s width, especially for spectra comparison and when analyzing coupling patterns. Therefore, at the bottom of the interactive editing form you can choose the scale type as well as its units.

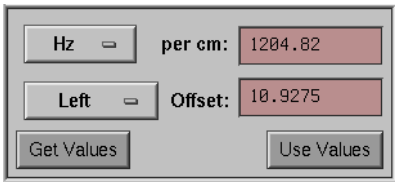


Figure 6.25 Changing units and offsets

The frequency scale can be normalized in Hz per cm or ppm per cm. The scale can also be justified with an offset. You can display the current settings with **Get Values**. The new data is applied to the current spectrum object with **Use Values**.

6.2.2 Additional functions for 2D spectrum objects

Called for a 2D NMR spectrum, the 1D/2D object editor provides facilities for interactively changing the appearance of 2D projections as well as maintaining the list of levels created with XWIN-NMR (Figure 6.26).

Scrolling and scaling of 2D projections works like already described for 1D spectra. The projection to be affected (top, bottom, left, right) is chosen with a radio button.

The 2D object editor displays a list containing the positive and negative 2D level values as defined within XWIN-NMR. New levels are added to this list by entering

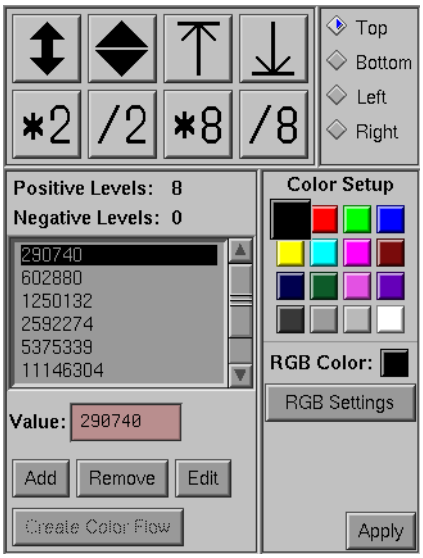


Figure 6.26 Editing a 2D spectrum and its projections

their value in the **Value** text field and clicking on **Add**. Use the **Remove** button to delete one or more entries from the list. After clicking on **Edit** the *2D Level Creator* window will pop up. There you can create an entirely new level list based on

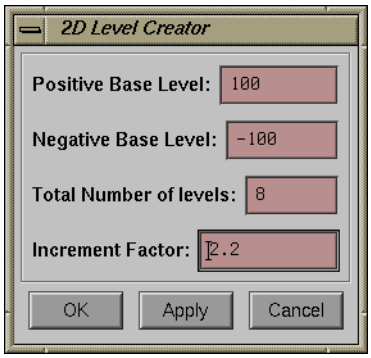


Figure 6.27 New level lists can be created with the *2D Level Creator*

base level values and an incremental factor[17]. If new positive levels are to be created enter a positive base level in the **Positive Base Level** input field. The positive base level must not be smaller than 100. The base level for negative levels must be -100 or lower and is entered in the **Negative Base Level** field. With **Total number of Levels** you can specify how many new levels will be created. The number of levels applies for positive and negative levels separately. For both negative and positive ranges new values are only created if a base level is supplied. Otherwise the already existing levels for each range (positive or negative) are preserved.

To change the color of a particular level, select this level in the level list and click on one of the color button in the 2D level **Color Setup**. The change will show an effect after clicking on **Apply**.

Often level data are represented best by a color flow where the colors between two adjacent levels differ only slightly. XWIN-PLOT creates this effect automatically when the button **Create Color Flow** is selected. This button is disabled unless exactly two levels are selected in the level list[18]. The colors of these levels are the basis for the creation of new RGB colors that will be assigned to all the levels between those chosen. Figure 6.28 gives an example of a 2D spectrum with colors automatically calculated by the **Create Color Flow** option.

It is recommended that you make some experiments with the color flow option in order to get an impression what the results look like.

When you use a layout with some assigned level colors on several different data sets the number of levels in the original layout and each data set might not match. XWIN-PLOT then automatically tries to adapt the colors to get an acceptable result.

If you always want to have one fixed color (e.g. blue) for all positive and another fixed color (e.g. red) for all negative levels simply create a 2D object with only two levels, one positive and one negative, assign the desired colors and save it. When using this layout on a data set with more than two levels XWIN-PLOT will extend your color assignment to ensure the desired result.

17) Note that any changes to the level list have an effect in XWIN-PLOT only and do not affect the level data created with XWIN-NMR.

18) Under Motif multiple selections are handled by using the modifier keys **Shift** or **Control** in addition to a mouse click.

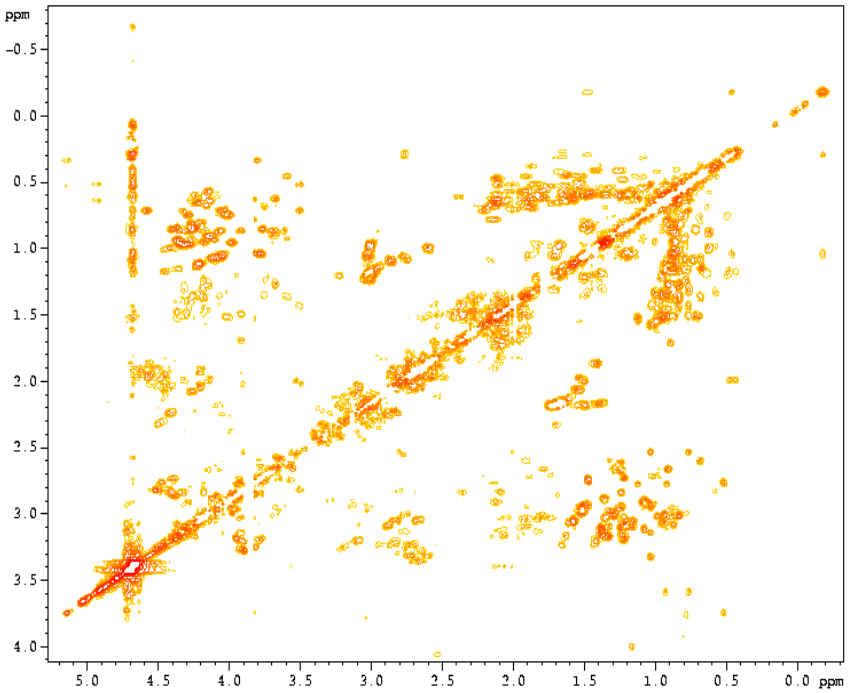


Figure 6.28 A 2D spectrum displaying automatically created colors

6.3 The NMR text object editor

In addition to the standard text objects that can be created in the **Basic** major editing mode XWIN-PLOT provides for special dataset-related text objects. These objects display a variable text instead of a fixed one. The text is read from a text file whose name is entered in the NMR text object editor (Figure 6.29). When

Figure 6.29 The NMR text object editor

entering the filename you can specify the path as specified on page 15. You can also use absolute paths.

7

Automation editors

The automation editors are called with the **Automation Parameters** entry in the **Edit** menu. This entry is only enabled if an object supporting automation parameters is selected.

7.1 Reset actions

The automation editors provide options for controlling the behavior of 1D and 2D objects in respect to a reset of these objects. Each automation editor contains options that affect an object‘s X and Y dimension separately.

7.1.1 General reset actions

All automation editors have some reset actions in common. For the X dimension these reset actions are:

- **Don‘t change:** Xmin/Xmax will not be changed on a reset.
- **Set to minimum/maximum:** Xmin will be set to the minimum x value. Xmax will be set to the maximum x value.

These are the general reset actions for the Y dimension:

- **Don‘t change:** Ymin/Ymax will not be changed on a reset.

- **Set to minimum/maximum:** Ymin will be set to the minimum y value. Ymax will be set to the maximum y value.

7.1.2 The FID automation editor

The FID automation editor (Figure 7.1) provides options that control the reset behavior of FID objects.

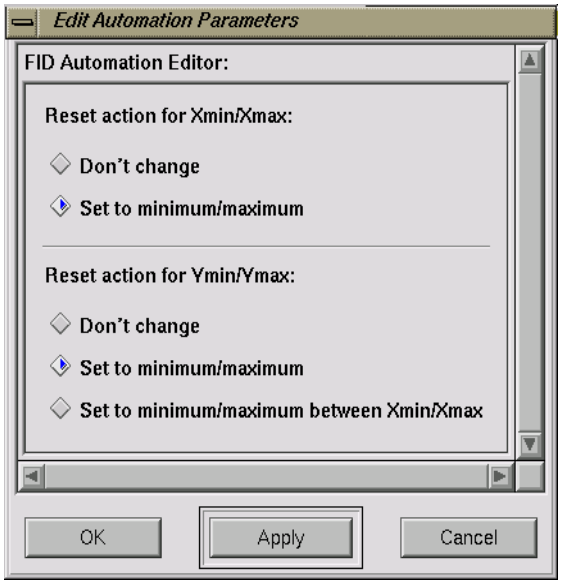


Figure 7.1 The FID automation editor

These are the additional reset actions for the Y dimension:

- **Set to minimum/maximum between Xmin/Xmax:** Ymin will be set to the minimum y value between Xmin/Xmax. Ymax will be set to the maximum y value between Xmin/Xmax.

7.1.3 The 1D automation editor

The way in which the 1D spectrum reacts in case of a reset can be selected within the 1D automation editor (Figure 7.2).

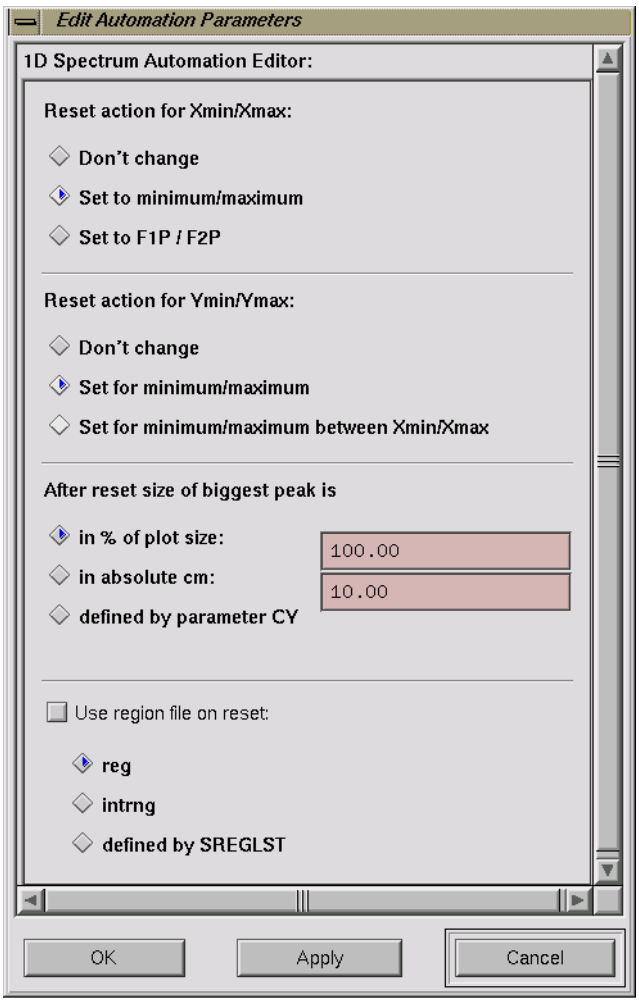


Figure 7.2 The 1D automation editor

The additional reset actions for the X dimension of a 1D spectrum have the following meaning:

- **Set to F1P/F2P**: Xmin will be set to the value of the parameter F1P in the data set, Xmax will be set to the value of F2P. Use this when the 1D spectrum should use the same axis limits as used in XWIN-NMR. This can also be useful in AU programs. Axis limits of the plot then can be controlled by setting the parameters F1P/F2P prior to the AUTOPLOT command.

These are the 1D spectrum object's specific reset actions for the Y dimension:

- **Set to minimum/maximum between Xmin/Xmax:** Ymin will be set to the minimum y value between Xmin/Xmax. Ymax will be set to the maximum y value between Xmin/Xmax.
- **After reset size of biggest peak is:** After Ymin/Ymax have been calculated according to the selected action, Ymax will be rescaled with a user-defined factor. You can choose to define the new size in percent of the object size (the default value 100% results in no changes). Alternatively, you can specify the absolute new size in centimeters here, or tell XWIN-PLOT to get the new size in centimeter from the parameter CY in the data set. Together with the F1P/F2P option above the last option can be used in AU programs to have full control over plot limits and scaling.

If **Use region file „reg“ on reset** is activated, the reset action for Ymin/Ymax will only take into account the regions defined in the file reg, intrng (See chapter 3.5 on page 19.), or defined by the contents of the parameter SREGLST in the data set.

7.1.4 The 2D automation editor

With this automation editor (Figure 7.3) you define how a 2D spectrum reacts to a reset.

The additional reset actions of a 2D spectrum have the following meaning:

- **Set to F2PLO/F2PHI**: Xmin will be set to the value of the parameter F2PLO in the data set, Xmax will be set to the value of F2PHI.
- **Set to F1PLO/F1PHI**: Ymin will be set to the value of the parameter F1PLO in the data set, Ymax will be set to the value of F1PHI.

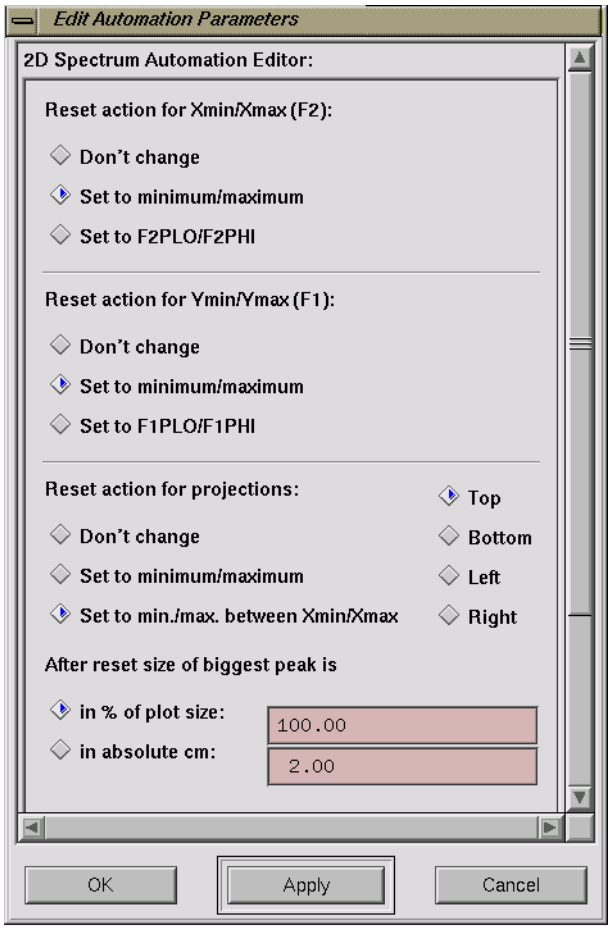


Figure 7.3 The 2D automation editor

Use these options when the 2D spectrum should use the same axis limits as used in XWIN-NMR. Again, this can also be used in AU programs to control axis scaling by setting the parameters `F2PLO/F2PHI/F1PLO/F1PHI`.

For each of the possible four projections then same reset actions are available as used for stand-alone 1D objects.

8

Reusing layouts

An outstanding feature of the XWIN-PLOT plot editor is its layout support. A layout is a graphics template that was created for particular data sets and saved for reuse with other data sets. When saving a layout, only the layout information, e. g. object positions and dimensions, are saved, not the actual data set information. This chapter describes how to reuse a layout in order to use XWIN-PLOT efficiently.

8.1 Layouts and data sets

The basic steps for reusing layouts are shown in Figure 8.1. This steps consists of:

- Loading the layouts
- Loading the data sets
- Resetting the layouts
- Printing

8.1.1 Loading layouts

Layouts can be loaded by using **Open** from the **File** menu. If you want to use more than one layout, first use **New** to get a new layout and then **Open** to load the additional layout.

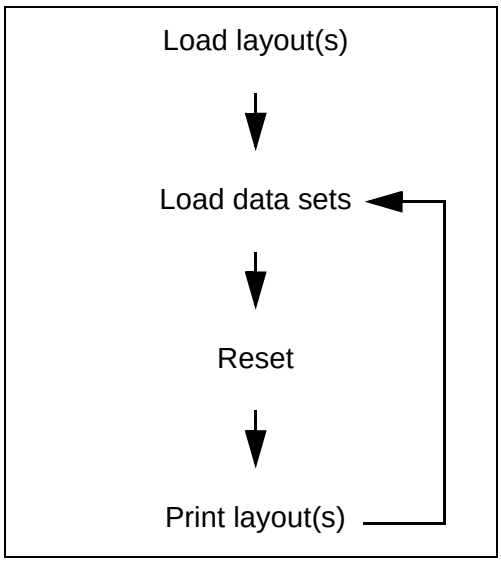


Figure 8.1 Reusing layouts

If you are using the stand-alone version of XWIN-PLOT, you can also load layouts by specifying the layout file names on the command line. (See chapter 2.2 on page 13.)

8.1.2 Loading data sets

Data sets may be loaded in the following ways:

- With the *Portfolio Editor* you can load arbitrary data sets. (See chapter 5.6.2 on page 47.)
- **Get Current Data Set** in the **XWIN-NMR** menu loads the current XWIN-NMR data set. Use **Get Current Data Set + Reset** if you also want to reset a layout. Use **Get Current Data Set + Reset + Print** to additionally print the layout. Note that these commands are only available in case XWIN-PLOT was started from within XWIN-NMR.

8.1.3 Reset

A reset executes the reset actions of NMR objects. The reset actions can be used to rescale a spectrum automatically. (See chapter 6.1.7 on page 66.)

To issue a reset you can either mark individual objects and use **Reset Marked Objects** in the **Edit** menu, or you can reset all objects with **Reset All Objects** in the **Edit** menu. A reset is done automatically by the **Get Current Data Set + Reset** command.

8.1.4 Print

To print a layout use the **Print** command from the **File** menu. (See chapter 5.8 on page 50.) If you use the command **Get Current Data Set + Reset + Print** from the **XWIN-NMR** menu, the layout will be printed automatically.

8.2 Printing a series of spectra

To reuse layouts is very convenient when a series of spectra is to be printed. With XWIN-PLOT several spectra can be printed easily using the plot editors **Multi-Print** capability, available in the **File** menu. In the *Multi-Print* dialog window you can print groups of data sets combined with all open layouts.

To use this feature the layouts that are to be used for printing have to be loaded first. Now the data set portfolio has to be prepared. In order to fill the Portfolio with data enter the *Portfolio Editor* and put all data sets that are to be printed in the data set portfolio. If more then one data set is used by the layouts, enter the number of data sets in the *Multi-Print* dialog. Now simply press the **Print** button to get printouts of all layout and data set combinations.

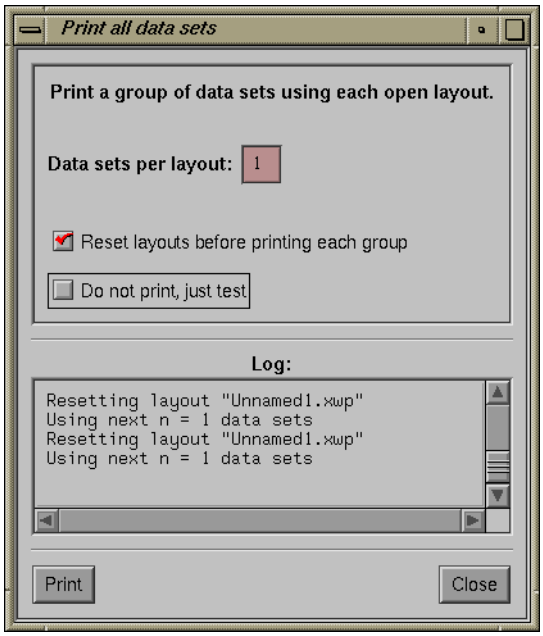


Figure 8.2 Printing multiple data sets

9

Autoplot AU Macro Reference

Once you have created some standard layouts according to your personal needs a simple `autoplot` command can be used to produce the plot without any further user interaction. `autoplot` can be typed at the XWIN-NMR prompt and becomes really important when you include plotting tasks in AU programs.

`autoplot`, together with the necessary arguments, can be entered and started on a standard shell prompt. For efficient use in AU programs a collection of AU macros is available. There are macros to autoplot itself as well as macros to collect several datasets in a portfolio. Use of a portfolio instead of the current dataset lets you include more than one dataset in the layout.

9.1 Plotting the current data set

`AUTOPLOT`

The macro `AUTOPLOT` executes the `autoplot` command without any further arguments.

The name of the layout will be taken from the `LAYOUT` parameter in the current dataset (see the `edo` dialog). A portfolio file `portfolio.por` will be loaded if found in the processing directory of the current dataset. Otherwise the default portfolio will be used. Its first entry will always be set to the current dataset. If projec-

tions have been calculated these will be included in the portfolio at positions two to five. Other entries remain unchanged. This works exactly the same way as if XWIN-PLOT was started within XWIN-NMR.

AUTOPLOT uses the printer that has been specified in the layout file. To change the printer setting of a layout, open the layout with XWIN-PLOT, choose anther printer setting in the Printer Setup dialog, and save the layout again.

Example code as it could be used in an AU program:

```
GETCURDATA
AUTOPLOT
```

9.2 Plotting arbitrary data sets

To plot more than one dataset in a layout you need to create a portfolio file specifying those datasets. The following AU macros are provided to create and declare portfolio files.

`DECLARE_PORTFOLIO`

This macro prepares the AU program for the use of the other portfolio macros. It must be included at the beginning of the AU program.

`CREATE_PORTFOLIO("filename")`

This creates a portfolio file named `filename`. You must do this before the first use of a `ADD_TO_PORTFOLIO` / `ADD_CURDAT_TO_PORTFOLIO` statement. The filename is taken without any further modification. It is a good idea to specify an absolute path to a location that can be safely used, e.g. in the temporary folder or in your home directory (see the example below).

`ADD_CURDAT_TO_PORTFOLIO`

The current data set is added to the portfolio list.

`CLOSE_PORTFOLIO`

Closes the portfolio definition and makes it ready for use.

`AUTOPLOT_WITH_PORTFOLIO`

Executes the `autoplot` command. Instead of the standard portfolio search order, the portfolio file is loaded that has been constructed with the recent `CREATE_PORTFOLIO` / `CLOSE_PORTFOLIO` instructions. Note that for technical reasons this macro will not automatically the peak list and / or parameter list as documented for the `autoplot` command on page 17.

`AUTOPLOT_WITH_PORTFOLIO_TO_FILE("filename.ps")`

This works like `AUTOPLOT_WITH_PORTFOLIO`. The output is not sent to the printer but to the specified Postscript file instead. The Windows version additionally supports the suffix "`.emf`" to create an Enhanced Metafile. Note that for technical reasons this macro will not automatically the peak list and / or parameter list as documented for the `autoplot` command on page 17.

Example

```
/* A small AU example
**
** The current dataset shall have three PROCNOs
*/
DECLARE_PORTFOLIO

GETCURDATA
CREATE_PORTFOLIO("/tmp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO

IPROCNO
ADD_CURDAT_TO_PORTFOLIO
```

```
IPROCNO
ADD_CURDAT_TO_PORTFOLIO

CLOSE_PORTFOLIO

/* Go back to the initial dataset to use
** the correct LAYOUT parameter
*/
DPROCNO
DPROCNO

AUTOPLOT_WITH_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIO_TO_FILE("/tmp/myPlot.ps")

QUIT
```

For more information you may want to check the AU programs `xwp_p1dlf`, `xwp_p2dpl` and `xwp_pcpd135`. They are usually installed with the command `expinstall`.

10

Tips and tricks

XWIN-PLOT offers a lot of useful features and it surely will take some time before you can exploit all of them. The more familiar you get with the plot editor the more you will learn how to use its tools to create sophisticated layouts. The intention of this chapter is to provide some valuable hints on the use of some of the editor‘s features that might not come to your mind immediately.

10.1 A shadow around a spectrum

XWIN-PLOT does not offer a predefined object of the type „Spectrum inside a frame“ like the one shown in the previous examples. It is easy, however, to create such an object by combining a filled rectangle with a spectrum. The result is shown in Figure 10.1. Figure 10.2 demonstrates how the layout in this example was combined with three objects, namely the spectrum a), a rectangle filled with the color white b) and finally a black rectangle c). The spectrum was surrounded by an empty rectangle and both objects were grouped with the **Group** command in the **Edit** menu. The resulting object was placed in front of a filled rectangle of the same size and both objects were combined to a group. This way you get a single object which looks like the one in Figure 10.1. Because the object‘s components are bound into a single group, the resulting object can be moved, scaled etc. like a single object.

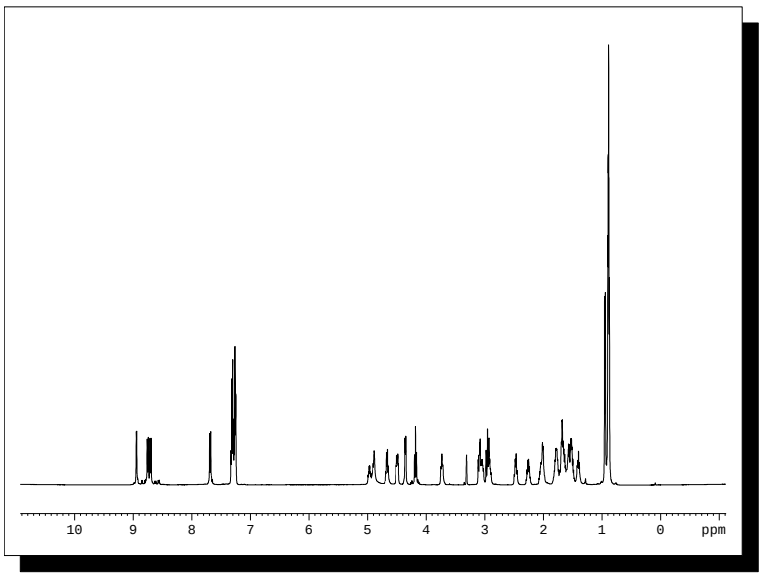


Figure 10.1 A spectrum surrounded by a shadowed frame

10.2 Import and export of graphics

XWIN-PLOT supports full import and export of graphics on both platforms Unix and Windows. On Unix systems the EPSI format (Encapsulated Postscript Image) is typically used, whereas on Windows the WMF/EMF format (Windows Metafile / Enhanced Metafile) is the *de facto* standard. Like EPSI, WMF graphics are completely rescalable without loss of quality. With EPSI and WMF objects, XWIN-PLOT is open to the best high-quality graphics on each platform.

The layout files are freely interchangeable between the two platforms. However, due to the missing support by the operating systems, WMF graphics will not be displayed or printed on Unix systems, and EPSI graphics will not be displayed or printed on Windows systems.

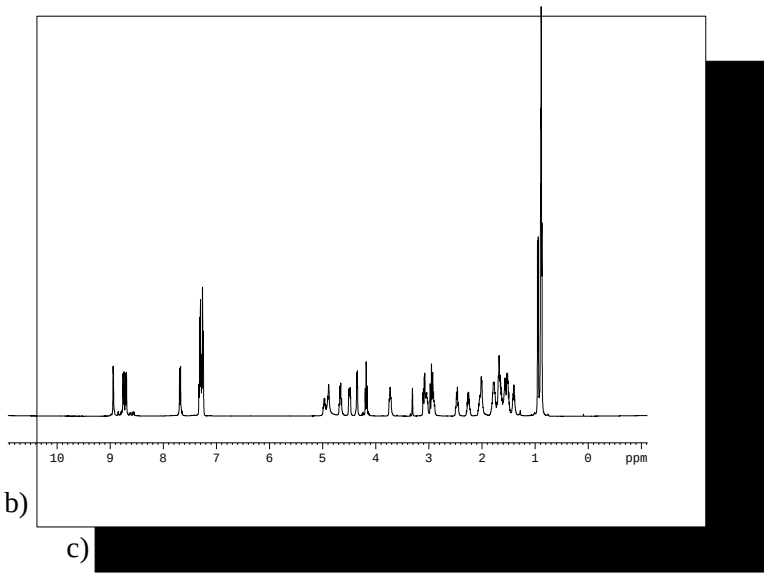


Figure 10.2 The building blocks of the graphic in Figure 10.1

10.2.1 EPSI support (Unix)

Compared to bitmap formats EPSI has the advantage of being scalable, i.e. you can rescale EPSI graphics without losing resolution.

To import an EPSI file create an EPSI object, enter the standard object editor for this object and choose the file name. (See chapter 6.1.3 on page 60.) With XWINPLOT you can print layouts with EPSI objects on any printer supported by XWINPLOT. The printer need not be PostScript compatible.

A layout can be exported as an EPSI file like this:

1. Enter the *Printer Setup* dialog, choose **EPSI** as printer type and press the **Apply** or the **OK** button. (See chapter 5.11.3 on page 54.)
2. Enter the *Print* dialog and press the **To File** button. Enter a file name for your EPSI file and press the **OK** button. By convention, EPSI files end with `.eps` or `.epsi`.

10.2.1.1 EPSI import to FrameMaker

This is how to import an EPSI file to FrameMaker:

1. From the **File** menu, choose **Import** and then **File**.
2. Select the file you want to import and press **Import**.

If you use FrameMaker 4 for Windows, please note:

- FrameMaker 4 cannot display EPSI directly and therefore uses a low-resolution preview bitmap. On a PostScript printer, however, the EPSI file will be printed in its full resolution.
- If you transfer the EPSI file generated by XWIN-PLOT from your workstation to your PC using the `ftp` program, you must use binary mode for the transfer.

10.2.1.2 EPSI import to CorelDraw

To import an EPSI file to CorelDraw 6 you must do the following:

1. From the **File** menu, choose **Import**.
2. Select **Postscript Interpreted (PS)** for **Files of type**.
3. Select the EPSI file and click on **Import**.
4. In the *Import PostScript* dialog, click on **OK**.

Like XWIN-PLOT CorelDraw supports the printing of drawings with imported EPSI files on non-PostScript printers.

10.2.2 Windows Metafile Support (Windows)

Like EPSI, WMF[19)] graphics are scalable without loss of quality. There are two ways WMF graphics can be used:

1. Create a Metafile object, enter the standard object editor for this object and choose the file name. The layout now includes the reference to an external WMF file. Note that this file must be still present to display and print the WMF graphics.
2. Import graphics of other Windows applications from the clipboard using **Paste** from the menu **Edit**. The metafile data are now part of the layout file and will

19) Some files use an .EMF suffix indicating that they are in *Enhanced Metafile Format*. XWIN-PLOT reads both formats WMF and EMF.

be saved with it. In that case there is no external file containing the image.

This way the storage location of the image data can be external or internal. The standard object editor for Metafile objects will show you this for each object with a short description.

To export your complete layout graphics to a Windows Metafile simply choose **Export** from the **File** menu. XWIN-PLOT will create an image in the EMF format (*Enhanced Metafile Format*) that is accepted by almost all graphically oriented Windows applications.

Of course you can copy some or all of your graphics in XWIN-PLOT to the clipboard. If you want to copy the complete layout choose **Mark All** and then **Copy** from the menu **Edit**. Then switch over to your target application and use **Paste** to insert the graphics.

Text marked in XWIN-PLOT will be exported as graphics. If you want to have a text object exported as text only, open the standard object editor for that text object, select the **Edit** button, mark the text and choose **Copy** after pressing the right mouse button.

10.3 Shortcuts

Some frequently needed XWIN-PLOT functions cannot only be called from the menu bar but also by using so called *shortcuts*. This means that a modifier key is pressed in addition to another key in order to call functions that are also available in the menus of XWIN-PLOT. The shortcut **[Control][A]**, for example, is an equivalent to the menu entry **Mark All**. Using shortcuts instead of the mouse can save time when working with XWIN-PLOT.

Note that shortcuts probably don‘t work with a key like **Num Lock**, **Scroll Lock** or **Caps Lock** pressed.

11

Notes for Windows Users

With the Windows NT / Windows 2000 version of XWIN-PLOT the graphical user interface was adapted to the Windows look-and-feel. Additionally, the behavior of some functions using operating system features was changed in order to improve the embedding in the Microsoft Windows environment.

11.1 Printing and the Printer Setup

XWIN-PLOT for Windows uses the Windows printer drivers. This means that any printer for which a driver is correctly installed under Windows can be selected as printing device in XWIN-PLOT.

Following the Windows style guidelines the option **Printer Setup** is called **Page Setup** and is available in the **File** menu. Selecting **Print** or **Page Setup** from the **File** menu will show standard dialogs. The **Split Page** option is part of the *Page Setup* dialog like it is under UNIX.

If the user creates a new layout XWIN-PLOT uses the **Document Defaults** of the currently selected default printer to determine the document size. To change the default paper size (which will be typically *Letter* or *A4*) click on **Start menu / Settings / Printers**, mark your current default printer and choose **Document Defaults** from the **File** menu. The dialog will be device-dependent.

XWIN-PLOT layout files created under Windows can be used by XWIN-PLOT under UNIX and vice versa. However, the name of the printer device will in most cases not be correct. Just open the *Page Setup* dialog to specify the correct printer name.

11.2 Support for WMF/EMF graphics

To easily integrate graphics from other Windows applications with your layouts XWIN-PLOT provides a “Metafile” graphics object. Use “Metafile” objects like the EPSI objects of the Unix version. XWIN-PLOT graphics can be exported to EMF graphics files or by use of the clipboard or choose Export from the menu File to create a graphics file in Enhanced Metafile Format. Refer to Chapter 10.2 for detailed information.

11.3 Clipboard

XWIN-PLOT fully supports the Windows clipboard for text and graphics. If you cut or copy one or more XWIN-PLOT objects to the clipboard you can not only paste them to other XWIN-PLOT layouts but can also import them using the **Paste** command from the **Edit** menu in applications like *WinWord* or *PowerPoint*. It is also possible to import text and graphics from other applications.

To view the current clipboard contents use the *Clipboard Viewer* by choosing **Start** / **Programs** / **Accessories** / **Clipboard Viewer**.

11.4 Support for Email Clients

XWIN-PLOT is able to send the current plot graphics as Email. Simply choose **Send...** from the **File** menu. Your default mail client will popup and create a new empty message with your plot added as a file attachment. For the attached graphics file the EMF (Windows Metafile) format will be used to ensure highest quality.

To enable mail support, you must have installed a *Simple MAPI Client* on your system. You can use the *Windows Messaging* package that is provided as part of the Windows setup. Another common client is *Outlook Express* that is part of *Microsoft Internet Explorer*. Please note that in *Outlook Express*, the *Simple MAPI Client* functionality must be explicitly enabled in the applications options. For other mail programs, please refer to the related product documentation.

11.5 Toolbar

Below the menu bar XWIN-PLOT for Windows displays an additional toolbar consisting of some common icons. These provide easy access to often used file and edit functions. Moving the mouse cursor over the toolbar gives a short explanation for each button in the status bar.

12

Appendix

12.1 Errors and warnings

12.1.1 Messages in the terminal window

Messages that appear in the terminal window (while running XWIN-PLOT usually signal fatal conditions. On Windows they will be displayed in an extra message window. Please submit a detailed report of such messages to Bruker.

12.1.2 Messages in dialog windows

A typical warning in XWIN-PLOT is shown in Figure 12.1. In most cases such warnings result from NMR data files that do not exist. All NMR data needed by the plot editor must have been created previously with XWIN-NMR as described in Chapter 3. In practical terms this means that if integral data is to be displayed in XWIN-PLOT, the spectrum must have been integrated in XWIN-NMR. If you want the plot editor to show peak labels, these labels have to be created in XWIN-NMR first. Remember that XWIN-PLOT is a program for displaying and printing NMR data, not for creating or processing them.

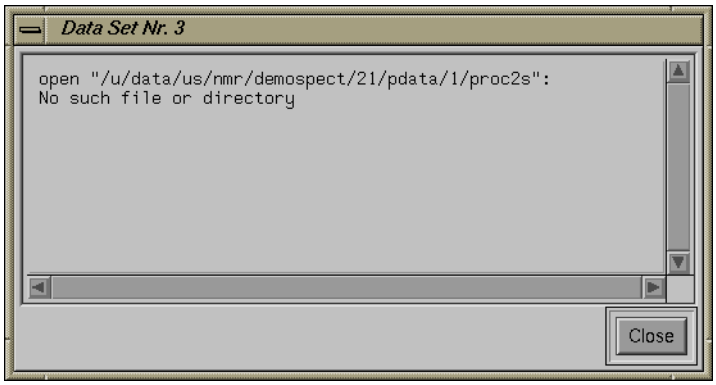


Figure 12.1 Warnings are displayed inside a dialog window

12.2 What‘s new?

This section gives an overview of the changes in the current version of the XWIN-PLOT software compared to previous versions. Beginning with version 2.5.1 bug fixes are documented in the Bruker Bug Database which is accessible on the Bruker WWW server.

12.2.1 Changes since XWIN-PLOT 3.0

- XWIN-PLOT is now available in a version for Linux.
- After installation a large number of pre-designed layouts for typical 1H / 13C measurements can be found in the `layouts` directory. Backup copies of all layouts are placed in the subdirectory `backup`. All layouts will be set to *read only* status after installation.
- Reset actions for 1D and 2D objects have been significantly enhanced to provide more flexibility of the axis scaling. Projections of 2D objects can have their own reset actions. It is now possible to use axis limits as defined within XWIN-NMR. (See Chapter 7.1.3 on page 83.)
- The new `xwp` command can be used instead of `xwinplot` in XWIN-NMR to let all 1D/2D objects use the axis limits as defined in XWIN-NMR, independantly from the limits and reset actions specified in the layout (page 11).
- The new `xwpr` command can be used instead of `xwinplot` on the XWIN-NMR command line. This will have XWIN-PLOT execute a **Reset on all objects** command after loading the layout, just as AUTOPLOT does it by default (page 11).
- When starting from within XWIN-NMR, XWIN-PLOT and AUTOPLOT will automatically execute the commands `xwp_lp` and / or `xwp_pp` on the current dataset if the parameter list and/or peak list is missing. (page 17, see also Chapter 9.2 on page 92).
- `AUTOPLOT` always stores an archive copy of the currently used layout file in the used dataset. (See Chapter 5.7.1 on page 50.)
- A new option for EPSI / Meta objects allows more flexibility in handling external graphics (page 60).
- The location of external EPSI / Meta objects can now be specified relative to the assigned data set. This allows to include different graphics files for different data sets. EPSI / Meta objects also understand the symbol $XWINNMRHOME. (Refer to page 16 in chapter 2.2.4.)

- XWIN-PLOT now tries to get a more intelligent assignment of colors to different levels when the number of levels in the layout and the data set do not match (Section 6.2.2).

12.2.2 Changes since XWIN-PLOT 2.6.0

- The new commands **Save Layout/Portfolio to Dataset** / **Load Layout/Portfolio from Dataset** provide a way to quickly save the layout to the current dataset. The portfolio is saved as `portfolio.por` in the current dataset.
- If a file `portfolio.por` is found in the current dataset it is loaded instead of the default portfolio during startup of XWIN-NMR. (See chapter 5.6.2).
- EPSI and Metafile objects now have an option to always keep the original aspect ratio if desired.
- Under Windows now two formats are provided for the export of layouts, PostScript (.ps) and Enhanced Metafile (.emf).
- The new option `-e` enables autoplot to create PostScript / Enhanced Metafiles instead of printer output. (See Chapter 2.2.2 on page 14.)
- An extended set of AU macros improves the handling of datasets, portfolios and file creation in AU programming (See Chapter 9).

12.2.3 Changes since XWIN-PLOT 2.5.1

- XWIN-PLOT under Windows NT can now include “Windows Metafile” graphics into its layouts. Pasting graphics from other Windows applications using the windows clipboard is supported. See Chapter 10.2 for details.
- With the Windows NT version you can send your current plot graphics as Email directly from within XWIN-PLOT (Chapter 11.4).
- Additional rescale factor for 1D objects for automation (See page 81).

12.2.4 Changes since XWIN-PLOT 2.0.1

- XWIN-PLOT is available in a version for Windows NT. See Chapter 11 on page 101 for details.
- Added dataset-related text object. (Refer to page 78.)

12.2.5 Changes since XWIN-PLOT 2.0.0

12.2.5.1 Bug fixes

- Fixed T1/T2 curve calculation algorithms.

12.2.6 Changes since XWIN-PLOT 1.4.4

12.2.6.1 General remarks

XWIN-PLOT 2.0 is released mainly in order to be compatible with XWIN-NMR 2.0. Note that XWIN-PLOT 2.0 is not compatible with old versions of XWIN-NMR.

12.2.6.2 New features

- The reset options for 1D and 2D NMR objects were moved to the automation editors. (See Chapter 7 on page 81.)
- Positive and negative 2D projections defined within XWIN-NMR are automatically added to the XWIN-PLOT data set selector if XWIN-PLOT is started from within XWIN-NMR. (Chapter 3.7 on page 19.)
- The settings made in the *Attributes Selector* can be loaded and saved.
- Additional help is provided by toolbar hints and startup tips. (Chapter 5.11.1 on page 52.)
- The on-line help is based on the Acrobat Reader only.
- The stand-alone versions of XWIN-PLOT and AUTOPLOT were renamed to `xwinplot` and `autoplot`, resp.

12.2.7 Changes since XWIN-PLOT 1.4.0

- Text files can be loaded into a text object. (Refer to page 62 in chapter 6.1.4.)
- 2D projections can be scaled and scrolled using the 2D object editor. (Chapter 6.2.2 on page 75.)

12.2.8 Changes since XWIN-PLOT 1.3.0

12.2.8.1 New features

- The main window layout was changed in order two support two major editing modes **Basic** and **NMR**.
- A special 2D editor, which includes a level editor, was added. (See Chapter 6.2.2 on page 75.)
- A new object for displaying T1/T2-Fit curves was added. (See Chapter 6.1.11 on page 70.)
- A facility to edit a list of data directories was added to the *Portfolio Editor*. (See Chapter 5.6.2 on page 47.)
- The handling of RGB colors in the *Attributes Selector* dialog window was simplified.

12.2.8.2 Bug fixes

- EPSI objects created by particular PC programs were not always displayed correctly. This bug has been fixed.
- Printing very large 2D spectra (e.g. on A0 size paper) required huge amounts of memory. This could cause the system to run out of swap space. This has been fixed.

12.2.9 Changes since XWIN-PLOT 1.2.0

12.2.9.1 New features

- A new program called AUTOPLOT is supplied. With AUTOPLOT layouts can be printed automatically without having to start XWIN-PLOT first. (See Chapter 2.)
- XWIN-PLOT and AUTOPLOT are now automatically started with the layout specified by the parameter `LAYOUT` if started from XWIN-NMR. The `LAYOUT` parameter can be set with the XWIN-NMR `edo` command. (See Chapter 2.1 on page 11.)
- White washed stacked plots are supported more directly. The stacked spectra object editor provides a new option for setting the correct curve attributes. (See 6.1.8 on page 67.)
- The *Portfolio Editor* supports appending of portfolio contents.

- New devices were added to the *Printer Setup*.
- A section about EPSI import and export has been added to the manual. (See Chapter 10.2 on page 96.)
- PostScript output created by XWIN-PLOT now works with programs like Corel Draw which have static limits for the maximum number of lines for a single object.

12.2.9.2 Bug fixes

- The scaling of FID objects did not always work. This bug has been fixed.
- Negative offsets with stacked plots now work correctly.

12.2.10 Changes since XWIN-PLOT 1.04

12.2.10.1 New features

- The *XWIN-NMR interface* dialog has been added. (See 3.9 on page 20.) With this dialog it is possible to run XWIN-NMR commands from XWIN-PLOT (not for the stand-alone version).
- **Get current data set** gets the current XWIN-NMR data set. This command can be combined with **Reset** and **Reset + Print** for fast layout printing. (See 8.1.2 on page 88.)
- **Update Data from Xwin-nmr** updates all data used by the plot editor from XWIN-NMR, i.e. all changes on the data sets done in XWIN-NMR are transferred to XWIN-PLOT. (See Chapter 3 on page 17).
- The *Multi-Print* dialog has been added. With this dialog a series of plots can be created very easily. (See Chapter 8.2 on page 89.)
- The EPSI (= Encapsulated PostScript Interchange) object has been added. (See Chapter 6.1.3 on page 60.)
- Text objects now can be adjusted not to change the font size then scaling by disabling **Allow automatic font resize** in the edit dialog. (See Chapter 6.1.5 on page 63.) For the title and parameter object this is the default.
- By activating **Use region file on reset** on a spectrum (using the edit menu) the text file `reg` in the processed data directory can be used to specify spectrum regions that will be used to determine y-scaling on a reset. (See Chapter 6.1.7 on page 66.)

- By pressing the **Alt** key while expanding a 1D in expand mode (See Chapter 5.2.2 on page 39.), portions of the spectra can be blown up according to the setup in *Global Setup*. (See Chapter 5.11.1 on page 52.)
- If modifier keys (**Shift**, **Ctrl**, **Alt**) are pressed while scaling or moving spectra, the spectrum will not change its position. This allows for the use of a spectrum object as a clipping window. (See Chapter 5.3.3 on page 42.)
- Pressing the right mouse button now automatically switches to mark mode, marks the object under the cursor and shows a popup menu which contains the most frequently used commands.
- **Undo** now can also undo zooming.

12.2.10.2 Bug fixes

- Titles without a newline character at the end did not work. This bug has been fixed.
- A 2D spectrum object now can display the spectrum in a range larger then the spectrum range, e.g. a spectrum ranging from 0 to 127 points in x and y direction can be displayed in a range of -100 to 300 points in x and y direction.
- Changing the units of 2D spectrum objects now changes the units of the projections immediately.
- **Scale bounding box** on a 2D with projections now works.
- Under certain circumstances, the attribute selector did contain weird values, resulting for example in spectra being drawn with wrong line thickness or line style. This has been fixed.
- In expand mode, integrals are scaled properly now.

12.3 Known bugs

Due to the poor scaling mechanism of the X11 font scaler, text objects do not always have a 100% WYSIWYG look. The width of text objects on the screen may appear different from their width on the printer. This can result in text objects to be clipped by the printer if the option **Allow automatic font resize** is enabled and the width of the text objects is made smaller. In this case the text object does not appear to be clipped on the display but it might be clipped by the printer.

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