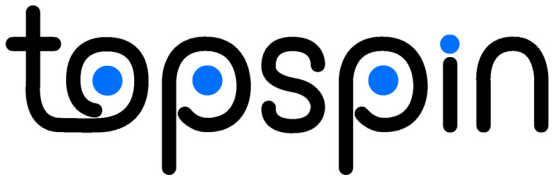

Installation Guide

TopSpin 2.1

Red Hat Enterprise Linux WS 4

Version 2.1.0

Bruker BioSpin

Part-No: H9556SL2/10
revision state: 19/10/2007 (Version 2.1.0)

Bruker software support is available via phone, fax, e-mail or Internet. Please contact your local office, or directly:

Address: Bruker BioSpin GmbH
Service & Support Department
Silberstreifen
76287 Rheinstetten
Germany
Phone: +49 (721) 5161 455
Fax: +49 (721) 5161 943
E-mail: nmr-software-support@bruker-biospin.de
FTP: ftp.bruker.de / ftp.bruker.com
WWW: www.bruker-biospin.de / www.bruker-biospin.com

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Chapter 1

Introduction

1.1 About this manual

This manual describes the installation of the ***TopSpin*** 2.1 under RED HAT ENTERPRISE LINUX WS 4.

It is available:

- as a hard copy 'Installation Guide for TOPSPIN RED HAT ENTERPRISE LINUX WS 4'. The print-version of the Installation Guide is actualized in planned intervals.
- as `pdf` file on the toplevel of the TOPSPIN 2.1 DVD
- as TOPSPIN 2.1 online Help: click ***Help → manuals → Installation Guide***
- as the up to date version on the Bruker BioSpin web-server:

  http://www.bruker-biospin.com/documentation_nmr.html
- Note that this manual does not contain the TOPSPIN Release letter. That is a separate document which is not available as a hard copy but delivered as `pdf` and `rtf` files on the TOPSPIN DVD and also on the Bruker BioSpin web-server (you can find it at the same URL as the Installation Guide)

This manual is subdivided into an introduction and three main parts. It depends on your local demands which of these are necessary for you at the moment.

The first part shows how to install and configure TOPSPIN and some essential additional software packages. It is recommended to follow the instructions step by step.
Part two describes the scratch installation of RED HAT ENTERPRISE LINUX WS 4 and some configuration steps like setup for network and printers. If you want to install Bruker BioSpin TOPSPIN on a PC which is already in use, you can skip this part.

In the last part, you can find some additional information for working with RED HAT ENTERPRISE LINUX WS 4 and TOPSPIN and also some tips for troubleshooting.

Note that all text-messages and graphics shown in this book are taken from the current version of the respective software products. Small differences to other versions are possible but generally speaking they should be very similar.

If you have any comments or suggestions, or if you find any errors in this manual, please do not hesitate to contact us at:

`nmr-software-support@bruker.de`

1.2 Conventions

The following conventions will be used throughout this manual:

`Bold-Courier`: Linux commands to be entered from the keyboard

Bold-Times: Linux commands/applications to be clicked with the mouse

`Bold-Courier-Italics`: NMR Suite commands to be entered from the keyboard

Bold-Times-Italic: NMR Suite commands to be clicked with the mouse

`Courier`: a file name or directory name

`Courier Small Italics`: responds of the system

`Courier Small`: the contents of a file

`Times italics`: any name which is not a file name e.g. host names, user names etc.

< >: place holder

1.3 Safety Regulations

In order to work safety in laboratories with NMR-spectrometers all users have to follow the safety regulations for magnetic, electrical, cryogenic and chemical safety. For detailed information please refer to the safety instructions in the Beginners Guide Manual provided on the TOPSPIN DVD.

1.4 Hardware and software requirements for TopSpin

1.4.1 Supported operating systems

TOPSPIN 2.1 on spectrometer computers is supported for:

- Windows XP Professional
- Windows Vista
- Linux Red Hat Enterprise WS 3
- Linux Red Hat Enterprise WS 4

All operating system updates (hot fixes and service packs) at the time TOPSPIN 2.1 was released have been tested and are supported.

TOPSPIN 2.1 on Datastations is supported for:

- Windows 2000
- Windows XP Professional
- Windows Vista
- Linux Red Hat Enterprise WS 3
- Linux Red Hat Enterprise WS 4
- Linux Red Hat Enterprise WS 5

Although not officially supported by Bruker, users reported that TOPSPIN is also running and is used for data processing, respective as storage unit:

- on other Linux systems

  and

- on Windows XP Home Edition

Bruker does not recommend these systems for the use of TOPSPIN. Please note

that Bruker cannot support the use of above-named systems. For detailed information please look up the software support matrix, provided in pdf-format, on the Bruker Web server under following address:

http://www.bruker-biospin.com/documentation_general.html

1.4.2 Special PC Hardware requirements

To run TOPSPIN 2.1 with Linux Bruker recommend the following computer hardware:

- PC[1] with CPU Clock ≥ 1 GHz
- Memory ≥ 512 MB
- Video (graphics)-card memory: 64 MB [2]
- 2 Ethernet cards (the second card is only required if your PC controls a spectrometer)
- DVD device[3]
- 3 button mouse or wheel mouse

If your hardware does not meet these requirements, TOPSPIN might still run but with a much lower performance.

Furthermore, display resolution must be set to 1280*1024 or higher.

The Installation was tested on a 'HP workstation xw4400' PC with a 'NVIDIA Quadro FX560' graphics card (128 MB) and two 'Broadcom 5751 NetXtreme Gigabit PCI4 Ethernet' cards.

1.4.3 Spectrometer requirements

TOPSPIN 2.1 is released for datastations, AVANCE, AVANCE II and AVANCE III spectrometers. If you are in doubt which kind of spectrometer do you have please refer to chapter 12.3 on page 172.

For upgrade possibilities of your spectrometer with TOPSPIN 2.1, please check with your local Bruker BioSpin office.

1. TOPSPIN only runs on x86-based PC's. It does not support 64bit architecture.
2. It is recommend not to use shared memory graphics, because in some cases memory problems have been observed.
3. ***TOPSPIN*** is delivered on DVD's with "-R" format.

Hardware components that are TOPSPIN version or operating system dependent are listed below. Components that are not listed here do not need an upgrade for TOPSPIN 2.1.

If your Avance spectrometer does not meet the above specifications, please get in touch with your local Bruker BioSpin representative for your upgrade options.

1.4.3.1 AVANCE-spectrometers and AVANCE II-spectrometers

- **CCU:**

LINUX, independent of your TOPSPIN version	
CCU	required minimum EC level
CCU 10 (part # H9503, EC level 00 to 19)	**06**
CCU 10 (part # H9503, EC level > 19)	**22**
CCU 11 [a] (part # H9503V1)	**00 (recommended 01)**

Windows, independent of your TOPSPIN version	
CCU	required minimum EC level
CCU 10 (part # H9503)	**any**
CCU 11 [a] (part # H9503V1)	**00 (recommended 01)**

a. Note that a different CCU 11 also exists for AQX/AQR spectrometers.

- **FCU 3:**

FCU 3	required minimum EC Level
part # H5822 (64k memory)	**04 (recommended 07)**
part # H9598 (256k memory)	**02 (recommended 05)**

- **FCU 4:**

FCU 4	required minimum EC Level
part # H9727	**any**
part # H9773	**any**

- **RCU:**

RCU[a]	EC level
RCU 1/2 (part # Z003678)	**any**
RCU 1/3 (part # Z022488)	**any**

a. AVANCE-spectrometers only

- **Multiple Receiver RCU:**

Multiple Receiver RCU[a]	EC Level
RCU 1/4 (part # Z052488)	**any**
RCU 2/4 (part # Z062488)	**any**
RCU 3/4 (part # Z072488)	**any**
RCU 4/4 (part # Z082488)	**any**
RCU 1/5 (part # Z003206)	**any**
RCU 2/5 (part # Z003207)	**any**
RCU 3/5 (part # Z003208)	**any**
RCU 4/5 (part # Z003209)	**any**

a. AVANCE-spectrometers only

- **TCU 3:**

TCU 3	required minimum EC Level
part # H5813, EC level 00 to 19	**09 (recommended 12)**
part # H5813, EC level ≥ 20	**28 (recommended 31)**
part # H5813V1	**any (recommended 01)**
part # H5813F2	**any (recommended 01)**
part # H5813F3	**any (recommended 01)**

- **RX22**:

RX22	EC Level
part # HZ002810	**any (recommended 08)**
part # Z012810	**any (recommended 02)**
part # Z032810	**any (recommended 01)**

1.4.3.2 AVANCE III-spectrometers

- **IPSO 19" H9987**

IPSO 19" H9987	required minimum EC Level
Baseboard part # H12519	**03**
TX-board (F-/T-/G-Ctrl) part # H12538F1	**01**
TX-board (F-/T-/G-Ctrl) part # H12538F2	**any**
RX-board (R-Ctrl) part # H12532	**any**
PCI-board part # H 12524	**01**

- **IPSO-AQSS H9984**

IPSO-AQSS H9984	required minimum EC Level
Ipso-ACQ host part # H12547	**any**
Ipso-ACQ acq part # H12549	**any**
PCI adapter board part # H12557	**any**
Hr-board part # H12553	**any**
FTMS-board part # H 12555	**any**

- **DPP1**:

DPP1	required minimum EC Level
part # H12513f1	**any**

1.4.4 Software requirements

! Because of the variety of Linux systems and their possible problems with some PC-hardware components, Bruker BioSpin can not support all of them. The supported Linux systems are RED HAT ENTERPRISE LINUX WS 4 and RED HAT ENTERPRISE LINUX WS 3 and the hardware components described in section 1.4.2. RED HAT ENTERPRISE is supported only for datastations, respective as storage-unit. This software/hardware combination was successfully tested with ***TOPSPIN*** 2.1. Any other Linux systems and PC hardware components might work, but are not tested and supported by Bruker BioSpin.
Please note that no additional hardware is required to run TOPSPIN 2.1 on a spectrometer or as datastation for processing data.

1.5 Important Red Hat Linux Enterprise WS 4 configurations

1.5.1 KDE - desktop manager: recommended by Bruker BioSpin

All information described in this manual is based on the desktop manager KDE. If you use GNOME, there will be some differences in handling. In the login window, type in:

- your login name
- your password
- choose as *Session* **KDE**[1] and press **Enter**

1. You can define your default login session with the command **`switchdesk`** when you are logged in.

Chapter 2

Express Installation and Configuration of TOPSPIN

2.1 About this chapter

This chapter gives a brief description of how to install Bruker BioSpin's TOPSPIN. In order to provide installation impressively and short, this chapter only handles with the main aspects of installation.

The following is dressed to users who would like to install TOPSPIN 2.1 on a PC, on which XWIN-NMR or a version of TOPSPIN is already installed and configured correctly. The Express Installation of TOPSPIN therefore provides a concise overview of the main installation aspects for TOPSPIN on Linux systems. Further details can be found in the following chapters.

For more details on the installation see chapter chapter 4 on page 35.

Extensive details about the ***TOPSPIN*** commands like ***cf, expinstall*** etc. are provided in the Acquisition Reference manual. Please refer to this document for detailed information.

2.2 Installing TOPSPIN

The main decision you have to make during installation is where do you want to install the new ***TOPSPIN*** version. If you a have previous NMR SUITE or TOPSPIN installation on this PC available, you can either:

- install the new version in parallel to the previous one
  (e.g. old version in `/opt/topspin2.0`, new in `/opt/topspin2.1`)

  or
- install the new version in the same directory as the previous one
  (e.g. old version in `/opt/topspin`, new in `/opt/topspin`)

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation you can start working with the new version and if you want to go back to the previous version for whatever reasons you can just start and reuse it.

The installation of TOPSPIN 2.1 offers an automatic import of your individual configuration of a previous version, so that there is no advantage to install the new version in the same directory as the old one.

2.2.1 Installation in parallel

1. Close ALL WINDOWS on the desktop.
2. Insert the DVD TOPSPIN *2.1*.
3. Start of the installation:
   - If the automatic start of the DVD is enabled, the shell described in the next step appears automatically, go to step 4.
   - If the shell of the next step does not appear automatically you have click on the DVD icon on your desktop and click on the file `install` [1].
4. If you are not logged in as root, a Linux shell will appear that asks you for the root password:

   ```
   Please enter root password if prompted for it:
   Password:
   ```

   - Enter root password and press enter

1. Please note that there is also a file called ‘install.cmd’ on the DVD. This file is the installation script for windows, under Linux you have to click on the file ‘`install`’.

5. The window *TOPSPIN Installation Manager* appears.

6. The window *Welcome!* appear.

- Click **Next**

7. The window *TOPSPIN Release Letter* will appear:

Please read the NMR Release letter! You can find therein all information about new features and bug fixes of the current version .

- When you have finished reading the Release Letter please click **Next.**

8. The window *Please select a target directory for TOPSPIN* will appear:

Enter an installation path which does not exist so far, e.g. **`/opt/topspin2.1`**

- Click **Next**

9. If the installation directory does not exist so far, you will be asked if the installation process should create it.

- Click **Yes**

10. A window *Please select the setup type* will appear:

a) Select the setup type. Do one of the following:

- Select *Data Processing only* if you want to use TopSpin for data processing.
- Select *Data processing, acquisition and automation* if you want to use TopSpin for spectrometer control. This will e.g. install **Diskless** automatically.
- *Customized setup* (allows components selection) if you want to install selected programs only.

b) Click **Next**

10.1. If *Customized* was selected please refer to step 10.

a) ... a window *Please select products to install* will appear:

- Select the packages which you want to install (note that DISKLESS is only required if your PC controls a spectrometer or you want to configure it like this (see chapter 6.2.2 on page 73).
- Click **Next**

11. The window *Select a spectrometer configuration to import* will appear. You can either import no spectrometer configuration, or browse for a spectrometer configuration or select one of the configurations you get offered within this win-

dow.[1]

12. If a previous ***TOPSPIN*** installation is available in the global environment variable Path, you will be asked if you want to define the current installation path instead. It is recommended to set the current installation into the PATH variable, so enable:[2]

Yes, add the new TOPSPIN installation directory to the global PATH

- Click **Next**

13. A window appear that asks for the installation path of FlexLM. It is strongly recommended to accept the default path[3]!

- Click **Next**

14. A window appear that displays the program selection of step 10a.

- Click **Next**

15. A window *Set NMR Super User* will appear:

a) Do one of the following:

- Accept the default NMR SUPERUSER (nmrsu) or
- Enter a special user for this purpose, e.g. named *nmr-admin* or
- Enter any other user

If the user does not exists, the installation will create it. For further details see chapter 4.1 or the TOPSPIN Users Guide.

b) Click **Next**

16. A window *Password Input* will appear and asks for the NMR ADMINISTRATION PASSWORD[4] (for more details about this feature see chapter chapter 4.1 on page 35).

---

1. The installation process will offer all configurations which are available in the TOPSPIN / XWIN-NMR installation that are defined in the /etc/profile.d/xwinnmr(.csh/.sh) resp. topspin(.csh/.sh) directory.
2. In case more than one ***TOPSPINTOPSPIN*** version is installed in parallel it is your decision which one should be defined here
3. It is strongly recommended to accept the default path for the FlexLM installation: /usr/local/flexlm ! If you choose a user defined path, it may cause some problems with other applications using the FlexLM
4. Certain commands like ***cf*** and ***expinstall*** ask for the NMR ADMINISTRATION PASSWORD.

a) Type in the NMR ADMINISTRATION PASSWORD
b) Re-enter the NMR ADMINISTRATION PASSWORD
c) Click **Next**

17. If *Data Processing, acquisition and automation* or *Customized* with the Diskless package was selected in step 8 a window will appear to inform that the spectrometer has to be shut down.

a) If the PC is not yet connected to a spectrometer or if the CCU is not booted[1] you can promptly.
   • Click **Next**
b) If your PC is currently connected to a spectrometer and the CCU is booted:
   a) Open a Linux shell
   b) enter the command:

      telnet spect

   c) login as *root*
   d) enter the command:

      init 5

      → this will shut down the CCU
   e) Close the Linux shell
   f) Click **Next** in the window that asked you about shutdown the CCU

Note: The CCU is now either down or switched off and should be turned on again at the end of this procedure.

→ The installation of TOPSPIN will start now.

18. After installation is finished a window appears that informs about all installed programs
   • Click **Seen**

19. Depending if you have installed DISKLESS one of the following windows will appear:
   • If you have installed DISKLESS a window will appear that asks you to reboot the PC. Make sure that you can reboot the PC now (check for any unsaved

1. Note that during a first time installation of the TOPSPIN the CCU can not be booted.

windows (e.g. an editor window) and check if no other users are logged in into this PC) then click **Yes.**

- If you have not installed DISKLESS a window will appear that informs you to log out and log back in before you start TOPSPIN, click **Seen.**

20. The window wherein you entered the root password informs you that you have to press *Enter* to close this window.

- Press **Enter**

21. If you have started the installation manually by clicking the file `install` in the Konqueror window, you have to close this Konqueror window.

22. To eject the DVD click right on the DVD icon on the desktop and choose **eject.**

2.2.2 What do you want to do with TOPSPIN?

- it should control a spectrometer or you want to use a special spectrometer configuration

  → you have to execute ***cf*** and ***expinstall***

- it should be used for data processing only?

  → you have to execute ***expinstall***

For more details please refer to the next chapter.

2.3 Configuring TOPSPIN

The following chapter offers the basic guidelines to configure TOPSPIN for using it as a datastation, respective as a storage unit, for data processing only or to control and operate a spectrometer.

In order to provide a short overview of the main actions, details about the commands are not discussed in here. Extensive details about the ***TOPSPIN*** commands like ***cf, expinstall*** etc. are provided in the Acquisition Reference manual. Please refer to this document for detailed information.

Start TOPSPIN:

- Click the icon TOPSPIN on the desktop[1], or
- Click **<redhat> → Other → TOPSPIN<vers.>**

1. How to create a icon? See chapter 15.7.1

When a user starts a new TOPSPIN version for the first time, a window LICENSE will appear:

a) Please read the license agreement for Bruker TOPSPIN !

b) If you agree, please click **I Accept**.

Now the window *Configuration check* will appear, that allows you to configure the software. If you have to click on ***Cf*** or ***Expinstall*** depends on what you want to do with TOPSPIN. You are mainly in one of the following situations:

1. You want to configure a processing-only-PC with a default configuration on a datastation → go to chapter 2.3.1 (for details see chapter 6.2.3)
2. You have installed the new software on the same PC as a previous XWIN-NMR/TOPSPIN installation, so the old spectrometer configuration is available on the same PC → go to chapter 2.3.2 (for details see chapter 6.2.1)
3. You want to configure a processing-only-PC like your spectrometer-PC and you have the spectrometer configuration on another computer → go to chapter 2.3.3 (for details see chapter 6.2.2)
4. You have to configure the software for controlling a spectrometer on a new hard disk without a backup of the spectrometer configuration, so you have no configuration files → go to chapter 6.2.4

2.3.1 If you want to use a default configuration on a datastation

A default configuration of TOPSPIN can be used for a datastation, respective a storage unit, meaning a PC that is used for processing only. During the installation of TOPSPIN ...

- in a new TOPSPIN installation directory
- if no TOPSPIN/XWIN-NMR was installed on this computer so far

the configuration process performs automatically (no ***cf*** is required).

There are two default configuration available *Bruker_default_av500* and *Bruker_default_avi300* which correspond to two different Avance spectrometer.

For data processing only you have to execute ***expinstall*** and select *Installation for Datastation (Default)*.

For further details please refer to the respective chapters (see chapter 6.2.3).

2.3.2 If your PC controls a spectrometer:

1. Be sure that the spectrometer is booted (see chapter 9.3.2 and 12.3.1.7)

2. Open a dataset

- Type ***new*** and create a new dataset.
- You can also select a dataset (e.g. *exam1d_1H*) acquired with another TOPSPIN or XWIN-NMR version

3. Enter ***cf*** (The command ***cf*** now configures the software according to the hardware of your spectrometer.)

a) A window will appear:
Password request. Please enter the NMR ADMINISTRATION PASSWORD

Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

b) A window will appear:
Spectrometer configuration: ...

Select your previous configuration and press **Edit** to confirm this configuration.

c) A window will appear:
Edit configuration. ...

The selected configuration is displayed. Choose whether to configure it as a spectrometer or datastation. Choose the type of your spectrometer e.g. ***AVANCE*** → **ENTER**. Check or type in the 1H frequency of the magnet e.g. ***500.13*** → **ENTER**. Use the debug mode only in case of troubleshooting.

d) In case the information window `mod hconfserver` appears:

- your spectrometer has not a BSMS rack with ECLB board: you may ignore this warning → **ENTER**. Nevertheless please check the configuration summary (`uxnmr.info` file) if all units are listed.
- your spectrometer has a BSMS rack with ECLB board and the DHCP server might not work correctly. For troubleshooting information see chapter 12.3.2

e) A window will appear:
Specify the channel to which external devices are connected. The RS232/485 channel for external devices-Table appears.

Check if the tty-numbers of the hardware components are set correctly.

f) A window will appear:
Additional configuration. Security check. Enable peak power check (POWCHK). Enable puls power check (PULCHK).

Choose the options if you want to use this security options. *Powchk* and *Pulchk* require special probes and *cortab*. If in doubt contact your local Bruker BioSpin representative, please.

g) Only if you have a sample changer!

Should the Sample Changer control the Lift? (yes/no)

The answer depends on how the air flow is connected, normally you will answer: ***yes*** → **ENTER**

If you have a sample changer, this question appears:

Delay between SX and next command [sec]?

Type in the length of the delay e.g. ***10*** → **ENTER**

h) The *nuclei-table* appear

Check if the frequency of the nuclei are set correctly. If in doubt click ***Restore*** then click ***Save***

i) The results of ***cf*** appears in a text window. Check this list carefully and compare the result with an list from an earlier configuration (if available) click ***Print*** and store the paper output with your other spectrometer documentation, then click ***OK.*** These data are saved in:
<TOPSPIN_HOME>/conf/instr/<spect>/uxnmr.info

If during 'cf' an error message occurs that invites you to do a firmware update see chapter 6.3

After finishing ***cf*** the window *config* will appear showing a list of configuration steps. You will be asked for the NMR ADMINISTRATION PASSWORD several times:

- Continue with ***expinstall***

a) Type in the NMR ADMINISTRATION PASSWORD and **ENTER**

b) Click **Next** if you either have not modified Bruker BioSpin Parameter files, AU-programs and Pulse-programs or if you have archived them in a different directory. Your individual Parameter files, AU-programs and Pulse-programs etc. that are named different to the original Bruker BioSpin files will not be destroyed during the installation.

c) A window appears: Check *Installation for Spectrometer* → Click ***Next***

d) In the appearing window: Check *the required system* → Click ***Next***

e) In the appearing dialog box: Select the spectrometer configuration name → Click ***Next***

f) In the appearing dialog box: Check the items you want to install or, accept the default selection → Click ***Next***

g) In the appearing dialog box: Select the default printer and plotter and the desired paper format → Click ***Next***

h) In the appearing window: Enter the desired spectrometer frequency, acquisition mode and pre-scan-delay or, accept the default values → Click ***Next***

i) In the appearing information box: Check the configuration selection and, if it is correct → Click ***Finish***
and wait ...

- Continue with ***edsolv***

  Check the list of lock solvents → click ***Save*** if it is correct → Click ***Close***

- Continue with ***edhead***

  Select the current probe → click ***Define as current probe*** → Click ***Exit***

  A window *Edit Spectrometer Parameter* will appear:
  Check if the connections between preamplifier and probe are set correctly → click ***Save*** if it is correct → Click ***Close***

- Continue with ***edprosol***

  Check the parameters for your observed nuclei, and if necessary change and/or recalculate them → Click ***Save*** to store to disk → Click ***Exit***

- Continue with ***edlock***

  Check the lock table values (field, lock phase, ...), change them and click ***Save*** if necessary, otherwise click ***Abort***

- Continue with ***edscon***

  Check the spectrometer constants, change them and click ***Save*** if necessary, otherwise click ***Cancel***

- After finishing the configuration a window `cron check` appears. Click on ***Automatic backup*** to set up an periodically backup of your TOPSPIN spectrometer configuration.
  If you click OK in the following window an automatic backup every 4 weeks will be initiated.

After ***cf***, ***expinstall***,... have finished insert a sample and make sure that you can lock on the lock solvent. Type ***ii*** and read with ***rpar*** a standard Bruker BioSpin parameter file (e.g. '***rpar PROTON all***'), type ***getprosol***, ***rga, wobb*** and ***zg*** and collect a normal ^{1}H NMR spectrum.

2.3.3 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer (see chapter 6.2.2).

Part I

TopSpin Installation and Configuration

Chapter 3

General Installation Information

3.1 Installation order

A complete new installation on a PC connected to a spectrometer involves the following steps:

1. Installing RED HAT ENTERPRISE LINUX WS 4 (see chapter 9.1)
2. Installing additional packages (see chapter 9.2)

Step 1 to 2 are normally already done by the manufacturer.

3. Configuring the network (see chapter Chapter 10)
4. Installing TOPSPIN (see chapter 4.3)
5. Installing TOPSPIN license (see chapter Chapter 5)
6. Configuring of TOPSPIN (see chapter 6.1)
7. Installing a printer (see chapter Chapter 11)

If your PC has already been used for TOPSPIN/XWIN-NMR, steps 1 and 2 are probably already done. In that case, you can start with step 3.

Chapter 4

Installing TOPSPIN

4.1 NMR SUPERUSER and NMR ADMINISTRATION PASSWORD

TOPSPIN offers a complete new password check for the configuration tools of TOPSPIN. During the TOPSPIN installation, you are prompted to define:

1. The username for the so called NMR SUPERUSER. The NMR SUPERUSER can be *nmrsu* (this is the default) or any other user (if the user does not exists so far, it will automatically be created during installation process).
   - After the installation, the NMR SUPERUSER is the owner of the TOPSPIN files, which are modified during configuration of the program. Log in as this user allows you to remove these files, change file permissions etc. The name of the NMR SUPERUSER will be stored in the readable text file: `<TOPSPIN_HOME>/conf/nmrsuperuser`
2. the NMR ADMINISTRATION PASSWORD to be used for TOPSPIN configuration commands. This password can be freely chosen and is not connected to any user. TOPSPIN asks for this password by commands like ***cf***, ***expinstall*** etc. The encrypted NMR ADMINISTRATION PASSWORD is stored in the file:

   `<TOPSPIN_HOME>/conf/nmradminpassword`

Note: The NMR SUPERUSER login password and the NMR ADMINISTRATION PASSWORD have different purposes and are totally independent. Changing one of

them does not affect the other.

With the information about the NMR ADMINISTRATION PASSWORD and NMR SUPERUSER TOPSPIN is ready to be configured. The NMR ADMINISTRATION PASSWORD will be asked for every time a configuration type command is entered. If this password is typed in correctly, the command will be executed regardless of which user is logged in the operating system. As a result all newly created configuration files will be owned by the user that was logged in at the time the configuration command was executed. Any other user can modify the configuration during his login session, just by knowing the correct NMR ADMINISTRATION PASSWORD. This is possible because all configuration files are read- and writeable for everybody, but TOPSPIN will not write them without the correct NMR ADMINISTRATION PASSWORD!

TOPSPIN also offers a so-called *Security Mode*. With this feature all configuration files are read- and writeable only for the NMR SUPERUSER.

4.1.1 How to change the NMR ADMINSTRATION PASSWORD

The *installnmr* script can be used to change the NMR ADMINISTRATION PASSWORD and the NMR SUPERUSER. If it is called with the option '-*secure*', it changes the permissions in a way, that only the NMR SUPERUSER can execute the configuration commands and the resulting files are readable and writable only for him, all other users have read-only permissions.

To change the NMR ADMINISTRATION PASSWORD, you have to:

1. Login as root
2. Open a Linux shell.
3. Go to the TOPSPIN installation directory, in a default installation this is

   `/opt/topspin`
4. Enter the command:

   `prog/bin/installnmr <TOPSPIN_HOME> <NMRSUPERUSER>`

   If you installed TOPSPIN in the default directory and you want to use the user 'nmrsu' as NMR SUPERUSER, you have to type in

   `prog/bin/installnmr /opt/topspin nmrsu`
5. Enter the old password and new password as requested.

4.1.2 How to define a new NMR ADMINSTRATION PASSWORD

To define a new NMR Administration Password, for example because you have forgotten it, you have to:

1. Open a Linux shell
2. Login as root with the command

   su -
3. Delete the file

   <TOPSPIN_HOME>/conf/nmradminpassword
4. Enter the command

   prog/bin/installnmr <TOPSPIN_HOME> <NMRSUPERUSER>
5. Enter new password as requested.

If you want to make sure that no meddler can do this, you have to modify the permissions, owner and group membership of this file accordingly.

4.2 Packages on the TopSpin DVD[1]

The TOPSPIN 2.1 DVD contains the following programs:

1. TopSpin: Acquisition, Processing and Plotting software
   - TOPSPIN Plot Editor: Object oriented WYSIWYG plot editor (automatically installed as part of TopSpin package)
2. Icon-NMR: Icon-driven interface for Routine Spectroscopy and Automation
3. NMR-GUIDE: Web-browser based teaching and training program
4. Diskless: Spectrometer CCU operating system
5. NMR-SIM: Program for numerical simulation of NMR experiments
6. AUTOLINK

The following programs are part of the TOPSPIN 2.1 DVD-content, but please note that they must be licensed separately in each case:

1. AMIX-Viewer: new multiple object viewer
2. SBASE: Spectra database (requires AMIX license)

1. Installation under Windows offers additionally the two programs Auremol and Perch

3. NMR-GLP: Program for 'Good Laboratory Practice' tests
4. FLEXLM: License manager required for starting TOPSPIN programs.
5. AUREMOL

Please note that all version information about the different programs can be found on the TOPSPIN DVD and in the latest version of the Release Letter.

4.3 Installing TOPSPIN

This chapter describes the installation of the TOPSPIN.

The main decision you have to make during installation is where do you want to install the new ***TOPSPIN*** version. If you have a previous NMR SUITE or TOPSPIN installation on this PC available, you can either:

- install the new version in parallel to the previous one
  (e.g. old version in `/opt/topspin2.0`, new in `/opt/topspin2.1`)

  or
- install the new version in the same directory as the previous one
  (e.g. old version in `/opt/topspin`, new in `/opt/topspin`)

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation you can start working with the new version and if you want to go back to the previous version for whatever reasons you can just start and reuse it.

The installation of TOPSPIN offers an automatic import of your individual configuration of a previous version, so that there is no advantage to install the new version in the same directory as the old one.

4.3.1 Installation in parallel

1. Close ALL WINDOWS on the desktop
2. Insert the DVD TOPSPIN *2.1*
3. Start of the installation
   - If the automatic start of the DVD is enabled, the shell described in the next step appears automatically, go to step 4

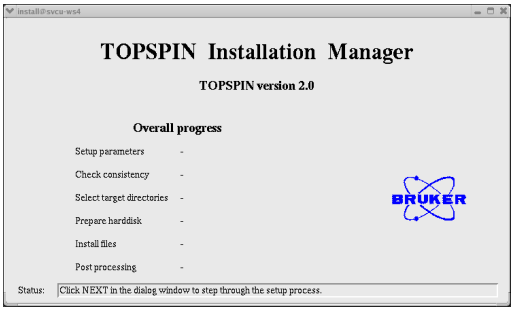
- If the shell of the next step does not appear automatically you have click on the DVD icon on your desktop and click on the file `install` [1]

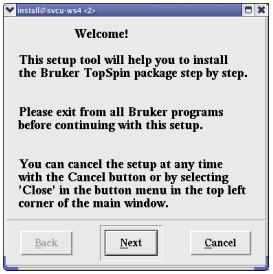
4. If you are not logged in as root, a Linux shell will appear that asks you for the root password:

```
Please enter root password if prompted for it:
Password:
```

- Enter root password and press enter

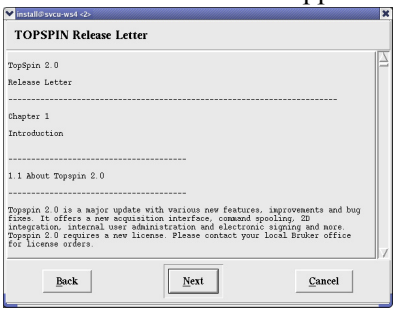
5. The windows *TOPSPIN Installation Manager* and *Welcome to the Bruker Software Installation Manager* will appear:





- Click **Next**

6. A window *Release Letter TOPSPIN* will appear:

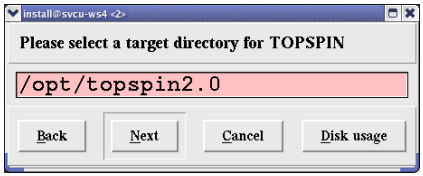


a) Please read the NMR Release letter! You can find therein all information about news and bug fixes of the current version.

b) When you have finished reading the Release Letter click **Next**

1. Please note that there is also a file called ‘install.cmd’ on the DVD. This file is the installation script for windows, under Linux you have to click on the file `install`

7. A window *Please select a target directory for TOPSPIN* will appear:



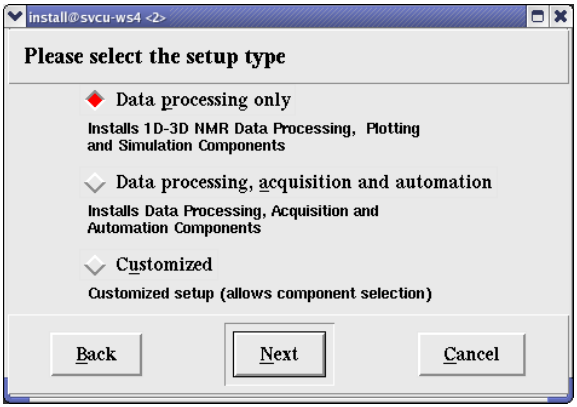
Enter an installation path which does not exists so far, e.g. ***/opt/topspin2.1***

- Click **Next**

8. If the installation directory does not exist you will be asked if the installation process should create it automatically

- Click **Yes**

9. A window *Please select the setup type* will appear:



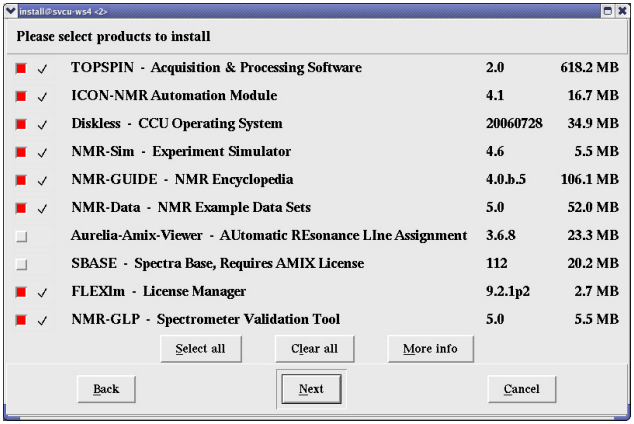
a) Select the setup type. Do one of the following:

- Select *Data Processing only* if you want to use TOPSPIN for data processing.
- Select *Data processing, acquisition and automation* if you want to use TOPSPIN for spectrometer control. This will e.g. install **Diskless** automatically.
- *Customized setup* (allows components selection) if you want to install selected programs only.

b) Click **Next**

9.1. If *Customized* was selected in step 9 ...

... a window *Please select products to install* will appear:

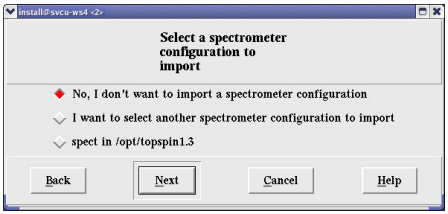


- Select the packages which you want to install (note that DISKLESS is only required if your PC controls a spectrometer or you want to configure it like this (see chapter 6.2.2).
  - TOPSPIN: Acquisition, Processing and Plotting software
  - ICON-NMR: Icon-driven interface for Routine Spectroscopy and Automation
  - DISKLESS: Spectrometer CCU operating system
  - NMR-SIM: Program for numerical simulation of NMR experiments
  - NMR-GUIDE: web-browser based teaching and training program
  - NMR-Data: spectroscopic example data
  - AURELIA-AMIX-Viewer: Viewer of 2D/3D/4D NMR data (requires separate license)
  - SBASE: Spectra database (requires AMIX license)

- FLEXlm: License manager required for starting TOPSPIN programs.
- NMR-GLP: Program for'Good Laboratory Practice' tests (requires separate license)

- Click **Next**

10. The window *Select a spectrometer configuration to import* will appear. You can either import no spectrometer configuration, or browse for a spectrometer configuration or select one of the configurations you get offered within this window.[1]



The configurations that are shown in this picture are just an example. On your PC this list could look different.

11. If a previous ***TOPSPIN*** installation is available in the global environment variable Path, you will be asked if you want to define the current installation path instead. It is recommended[2] to set the current installation into the PATH variable, so enable:

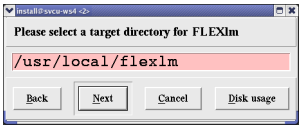
Yes, add the new TOPSPIN installation directory to the global PATH

- Click **Next**

12. A window appear that asks for the installation path of the FlexLM. It is strongly

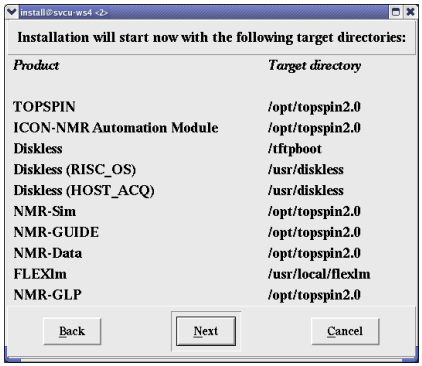
1. The installation process will offer all configurations which are available in the TOPSPIN / XWIN-NMR installation that are defined in the /etc/profile.d/xwinnmr(.csh/.sh) resp. topspin(.csh/.sh) directory.
2. In case more than one ***TOPSPIN*** version is installed in parallel it is your decision which one should be defined here

recommended to accept the default path! [1]



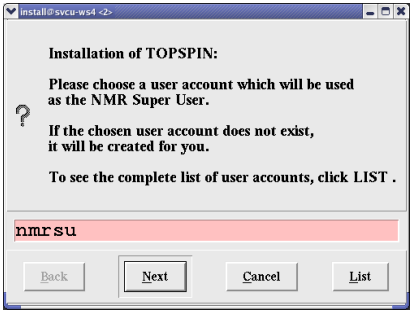
- Click **Next**

13. A window appear that displays the programs which will be installed



- Click **Next**

14. A window will appear that prompted for a definition of an NMR SUPERUSER



a) Do one of the following:

- Accept the default NMR SUPERUSER (*nmrsu*) or
- Enter a special user for this purpose, e.g. named *nmr-admin* or

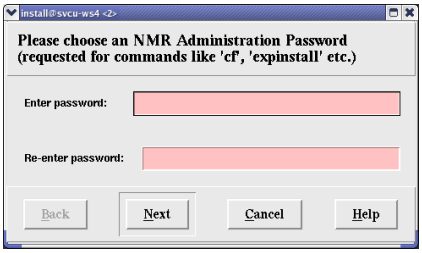
1. It is strongly recommended to accept the default path for the FlexLM installation: /usr/local/flexlm ! If you choose a user defined path, it may cause some problems with other applications using the FlexLM

- Enter any other user

  If the user does not exists, installation will create it. For further details see chapter 4.1 or the TOPSPIN Users Guide.

b) Click **Next**

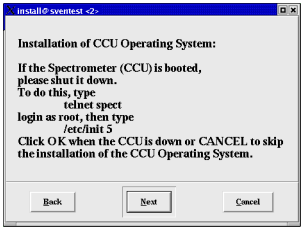
15. A window *Password Input* will appear and asks for the NMR ADMINISTRATION PASSWORD[1] (for more details about this feature see chapter 4.1)



- Type in the NMR ADMINISTRATION PASSWORD
- Re-enter in the NMR ADMINISTRATION PASSWORD

c) Click **Next** → The installation of TOPSPIN will start now.

16. If *Data Processing, acquisition and automation* or *Customized* with the Diskless package was selected in step 8 a window will appear to inform that the spectrometer has to be shut down



a) If the PC is not yet connected to a spectrometer or if the CCU is not booted[2] you can promptly

- Click **Next**

1. Certain commands like ***cf*** and ***expinstall*** ask for the NMR ADMINISTRATION PASSWORD.
2. Note that during a first time installation of the TOPSPIN the CCU can not be booted.

b) If your PC is currently connected to a spectrometer and the CCU is booted (see chapter 9.3.2 and 12.3.1.7)

a) Open a Linux shell

b) enter the command:

telnet spect

c) login as *root*

d) enter the command:

init 5

→ this will shut down the CCU

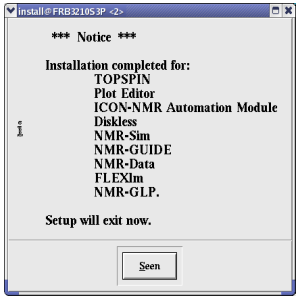
e) Close the Linux shell

f) Click **Next** in the window that asked you about shutdown the CCU

Note: The CCU is now either down or switched off and should be turned on again at the end of this procedure.

→ The installation of TOPSPIN will start now.

17. After installation is finished the window *Setup is complete* will appear:

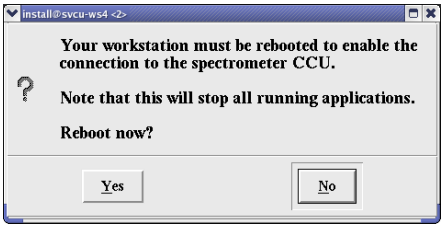


- Click **Seen**

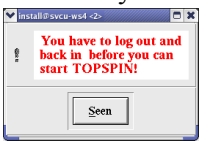
18. Depending if you have installed DISKLESS one of the following windows will appear:

- If you have installed DISKLESS a window will appear that asks you to reboot the PC. Make sure that you can reboot the PC now (check for any unsaved

windows (e.g. an editor window) and check if no other users are logged in into this PC) then click on **Yes**



- If you have not installed DISKLESS a window will appear that informs you to log out and log back in before you start TOPSPIN, click **Seen**



19. The window wherein you entered the root password informs you that you have to press *Enter* to close this window
    - Press **Enter**
20. If you have started the installation manually by clicking the file `install` in the Konqueror window, you have to close this Konqueror window.
21. To eject the DVD click right on the DVD icon on the desktop and choose **eject**
22. To start TOPSPIN log out and log back in

4.3.2 What do you want to do with TOPSPIN?

- it should control a spectrometer or you want to use a special spectrometer configuration

  → you have to execute ***cf*** and ***expinstall***
- it should be used for data processing only?

  → you have to execute ***expinstall***

For more details please refer to the next chapter

4.4 Perl and GCC

The packages Perl and GCC are automatically installed in the directory <TOPSPIN_HOME>/gnu and <TOPSPIN_HOME>/perl where <TOPSPIN_HOME> is the directory where ***TopSpin*** is installed (default /opt/topspin). Perl and GCC are needed for compiling ***TopSpin*** AU programs.

4.5 Installing TopSpin patches

TopSpin patches are parts of ***TopSpin*** which contain bug fixes. They are available on the Bruker BioSpin WWW server. We recommend to install new patches whenever the *patchlevel* on your system is older than the one on the WWW server.

Perform the following steps:

1. Start TopSpin
2. Enter the command ***about***

   The upcoming window will show information about your TopSpin installation and configuration. *Version*, *Server patchlevel* and *GUI build number* of your TopSpin installation can be used for an update check.

Download from WWW server

1. Log in on a computer which is connected to the internet
2. Open your web browser
3. Go to *http://www.bruker-biospin.de*
4. Click on **NMR → tech support → Software → Downloads → Linux PC** and select the package you want to download

Note, that in the past it was also possible to download patches from the German Bruker BioSpin FTP server. Bruker BioSpin Germany has now moved some parts of the information from the German Bruker BioSpin FTP server to the German Bruker BioSpin Web server. We did this because we want to offer relevant information about patches and documentation, for instance, in only one area. Should we have forgotten or omitted to put relevant information onto the web, please notify us at:

nmr-software-support@bruker.de

We will then send you the information by email.

4.6 The usage of the NMR-GUIDE

NMR-GUIDE 4.0 that comes with TOPSPIN 2.1 uses an own web server and the TOPSPIN internal java package. Therefore it is not necessary anymore to have these packages installed/configured separately!

4.6.1 Requirements for NMR Guide 4.0

The using of NMR-GUIDE 4.0 requires the installation of TOPSPIN 2.1. Also be sure that the following components are installed:

1. Web browser
2. *PDF viewer*

   NMR-GUIDE offers among other things a lot of PDF documents. To display these documents it is necessary to install the acrobat reader. For an installation description see chapter 9.3.1
3. NMR-GUIDE license (contact license@bruker.de for a three month demo license or order a official license from your local Bruker BioSpin representative). Note that the NMR-GUIDE license is already part of a full or demo ***TOPSPIN*** 2.1 license.

The WWW browser gets documents from the locally installed WWW server. The client - server communication is established over a network socket connection, but the communication partners only use the localhost TCP/IP host identifier. These pages are shown in the right-hand side window of the browser.

The WWW browser also gets dynamically created pages from the localhost. These workstation specific pages are coming from a *gserver*. This is a platform independent Java web server written by Bruker BioSpin and acts as a daemon running on the locally installed JAVA virtual machine. The gserver is included in the NMR Guide&Encyclopedia package. The table of contents is generated dynamically and displayed in the left-hand side window of the browser.

TOPSPIN commands can be invoked from the WWW browser. This process is also managed by the gserver. The gserver is an essential component of the NMR Guide&Encyclopedia and requires an NMR-GUIDE license.

4.6.2 Java Requirements for NMR-GUIDE 4.0

For using NMR-GUIDE 4.0 that comes with the ***TOPSPIN*** 2.1 version it is not necessary to install/configure a special Java package. NMR-GUIDE uses the ***TOPSPIN*** internal Java package that is automatically installed and configured during installation of ***TOPSPIN***.

4.6.3 Working with the NMR-GUIDE

In order to work with the NMR-GUIDE, the following procedure must be followed.

4.6.3.1 Start up of the NMR-GUIDE

1. Start TOPSPIN and enter the command:

   ghelp

   or enter the command (this allows to start a search also within NMR-GUIDE):

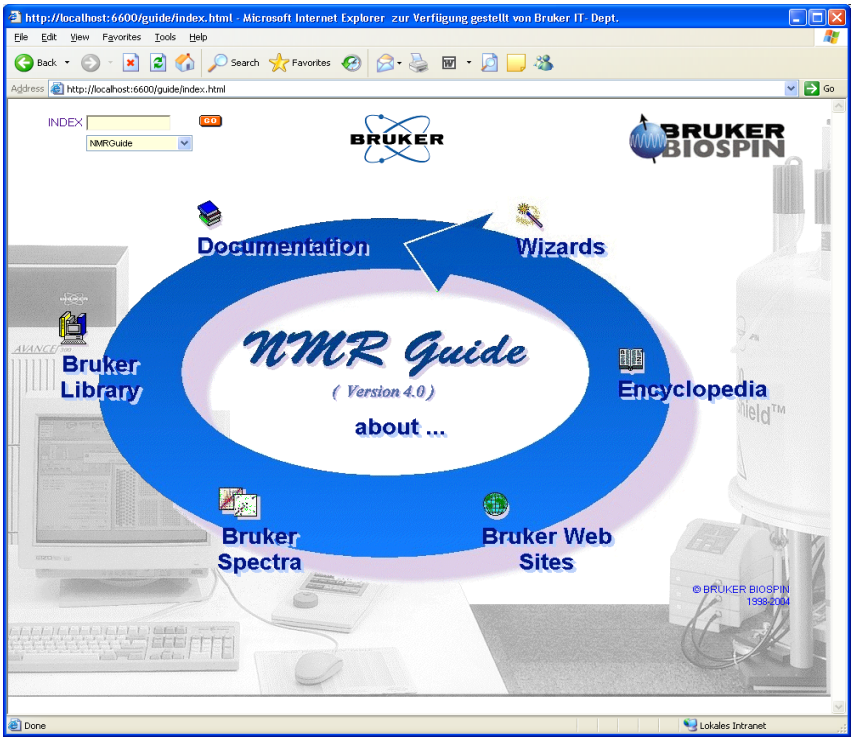
   help

   or select from the ***Help*** pull-down menu of TOPSPIN the entry:

   NMR-GUIDE

2. Your standard web browser will automatically starts and shows the page

http://localhost:6600/guide/index.html



You can now use the functionality of NMR-GUIDE

4.6.3.2 Using the NMR-GUIDE search engine

One of the very important and useful tools of NMR-GUIDE is its search engine. It offers the possibility to search within thousands of html pages that contain a huge amount of information about NMR spectroscopy.

For using this search engine you can start NMR-GUIDE and enter the keyword therein (or select an entry of the list of commonly used keywords). With NMR-GUIDE 4.0 you have also the possibility to search directly from within TOPSPIN, just enter the command:

help <keyword>

Chapter 5

The TOPSPIN license

5.1 Questions and answers about the TOPSPIN license

1. *Which programs need a license?*

TOPSPIN, NMR-SIM and NMR-GUIDE need a license.

If you do not have a license for TOPSPIN, it will start up in an emergency mode if your PC is connected to a spectrometer. However, NMR-SIM and NMR-GUIDE will not run without a valid license.

ICON-NMR is always used in connection with TOPSPIN and does not need an individual license.

TOPSPIN PLOT EDITOR has an individual license but it comes in a bundle with every kind of ***TOPSPIN*** license, so if you have a ***TOPSPIN*** license you have also a TOPSPIN PLOT EDITOR license. If ***TOPSPIN*** is running with the spectrometer license TOPSPIN PLOT EDITOR offers limited functionality only.

AURELIA, AMIX, MAXENT, GLP and PARAVISION do need a license which must be ordered for each program separately.

2. *Which license types are available and what programs may be run with each?*

There are six different license types, details of each are given in the following table. For more information please refer to the Bruker BioSpin license order page on the web server:

https://www.bruker-biospin.de/NMR/nmrsoftw/licenses

or contact your local Bruker BioSpin representative.

License type	Contents
Full	Acquisition, Processing, Automation (ICON-NMR), Plotting, Experiment Simulation and NMR-GUIDE
	license period: 15 years
	Floating
Demo	Acquisition, Processing, Automation (ICON-NMR), Plotting, Simulation and NMR-GUIDE
	license period: 3 months
	Node locked, uncounted, free of charge
Processing-Only	Processing and Plotting
	license period: 15 years
	no Acquisition, no NMR-SIM, no NMR-GUIDE
Presenter	Viewing and Plotting
	license period: 15 years
	no Acquisition, no Processing, no NMR-SIM, no NMR-GUIDE
Teaching	NMR-SIM and restricted Processing and Plotting
	license period: 15 years
	TOPSPIN can only process datasets created with XWIN-NMR $\geq$ 3.1 that are older than 4 weeks or datasets created by NMR-SIM. One ***TOPSPIN***-plot session (without portfolio editor) can be started, Node locked, count 1.
Developer	Special license for extending TOPSPIN with own functionalities. Allows viewing of data.
	license period: unlimited
	no Acquisition/Processing/Plotting/NMR-SIM/NMR-GUIDE, free of charge

3. *What kind of licenses do I need?*

If you want to use TOPSPIN 2.x you need a FEATURE line '*TOPSPIN2*' in your `license.dat` file. If you have 'TOPSPIN 1.x' you can only start TOPSPIN 1.x.

If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously.

4. *Which licensing program is used for TopSpin?*

The Flexlm license manager is used and is delivered on the TopSpin DVD. It contains the '*bruker_lmgr*' license manager, the '*lmutil*' program, Help files and example `license.dat` file.

5. *What are the requirements for the Flexlm to function:*

Your PC must have an Ethernet card

6. *What is a Floating license?*

Floating licenses are licenses that are available for more than one computer in a network. *Floating* licenses are issued based on the Host-ID of one particular computer. This computer becomes the ‚license server'. All computers that can communicate with this ‚license server' computer can use the licenses managed by this computer. For this to work, the same license file must be installed on all participating computers, including the ‚license server'. The Flexlm license manager software must only run on the ‚license server' computer.

A *Floating* license can have just one license for a program like TopSpin. In such a case, the respective program can be started once on one computer in the network. If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously. For example, if you have a license file with 5 licenses for TopSpin, TopSpin can be started 5 times from any 5 computers in the network.

The number of licenses is stated in the FEATURE for the respective program.

7. *What is the difference between 1-Server / 3-Server Licenses?*

Floating licenses can be ordered as 1-server or 3-server licenses. In a 1-server license you have only one license server, and in a 3-server license there are three license servers defined in the license file.

- The advantage of a 1-server license is that it is only necessary to have one computer active at a time to make the license available.
- The advantage of a 3-server license is that any of the three license servers can be inactive and the license management is then done by the remaining two servers.
- One requirement for the three license servers is that all of them have TCP/IP active.

- The operating system on the three computers can be the same or can be different (Linux, Windows).

8. *What is a Node Locked license?*

A node-locked license allows you to start the respective program only on the computer with the Host-ID for which that license was generated. Typically, this license form is used for Demo and Teaching licenses. No other computer can use the license in the way described above for floating licenses.

9. *How do I know if my license is* Floating *or* Node Locked*?*

You can recognize this from the syntax of the license FEATURES in the `license.dat` file:

`/usr/local/flexlm/Bruker/licenses/license.dat`

If the entry '*HOSTID*=' appears after the encrypted password, the license is Node locked and can only be used on the local PC

```
FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 9B1EA0113CD53A883974 HOSTID=006008d244fe vendor_info=....
```

→ *Node locked* license for three parallel sessions of TOPSPIN that can be started on the local PC

```
FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3  9B1EA0113CD53A883974 vendor_info=....
```

→ *Floating* license for three parallel sessions of TOPSPIN that can be started on every PC in the local network

10. *If I have a* Floating *license and I have a dual-boot PC (e.g Windows XP and Linux), can I use the license on both operating systems?*

Yes, the license is based on the physical address of the Ethernet card and not on the operating system. Copy the license file `license.dat` to:

Windows:

`c:\flexlm\Bruker\licenses\license.dat`

Linux:

`/usr/local/flexlm/Bruker/licenses/license.dat`

11. *How can I determine the hostid of my PC?*

See chapter 5.2.2.

12. *How do I install a license (full or demo) on my PC?*

See chapter 5.2.

13. *Does a Demo license require SERVER/DAEMON lines in `license.dat`?*

No, a Demo license is *Node Locked uncounted* and therefore only requires FEATURE lines. If SERVER and/or DAEMON lines exist, they are ignored.

14. *I have a* Floating *license. Must the file* `license.dat` *be identical on all hosts, server and clients?*

Yes, you have to install the `license.dat` on the server and copy it to all clients.

15. *Must the Flexlm license manager run on all hosts in the network?*

No, it only needs to run on the license server. If the license manager also runs on a license client, this is simply ignored.

16. *Must the Flexlm license manager run on a host with a Demo license?*

No, it only needs to run on the server for counted licenses, a demo license is uncounted.

17. *What can I do if TOPSPIN does not start after I installed the license?*
See chapter 12.1

18. *How is it possible that TOPSPIN starts even though I do not have a license?*

If you do not have a license for TOPSPIN, it will start up in an emergency mode if your PC is connected to a spectrometer. Also one TOPSPIN PLOT EDITOR session (without portfolio editor) can be started from within TOPSPIN. However, NMR-SIM and NMR-GUIDE will not run without a valid license.

19. *What can I do if TOPSPIN cannot find the license server?*

Try to restart the license server:

```
service bruker_lmgr start
```

5.2 Ordering and installing the TOPSPIN license

5.2.1 Ordering a license

You can order a license from Bruker BioSpin Germany. Demo licenses are free of charge. For all licenses you must specify:

- the hostid of your PC
- the program for which you want to get a license, e.g. TOPSPIN
- the type of license (full, demo, processing-only, presentation or teaching)

- the number of licenses and your order number (not necessary for demo license)

Licenses can be ordered from the German Bruker BioSpin web server:

https://www.bruker-biospin.de/NMR/nmrsoftw/licenses

5.2.2 How do I determine the correct hostid

The hostid is a 12-digit hexadecimal number. It is the physical address (also called Mac address or Node address) of the Ethernet card. After installing TOPSPIN, including the Flexlm license manager, you can determine the hostid in two ways:

- Start TOPSPIN; a command prompt will pop up, which will list the hostid, if no licence.dat file is available.
- Open a Linux shell and enter:
  `/sbin/ifconfig eth0`
  take the numbers of the *HWaddr*.

5.2.3 Installing a Demo license

A Demo license can be installed as follows:

1. Log in as Administrator
2. Install the Flexlm license manager as described in chapter 4.3
3. Open a Linux shell and enter:
   `nedit /usr/local/flexlm/Bruker/licenses/license.dat`
   enter the FEATURE lines, save and exit the file

5.2.4 Installing a full license on a license server

The Flexlm license manager must always be installed and run as a service on the license server. It is delivered on the TOPSPIN DVD and can be installed as described in chapter 4.3. In case the license file identifies the PC as license server, Flexlm is automatically installed as a service which is then automatically started during boot time

On the license server, the file `license.dat` must contain a SERVER line, a DAEMON line and FEATURE lines. An example would be:

```
SERVER tulip 0060080e830d 1700
```

```
DAEMON bruker_ls /usr/local/flexlm/Bruker/bruker_ls
FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 0B0E4011FF0CD32FBFF1 \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE TOPSPIN_1D bruker_ls 0.0 6-aug-2018 3 9B3EA021818829E2716A \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE TOPSPIN_2D bruker_ls 0.0 6-aug-2018 3 AB3E80014D54F0FB3887 \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE XWINPLOT bruker_ls 0.0 6-aug-2018 3 DB4E50F1618A2B2383D3 \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE TOPSPIN_ACQU bruker_ls 0.0 6-aug-2018 3 9BDE3051D4CB63255DCC \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE NMRSIM bruker_ls 0.0 6-aug-2018 3 2B4EC041E98523510FCB \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
```

where *tulip* is the hostname and *0060080e830d* the hostid of the computer. Note that the second part of the FEATURE lines, the vendor_info, does not necessarily exist. In that case a FEATURE line would look like:

```
FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 0B0E4011FF0CD32FBFF1""
```

To inform Flexlm about the new license enter in a Linux shell:

```
/usr/local/flexlm/Bruker/lmreread -c /usr/local/flexlm/Bruker/licenses/license.dat
```

5.2.5 Installing a full license on a license client

On a license client, license can be installed in two different ways, as described for a Demo license chapter 5.2.3. The only difference is that you do not have to setup a new file `license.dat`. You can just copy it from the license server which can be another PC (see question 10 in chapter 5.1).

5.2.6 Modifying the license file

If you have modified a license file, you have to inform Flexlm about the modified license with the command:

```
/usr/local/flexlm/Bruker/lmreread -c /usr/local/flexlm/Bruker/licenses/license.dat
```

Chapter 6

Configuration of TOPSPIN

The idea of this chapter is to give you some guidelines to full spectrometer or workstation configuration. We do not discuss the commands in detail here. For a full description refer to the TOPSPIN manual.

6.1 Take over the configuration of XWIN-NMR/TOPSPIN into TOPSPIN 2.1

The decision how to install TOPSPIN is very important in case you have already XWIN-NMR or TOPSPIN installed on the same or another PC. If so, you might want to take over the configuration of a previous XWIN-NMR/TOPSPIN into TOPSPIN 2.1 because of:

- in case the XWIN-NMR installation was used for controlling a spectrometer there are very important configuration files like the spectrometer configuration, shim files, your own pulse programs, parameter sets, etc.
- if XWIN-NMR was used for processing only there can be also very important configuration files like AU programs, macros, plot layouts etc.

! *Note: Transferring files could cause permission problems especially if they are transferred from one PC to another.*

6.1.1 You have a TopSpin/XWIN-NMR configuration that you like to use for TopSpin (on the same PC)

You can take over the configuration during the Installation of TOPSPIN 2.1 (see chapter 4.3) or after the installation with the ***TOPSPIN*** command ***nmr_save***.

During the installation you will be asked if you want to import a spectrometer configuration. If you want to take over the configuration after installation is finished, start TOPSPIN

- and type in the command:

  nmr_save

- or click

  Options → Manage Configuration → Save installation specific files

A window *NMR_Save* appears.

- Accept or modify the '*Location of Backup file*' (default: `<TOPSPIN_HOME>\nmr_backup`).
- Enter the location of the installation to be saved (e.g. `/opt/xwinnmr`).
- Click on ***Save***.

This will create a tar file of all necessary information from the TOPSPIN/XWIN-NMR installation. The tar-file is called `nmr_backup.tar` and will be stored in the directory you selected.

To take over this information into TOPSPIN, start ***nmr_backup*** and ...

- Make sure that *Location of Backup file* contains the correct path to your backup file
- Make sure that the *restore destination* is correct (previous settings might be overwritten in the restore destination!)
- Click on ***Restore***.

A window *Password request* will appear. Please enter the NMR administration password and click ***OK***.

After this process is finished, execute ***cf***.

If you like to get more information about the command ***nmr_save*** refer to chapter 6.5.

6.1.2 You have a TopSpin/XWIN-NMR configuration that you like to use for TOPSPIN (on another PC)

Before you start installation of TOPSPIN on PC-A you have to copy the two directories:

`conf` , `plot` and `exp`

from the TOPSPIN/XWIN-NMR installation on the PC-B into the directory where TOPSPIN will be installed. The default installation directory of TOPSPIN for Linux is:

`/opt/topspin`

In case you will use the default installation path you have to create these directories and as a second step copy the two directories `conf` and `exp` into them. After these two directories are available on PC-A you can start the TOPSPIN installation.

6.2 Configuring TOPSPIN

Start TOPSPIN:

- Click the icon TOPSPIN on the desktop[1], or
- Click **<redhat> → Other → TOPSPIN<vers.>**

When a user starts a new TOPSPIN version for the first time, a window 'LICENSE' will appear:

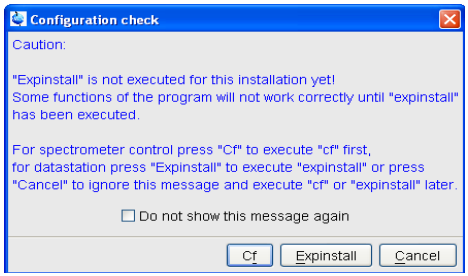
a) Please read the license agreement for Bruker TOPSPIN !

b) If you agree, please click **I Accept**.

Now the window *Configuration check* will appear, that allows you to configure the

1. How to create a icon? See chapter 15.7.1

software. If you have to click on ***Cf*** or ***Expinstall*** depends on what you want to do



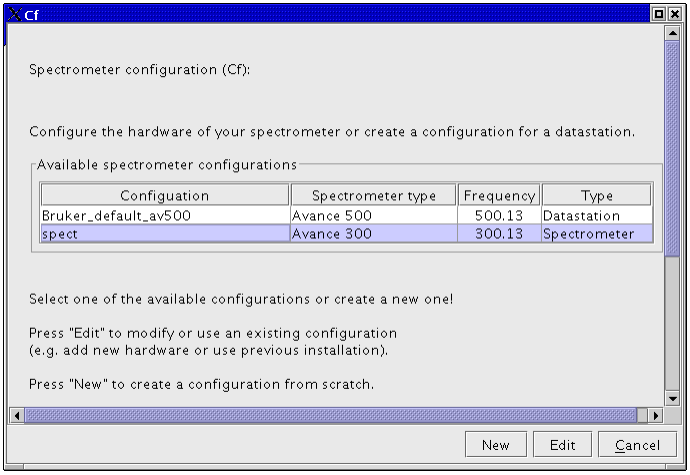
with TOPSPIN. You are mainly in one of the following situations:

1. You want to configure a processing-only-PC with a default configuration on a datastation → go to chapter 2.3.1 (for details see chapter 6.2.3)
2. You have installed the new software on the same PC as a previous XWIN-NMR/TOPSPIN installation, so the old spectrometer configuration is available on the same PC → go to chapter 2.3.2 (for details see chapter 6.2.1)
3. You want to configure a processing-only-PC like your spectrometer-PC and you have the spectrometer configuration on another computer → go to chapter 2.3.3 (for details see chapter 6.2.2)
4. You have to configure the software for controlling a spectrometer on a new hard disk without a backup of the spectrometer configuration, so you have no configuration files → go to chapter 6.2.4

6.2.1 If your PC controls a spectrometer

1. Be sure that the spectrometer is booted (see chapter 9.3.2 and 12.3.1.7)
2. Open a dataset
   - Type ***new*** and create a new dataset **.**
   - You can also select a dataset (e.g. *exam1d_1H*') acquired with another TOPSPIN or XWIN-NMR version.
3. Enter ***cf*** (The command ***cf*** now configures the software according to the hardware of your spectrometer):
   a) A window will appear:
   Password request. Please enter the NMR ADMINISTRATION PASSWORD
   Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

b) A window `Cf` will appear:

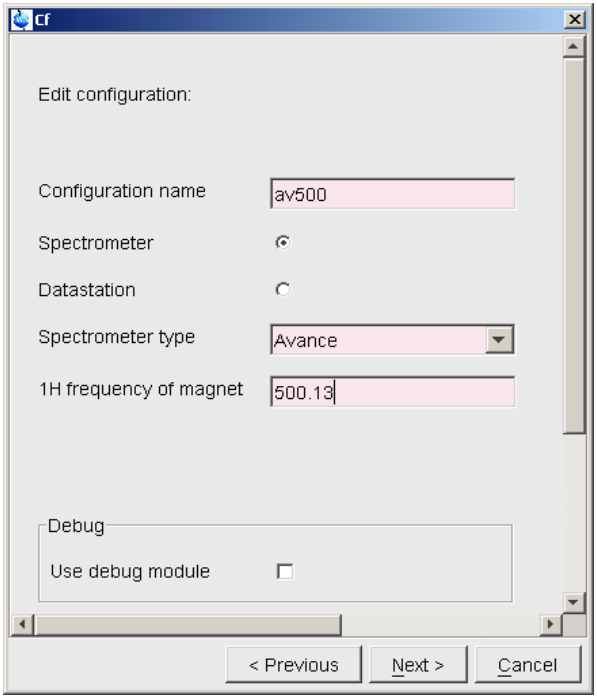


Most likely you will select an existing configuration and press ***Edit*** to confirm this configuration.

c) A window will appear:

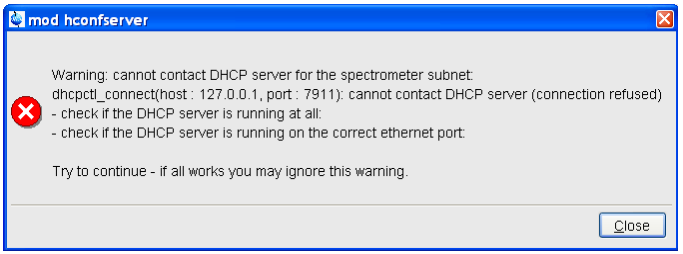
The selected configuration is displayed. Choose the type of your spectrometer e.g. ***AVANCE*** → **ENTER**. Check or type in the 1H frequency of the magnet e.g. ***500.13*** → **ENTER**. Use the debug mode only in a case

of trouble-shooting.



d) In case the information window `mod hconfserver` appears:

- your spectrometer has not a BSMS rack with ECLB board: you may ignore this warning → **ENTER**. Nevertheless please check the configuration summary (`uxnmr.info` file) if all units are listed.
- your spectrometer has a BSMS rack with ECLB board and the DHCP server might not work correctly. For troubleshooting information see chapter 12.3.2



e) A window will appear:

Specify the channel to which external devices are con-

nected. The RS232/485 channel for external devices-Table appears.

Check if the tty-numbers of the hardware components are set correctly.

f) A window will appear:
Additional configuration. Security check. Enable peak power check (POWCHK). Enable puls power check (PULCHK).

Choose the options if you need this security options.

g) Only if you have a sample changer! A window will appear:

Should the Sample Changer control the Lift? (yes/no)

The answer depends on how the air flow is connected, normally you will answer: ***yes*** → **ENTER**

In this cases the question appear:

Delay between SX and next command [sec]?

Type in the length of the delay e.g. ***10*** → **ENTER**

h) The *nuclei-table* appear.

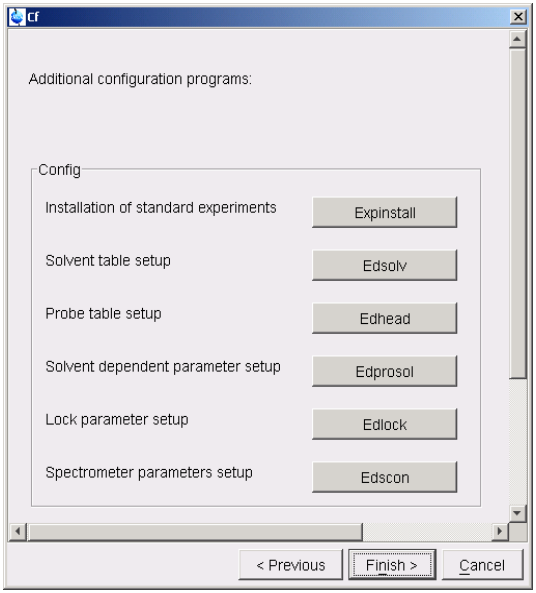
Check if the frequency of the nuclei are set correctly. If in doubt you can use default values by clicking on ***Restore*** then click ***Save***

i) The results of ***cf*** appears in a text window. Check this list carefully and compare the result with an list from an earlier configuration (if available) click ***Print*** and store the paper output with your other spectrometer documentation, then click ***OK.*** *These data are saved in <TS_HOME>/conf/instr/<spect>/uxnmr.info.*

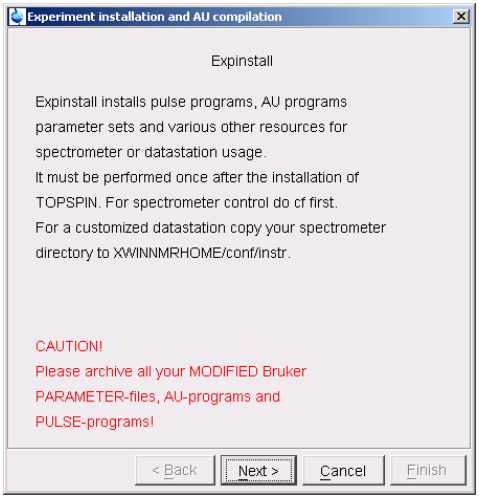
If during 'cf' an error message occurs that invites you to do a firmware update see chapter 6.3

After finishing ***cf*** the window *configure* will appear showing a list of configuration steps. Accept the default selection and click ***Start*** (You will be asked for

the NMR ADMINISTRATION PASSWORD a couple of times):

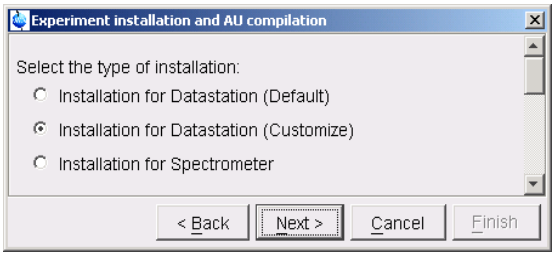


- Continue with ***expinstall***
  a) Type in the NMR ADMINISTRATION PASSWORD and **ENTER**
  b) Click **Next** if you either have no modified Bruker BioSpin-Parameterfiles,

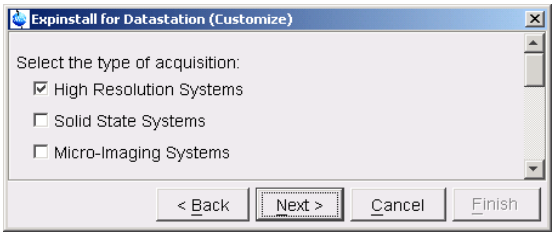


AU-programs and Pulse-programs (If you have some, you have to archive them in a different directory before executing ***expinstall***). Your individual Parameterfiles, AU-programs and Pulse-programs that have different names to the original Bruker BioSpin files will not be destroyed during the installation

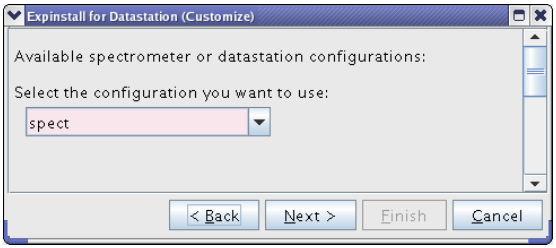
c) In the window that appears → Check *Installation for Spectrometer* → Click ***Next***



d) In the window that appears → Check the boxes of the NMR categories you are interested in[1] → Click ***Next***

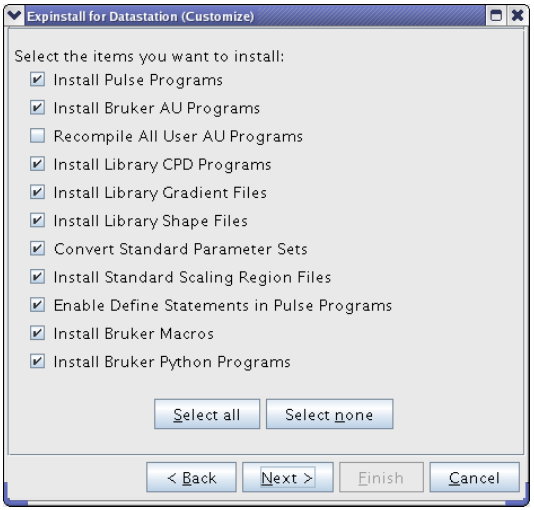


e) In the dialog box that appears → Select your spectrometer configuration name → Click ***Next***

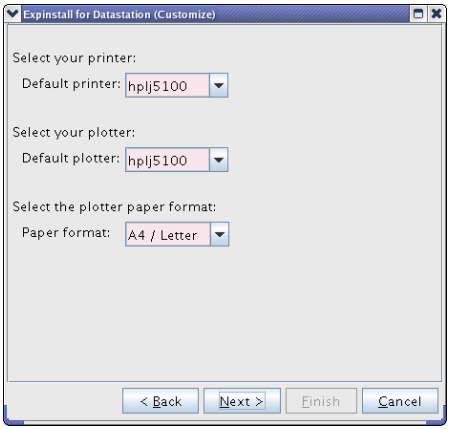


1. This selection defines which parametersets and pulse programs are available for usage after configuration is finished. It is possible to rerun ***expinstall*** later to add another selection afterwards

In the dialog box that appears → Check the items you want to install or, accept the default selection → Click ***Next***

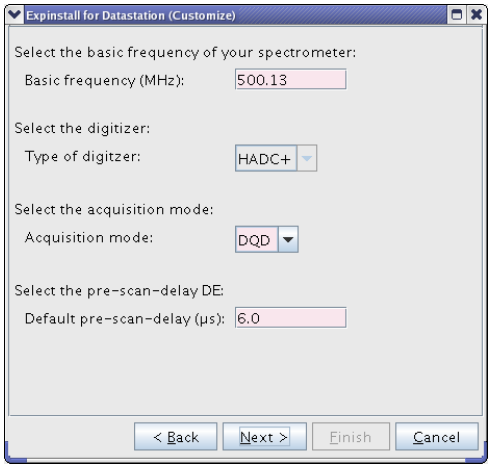


f) In the dialog box that appears → Select the default printer and plotter and the desired paper format → Click ***Next***



g) In the window that appears → Enter the desired spectrometer frequency, acquisition mode and pre-scan-delay or accept the default values

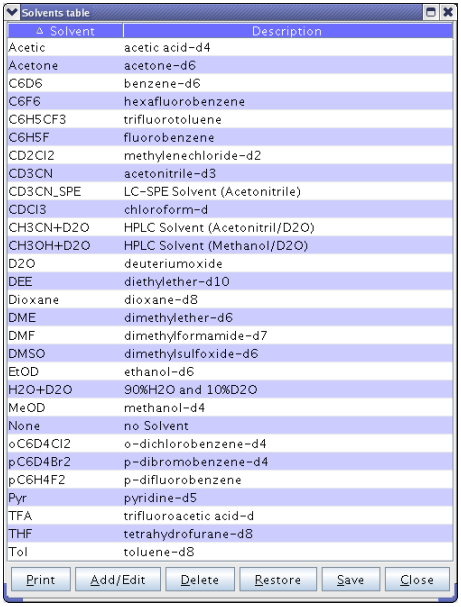
→ Click ***Next***



h) In the information box that appears → Check the configuration selection and, if it is correct → Click ***Finish***

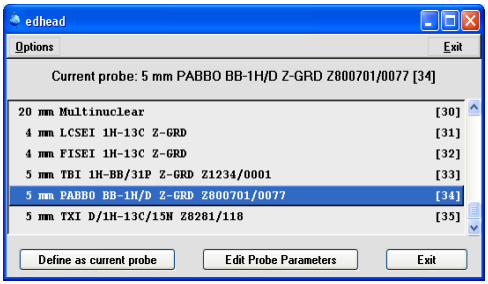
When *expinstall* is finished you can go ahead with the other configuration commands.

- Continue with ***edsolv***



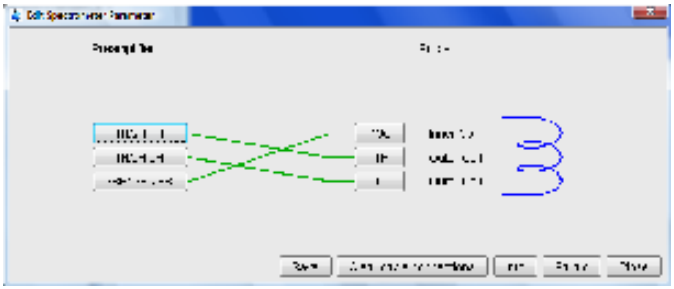
Check the list of lock solvents and click ***Save*** if it is correct → Click ***Close***

- Continue with ***edhead***



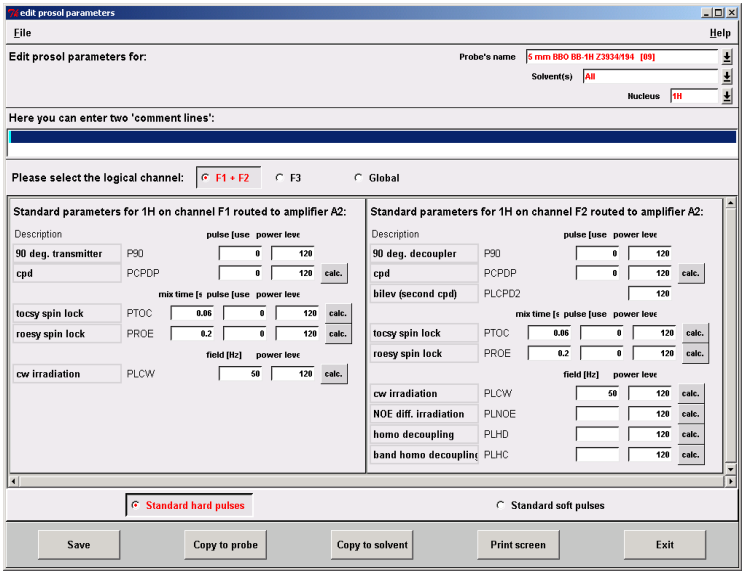
Select the current probe, click the button ***Define as current probe*** → Click ***Exit***

- A window '*Edit Spectrometer Parameter*' will appear:



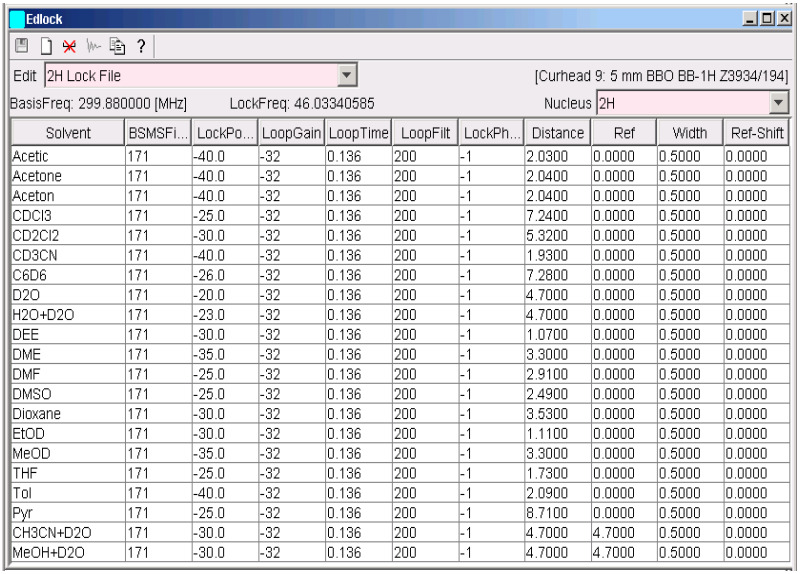
Check if the connections between preamplifier and probe are set correctly → click ***Save*** if it is correct → Click ***Close***

- Continue with ***edprosol***



Check the parameters for your favorite nuclei, change them and calculate them, if necessary → Click ***Save*** to store to disk → Click ***Exit***

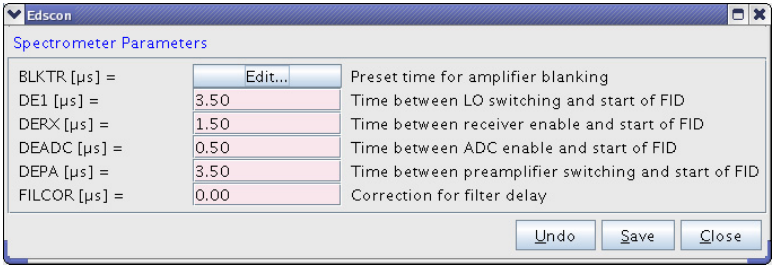
- Continue with ***edlock***



Solvent	BSMSFi...	LockPo...	LoopGain	LoopTime	LoopFilt	LockPh...	Distance	Ref	Width	Ref-Shift
Acetic	171	-40.0	-32	0.136	200	-1	2.0300	0.0000	0.5000	0.0000
Acetone	171	-40.0	-32	0.136	200	-1	2.0400	0.0000	0.5000	0.0000
Aceton	171	-40.0	-32	0.136	200	-1	2.0400	0.0000	0.5000	0.0000
CDCl3	171	-25.0	-32	0.136	200	-1	7.2400	0.0000	0.5000	0.0000
CD2Cl2	171	-30.0	-32	0.136	200	-1	5.3200	0.0000	0.5000	0.0000
CD3CN	171	-40.0	-32	0.136	200	-1	1.9300	0.0000	0.5000	0.0000
C6D6	171	-26.0	-32	0.136	200	-1	7.2800	0.0000	0.5000	0.0000
D2O	171	-20.0	-32	0.136	200	-1	4.7000	0.0000	0.5000	0.0000
H2O+D2O	171	-23.0	-32	0.136	200	-1	4.7000	0.0000	0.5000	0.0000
DEE	171	-30.0	-32	0.136	200	-1	1.0700	0.0000	0.5000	0.0000
DME	171	-35.0	-32	0.136	200	-1	3.3000	0.0000	0.5000	0.0000
DMF	171	-25.0	-32	0.136	200	-1	2.9100	0.0000	0.5000	0.0000
DMSO	171	-25.0	-32	0.136	200	-1	2.4900	0.0000	0.5000	0.0000
Dioxane	171	-30.0	-32	0.136	200	-1	3.5300	0.0000	0.5000	0.0000
EtOD	171	-30.0	-32	0.136	200	-1	1.1100	0.0000	0.5000	0.0000
MeOD	171	-35.0	-32	0.136	200	-1	3.3000	0.0000	0.5000	0.0000
THF	171	-25.0	-32	0.136	200	-1	1.7300	0.0000	0.5000	0.0000
Tol	171	-40.0	-32	0.136	200	-1	2.0900	0.0000	0.5000	0.0000
Pyr	171	-25.0	-32	0.136	200	-1	8.7100	0.0000	0.5000	0.0000
CH3CN+D2O	171	-30.0	-32	0.136	200	-1	4.7000	4.7000	0.5000	0.0000
MeOH+D2O	171	-30.0	-32	0.136	200	-1	4.7000	4.7000	0.5000	0.0000

Check the lock table values (field, lock phase, ...), change them and click ***Save*** if necessary, otherwise click ***Abort***

- Continue with ***edscon***



Check the spectrometer constants, change it and click ***Save*** if necessary, otherwise click ***Cancel***

After ***cf, expinstall***,... have finished, insert a sample and make sure that you can lock on the lock solvent. Type ***ii*** and read with ***rpar*** a standard proton parameter file, type ***getprosol*** and ***rga*** and collect a normal ^{1}H NMR spectrum.

6.2.2 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer. For example the spectrometer is a AV300 configured with the name 'av300'. Do the following.

a) Copy the configuration directory '<TOPSPIN_HOME>/conf/instr/av300' from the spectrometer AV300 to the workstation.

b) On the workstation paste this 'av300' directory to '<TOPSPIN_HOME>/conf/instr'.

(in a default installation this is the path: /opt/topspin/conf/instr)

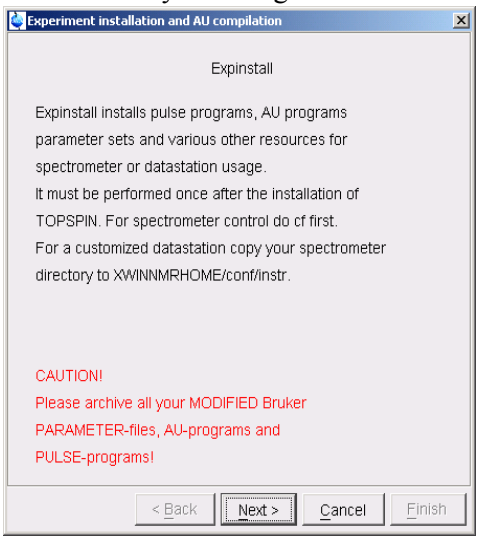
c) Start TOPSPIN as normal user.

d) Perform ***expinstall*** as follows:
Type in the command line ***expinstall*** or
Click ***Open*** → ***Setup*** → ***Experiment Installation*** [***expinstall***]

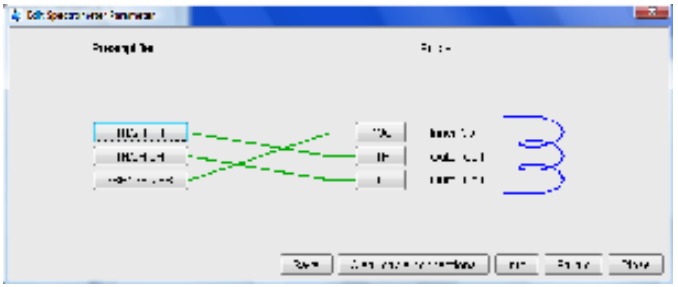
e) Type in the NMR ADMINISTRATION PASSWORD and **ENTER**

f) In the appearing information box → Click ***Next*** if you either have no modified Bruker BioSpin-Parameterfiles, AU-programs and Pulse-programs (If you have some, you have to archive them in a different directory before executing ***expinstall***). Your individual Parameterfiles, AU-programs and

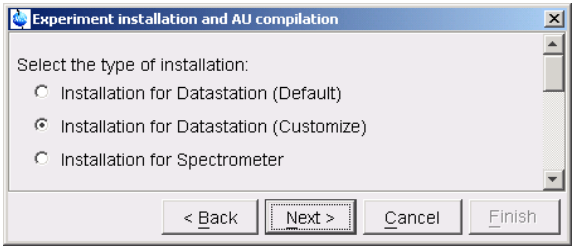
Pulse-programs that have different names to the original Bruker BioSpin files will not be destroyed during the installation



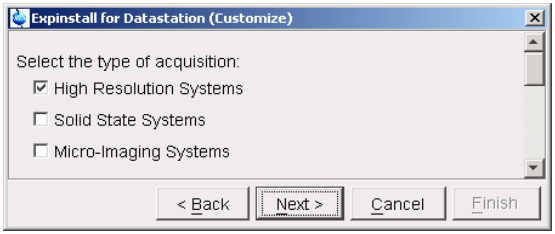
g) In the appearing window → Edit Spectrometer Parameter, check if the connections between preamplifier and probe are set correctly → click ***Save*** if it is correct → Click ***Close***



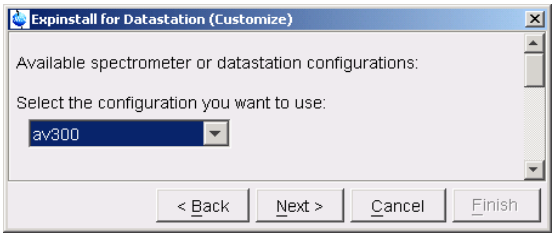
h) In the appearing window → Check *Installation for Datastation (Customize)* → Click ***Next***



i) In the window that appears → Check the boxes of the NMR categories you are interested in[1] → Click ***Next***

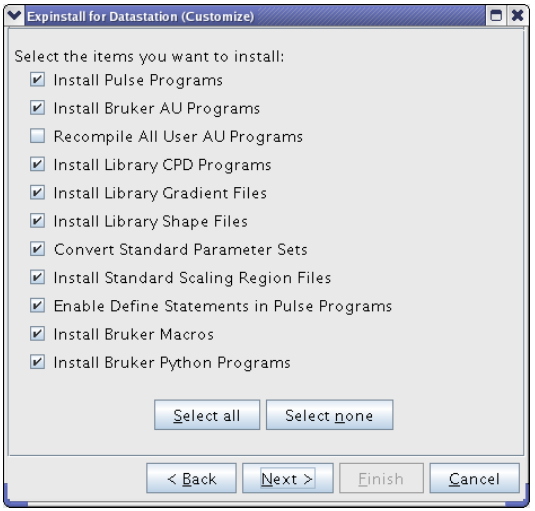


j) In the appearing dialog box → Select the spectrometer configuration name → Click ***Next***

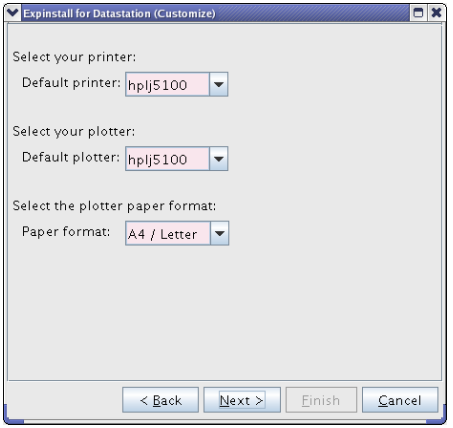


1. This selection defines which parametersets and pulse programs are available for usage after configuration is finished. It is possible to rerun ***`expinstall`*** later to add another selection afterwards

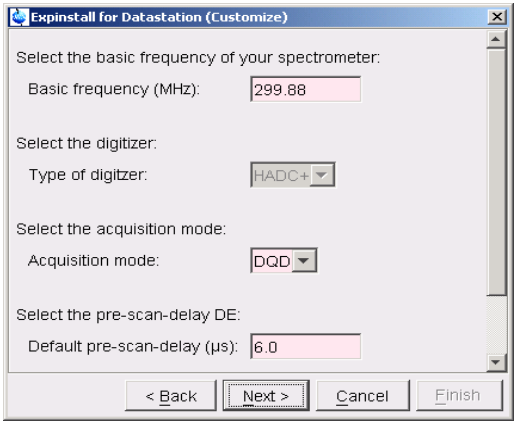
k) In the appearing dialog box → Check the items you want to install or, accept the default selection → Click ***Next***



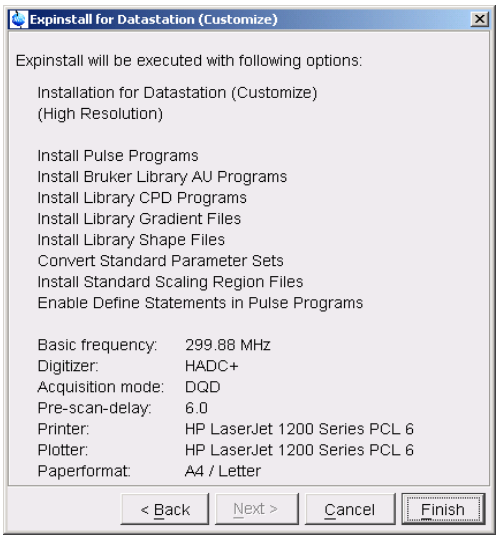
l) In the appearing dialog box → Select the default printer and plotter and the desired paper format → Click ***Next***



m) In the appearing window → Enter the desired spectrometer frequency, acquisition mode and pre-scan-delay or, accept the default values → Click ***Next***



n) In the appearing information box → Check the configuration selection and, if it is correct → Click ***Finish***



The installation of the selected items, will start now. Wait until this process has finished.

For more details on ***expinstall***, please refer to the description of this com-

mand in the Acquisition Reference manual.

6.2.3 If you want to use a default configuration on a datastation

A default configuration can be used on a datastation. It is automatically performed (no ***cf*** required) during the installation of TOPSPIN on a new computer, a new disk or in a new TOPSPIN installation directory. There are two default configuration available *Bruker_default_av500* and *Bruker_default_avi300* which correspond to two different Avance spectrometer.

It is required for a convenient usage of ***TOPSPIN*** to execute ***expinstall*** also in case of a datastation. In this case select *Installation for Datastation (Default)*.

6.2.4 If you do not know the configuration of your spectrometer

If you do not have any spectrometer configuration information, e.g. after a head-crash, then you have to recreate the configuration information.

For this you have to do ***cf*** and give the correct information for the '*Type of Spectrometer*'. You will get the correct list of your hardware in the '*RS232 table*'. You only have to type in the correct tty's of the interfaces.

6.3 Firmware update of the spectrometer hardware

This chapter describes how to update the firmware of certain spectrometer components. This is only necessary if the ***cf*** command has popped up a message window which informs that you have to do a firmware update of a component.

It is strongly recommended to do the firmware update only in this case, because the hardware component could get unusable if the update would be done incorrectly.

If you have further questions according firmware updates, please get in contact with your local Bruker BioSpin office. Addresses of several offices can be found in chapter 17, for contact information about all Bruker BioSpin office please go to our web server:

`http://www.bruker-biospin.de/NMR/about/offices`

6.3.1 Firmware Update for boards without ethernet connection

This chapter describes how to update the firmware for boards without ethernet connection on the example *LCB board*.

If you answer the question about the setting of the default path during the installation of the NMR Suite with ***yes***, you can start the following service tools in a shell by typing their names:

acb

bsms

grad

hpcu

hppr

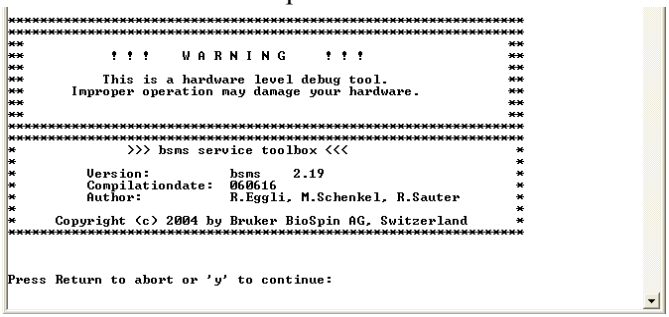
rx22

If you answer ***no*** you have to type in the name with the entire path:

<TOPSPIN_HOME>/prog/bin/scripts/<service-tool-name>

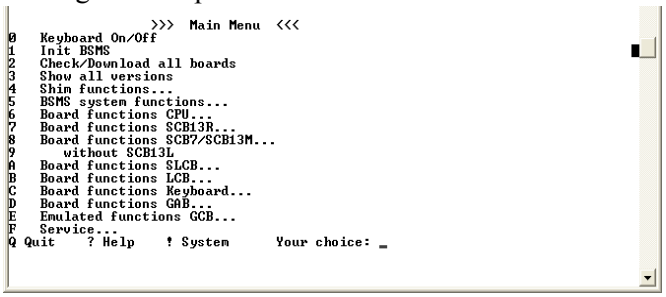
The following example shows the check of the *bsms service tool* with the entire pathname

1. Open a shell
2. Type **<TOPSPIN_HOME>/prog/bin/scripts/bsms**
   - An automatic interactive procedure starts in this shell



3. Type ***y*** → **ENTER**

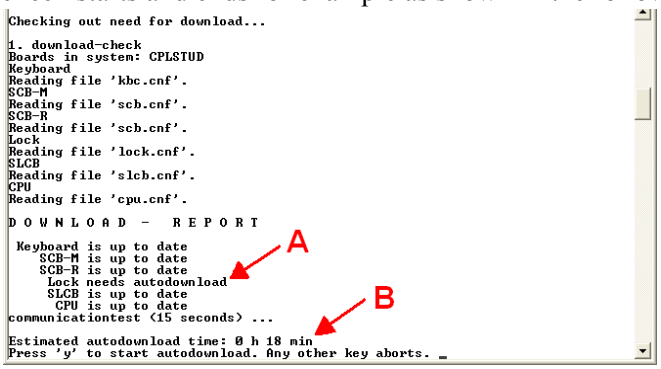
- A dialog comes up in the shell



4. To check and eventually download a new firmware (from TOPSPIN)

- type ***2*** → **ENTER**

The check starts and ends for example as shown in the following picture



if there is a problem with a component you get an information to contact your service office

if you need a firmware update you will get a message (A) with the length of time for the download (B). It is recommended to do the download as soon as possible.

5. Press ***y*** → **ENTER** to start the download

During the download it is absolutely necessary that spectrometer and workstation are not disturbed! Make sure that no one pulls a cable out of the spectrometer or will crash the Linux system while using it in parallel! (Yes we know this seems very improbable, but if the download would crash, your board might be unusable afterwards)

- A 'normal' error during downloading the new firmware (you will see a comment in the shell) requires to do the download once again!

- If you have done a download of newer firmware, you have to do ***cf*** again!
- If you do not need any downloads, you can follow the instructions in the command prompt to exit this tool.

6.3.2 Firmware Update for boards with ethernet connection

This chapter describes how to update the firmware for boards with ethernet connection on the example *ELCB board*. Please note, that the following procedure is only available if you have a spectrometer with boards with ethernet connection.

To check which ethernet connected hardware units are available you can use the TopSpin command ***ha***:

- Open TOPSPIN and enter the command ***ha***. A window appears that shows available hardware modules connected via ethernet.

or the shell command:

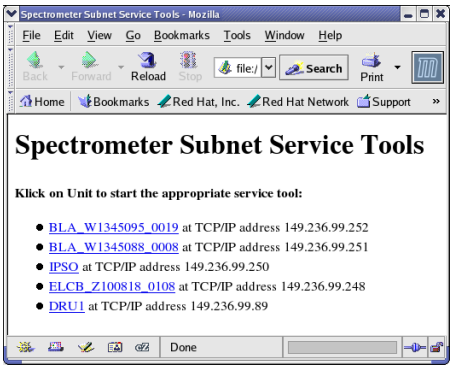
ethernet-service-tools

- Open a shell and enter the commands:

  cd <TopSpin_HOME>/prog/bin

  ./ethernet-service-tools

  A window appears that shows available hardware modules connected via ethernet.

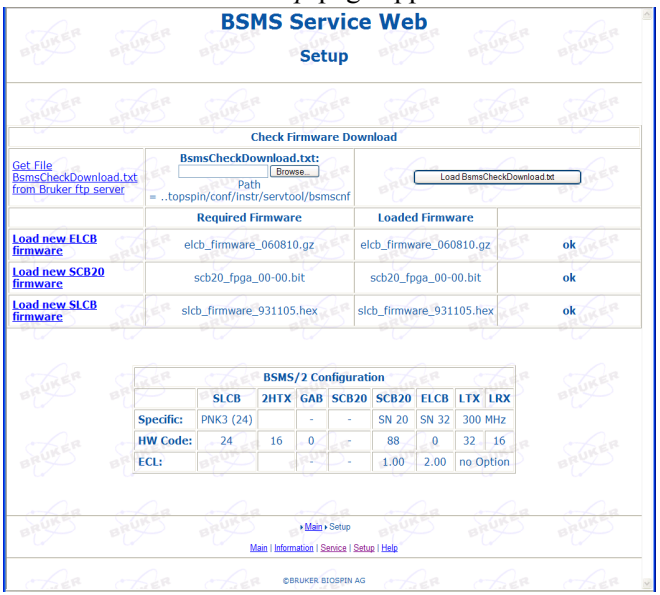


In the following a description is given how to update the firmware for boards with ethernet connection on the example *ELCB* board (BSMS with ELCB board)

1. In either the ***ha*** or **ethernet-service-tools** window click on the name of the hardware device. A browser window will appear with a connection to this device.

2. A window *BSMS Service Web - Main* appears. Click on ***Device Setup***.

3. The *BSMS Service Web - Setup* page appears.



Click on the button ***Browse*** to select the `BsmsCheckDownload.txt` file. In a default installation this file is stored in the directory:
`C:\Bruker\TOPSPIN\conf\instr\servtool\bsmscnf\`

Note: *Selecting* ***Get File BsmsCheckDownload.txt from Bruker ftp server*** *is only necessary if a Bruker Service Engineer recommends to do this.*

4. After the selection click on the button ***Load BsmsCheckDownload.txt***.
5. If a difference is displayed between *Required Firmware* and *Loaded Firmware* please click on ***Load new ELCB firmware***.

6. The *BSMS Service Web - ELCB Firmware Download* page appears.

   Click on the button ***Browse*** to select the firmware version which is mentioned in the line *Select the file...*. In a default installation the file is stored in the directory: `C:\Bruker\TOPSPIN\conf\instr\servtool\bsmscnf\`

7. Click on the button ***install firmware***.

Note: Selecting ***Get File elcb_firmware_XXXXXX.gz from Bruker ftp server*** is only necessary if a Bruker Service Engineer recommends to do this.

The ELCB firmware releases 06xxxx and up are distributed as `*.gz` files.
To be able to load this file format to the ELCB the firmware:

`elcb_firmware_051116.hex`

or newer has to be running on the ELCB. If an older firmware is running first download the `elcb_firmware_051116.hex` distribution.

The `*.gz` file has to be loaded as is, do not unzip it!

6.3.2.1 ELCB board: Save user configuration

You can save the user specific configuration of the ELCB board in a Text file.

1. Please open the *BSMS Service Web* page. Click on ***Service***.

2. The *ELCB Service Web* page appears. Click under *Active User Configuration / Parameters* on ***Save to Disc***.

3. The *BsmsSaveUsrNvm.txt* page appears. Click in the browser window on ***File*** → ***Save as...*** and choose the directory where the file `BsmsSaveUsrNvm.txt`

should be stored.

6.3.2.2 ELCB board: Restore user configuration

1. Please open the *BSMS Service Web* page. Click on ***Service***.

2. The *ELCB Service Web* page appears. Click under *Active User Configuration /*

Parameters on ***Save to Disc***.

3. The *ELCB Service Web* page appears. Under *User Level* you have to enter the *User* and *Password* and click on **Login**.

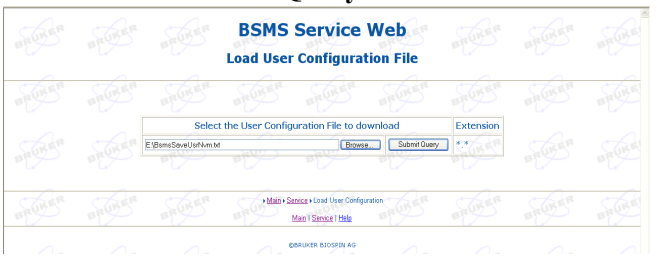
Note: To get these two information please get in contact with your local Bruker BioSpin office. Addresses of several offices can be found in chapter 17, for contact information about all Bruker BioSpin office please go to our web server:

`http://www.bruker-biospin.de/NMR/about/offices`

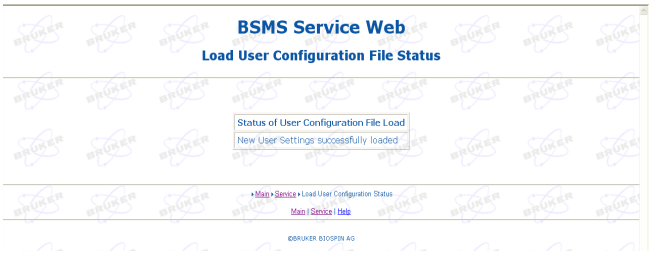
4. The *ELCB Service Web* page will be changed. Under *Active User Configuration / Parameters* click on **Load From Disk**.

5. The *BSMS Service Web - Load User Configuration File* appears. Click on **Browse** to select the user configuration file (`BsmsSaveUsrNvm.txt`) to

download. Click on **Submit Query**.



6. The *BSMS Service Web - Load User Configuration Status* appears. Please check if the *Status of User Configuration File Load* is *New User Settings successfully loaded*.



6.4 A log of the entire system configuration

The ***showconf*** command provides you with various information about your hardware and software, both of the PC and of the spectrometer. Here is how showconf works: You type ***showconf*** in a shell - and wait the about 2 minutes until it has finished. After that showconf has produced a file called `confout` that contains all you need. `Confout` is located in your home directory. The size of this report is usually less then 100 kbytes.

DO KEEP A COPY OF THIS FILE IN A SAFE PLACE!

6.5 Backup of VIFs (=Very Important Files) with nmr_save and user_save (nmr_restore and user_restore)

6.5.1 Introduction

It is not only necessary to create some backups for the operating system like Boot

Disks and to store the acquired datasets.

! It is strictly recommended to create a frequently backup of the 'VIFs' - the 'Very Important Files' - of the configuration of TOPSPIN, in order to make sure to get the information saved and to restore in special cases.

There are many reasons like e.g. head crash or theft of the hard disk that makes it important that a weekly or monthly backup is made of important data, so that you would be able to restore the spectrometer configuration in a very short time.

TOPSPIN offers the command[1] ***nmr_save*** for saving those important files that are not delivered by Bruker BioSpin. With ***nmr_save*** all global files (installation specific files), like spectrometer information, licenses etc. are saved. Even the default directories, listed in the ***Source Directories***, like e.g. '*pp*' and '*pp/user*' are saved. All these global files will be put together into one archive file.

With ***nmr_save*** installation specific files can now be saved periodically at a specific time and date.

Same functions like for nmr_save are even available for user specific files with the command ***user_save***. Only user-specific configuration files will be saved with this command. The additional directories, added by user which are listed in the ***Source Directories***, and the user-specific directory *<USER_HOME>/.topspin-<PC_NAME>/prop* are saved.
All these user-specific files will be put together into one archive file.
The periodic saving function, described below for ***nmr_save*** is also available for ***user_save***.

The commands ***nmr_restore*** and ***user_restore*** respectively restore installation and user-specific files to the same or to a different installation.

6.5.2 How to use nmr_save

nmr_save can be used for saving and restoring configuration information of the ***TOPSPIN*** installation where the command is executed. Furthermore, it is possible to use ***nmr_save*** in one ***TOPSPIN*** installation to backup data from another ***TOPSPIN*** or XWIN-NMR installation.

! In fact, if you have several versions of Bruker software installed in parallel, you

1. Bruker BioSpin also offers a script (*xwinnmr.save*) which can be used for saving the 'VIF's from within a shell or a cronjob (see chapter 16.2).

should always use the ***nmr_save*** command from the highest software version.

If your previous ***TOPSPIN***/XWIN-NMR installation is not located on the same PC, you can even mount the respective network path on your local PC and tell ***nmr_save*** to take over the necessary information over the network.

6.5.3 How to save information with nmr_save

nmr_save can be easily started as follows:

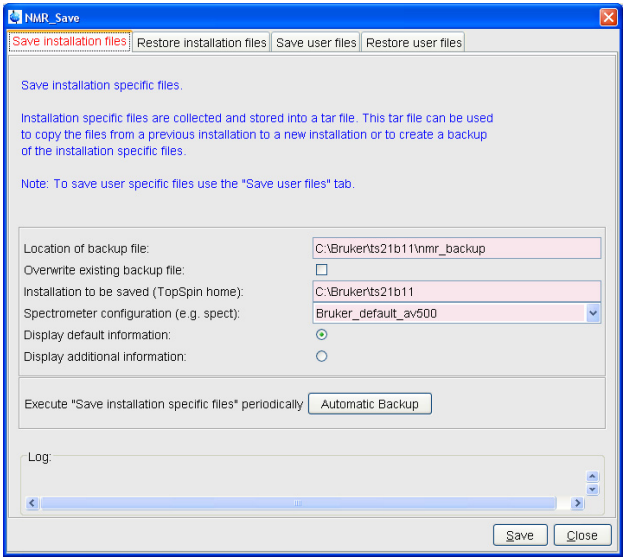
- Start TOPSPIN and type in the command:

  nmr_save

- or start TOPSPIN and click

  Options → Manage Configuration → Save installation Specific files

A window *NMR_Save* will appear.



1. Accept or modify the *Location of Backup file*
   (default is: `<TOPSPIN_HOME>\nmr_backup`).

2. Enter the location of the *Installation to be saved*

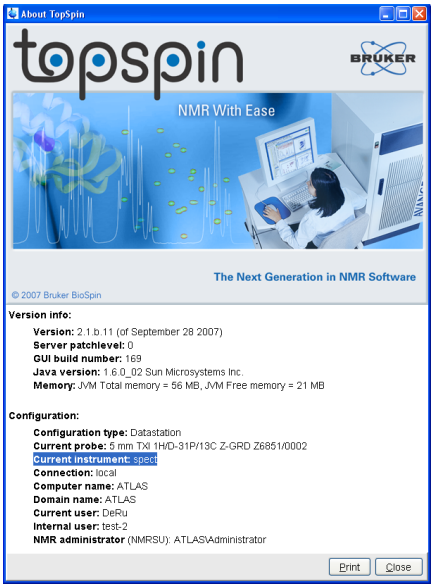
   (default is: <TOPSPIN_HOME>).

3. ***nmr_save*** will then offer a list of all available spectrometer configurations which are located in this respective installation. Select the correct configuration in the field *Spectrometer connfiguration (e.g. spect)*. In a typical setup your spectrometer configuration is called *spect*.

   In a typical installation three configuration names will be listed here, your current instrument name and the two Bruker default configurations, *Bruker_default_avanceII300* and *Bruker_default_av500*.

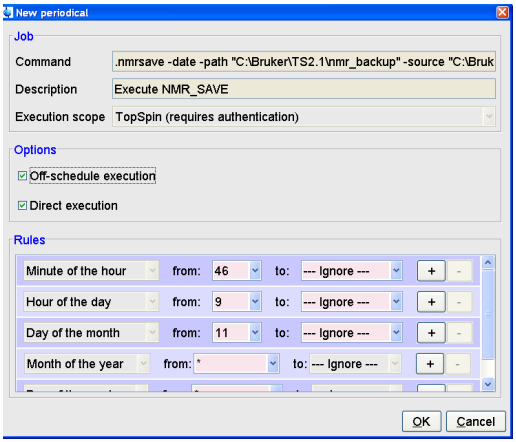
   If you are in doubt about the name of your current spectrometer configuration exit the nmr_save window and enter the ***TOPSPIN*** command ***about***. You can find the name of your current configuration in the upcoming window under *Configuration* → *Current Instrument*.

   Start ***nmr_save*** again. Now you can select the correct Spectrometer name.



TOPSPIN even saves your installation specific files automatically. If you want to execute „Save installation specific files“ periodically please click on the Button ***Automatic Backup***. This action will open a new window for a command schedul-

ing. Clicking ***OK*** will accept the default values an execute ***nmr_save*** once in a month.



This Automatic Backup functionality is offered by the TopSpin command **cron** described below.

4. Now you can click on ***Save***.

This will create an archive file of all necessary information from the selected installation/spectrometer configuration. This file is called
`nmr_backup_<data>-<time>.tar`
(e.g. `nmr_backup_20071910-2348.tar`
and is stored in the directory you selected above, typically:

`<TOPSPIN_HOME>\nmr_backup`

Shortly defined the command cron allows TOPSPIN executing a command periodically at a specific time/date.

- It is possible to define „*User*“ or „*TOPSPIN*“ commands. Latter one will be executed independent of the user who currently works with TOPSPIN.
- The functionality „off-schedule“ offers that the last one of a series which cannot be executed because TopSpin did not run, would be performed when TopSpin is started next time.

The command ***cron*** performs command scheduling. It allows to execute commands periodically at predefined date/time in planned intervals. These intervals

can be defined user-specifically or by default. It offers full flexibility in time definition, off-schedule execution and user control. Here you can specify the command to be scheduled, some scheduling options and the starting time and date. The following fields are available:

1. ***Command***: The command to be executed.
2. ***Description***: A description of the command.
3. ***Execution scope***: The scope of the command execution, *User* of *TOPSPIN*. For scope *User*, the scheduled command will only be executed if TOPSPIN is running by the same user that is active during cron definition. If the scope is *TOPSPIN*, the scheduled command will be executed for any user. Scheduled command with *TOPSPIN* execution scope can only be defined, cancelled or modified after entering the Administration password.
4. ***Off-schedule execution***: this flag allows you to execute commands that were scheduled to run at the time when TOPSPIN was off. These commands are executed after the next TOPSPIN startup.
   Please note that commands that were scheduled to run multiple times during TOPSPIN downtime are only executed once.

The following time scheduling rules exist:

- Minute of the hour: betwenn 00 and 59
- Hour of the date: between 00 and 23
- Month of the year: January to december
- Day of the week: Sunday to saturday

For each of these fields, you can define an interval by selecting a value in the *From* and a value in the *To* field. Setting the *To* field to ***Ignore*** schedules the command for execution only at the time/date selected in the *From* field. An asterix (*) in the *From* field indicates all possible times. Clicking the „+“ button to the right of a filed, adds an extra field of the same type, allowing multiple interval definition. Clicking the „-“ button removes the extra field.

6.5.4 Which information is stored with nmr_save?

nmr_save archives some directories completely, in some other directories only specific files. Files that start with an "." are ignored. The internal ***TOPSPIN*** database for pulse and cpd programs, macros and python scripts is saved completely. Which information is stored with nmr_save can be found below.

The following directories are saved completely (hidden files are ignored!):

<TOPSPIN_HOME>/conf/instr/autoshim/refmaps/

<TOPSPIN_HOME>/conf/instr/probeheads/

<TOPSPIN_HOME>/conf/instr/<spect>/prosol/

<TOPSPIN_HOME>/conf/instr/<spect>/cortab/

<TOPSPIN_HOME>/conf/instr/<spect>/inmrusers/

<TOPSPIN_HOME>/conf/instr/topshim/parameters/user

<TOPSPIN_HOME>/conf/instr/topshim/solvents/user

<TOPSPIN_HOME>/data/final/nmr/protocolfiles/

<TOPSPIN_HOME>/exp/stan/nmr/lists/best-nmr/user/subset/fi

<TOPSPIN_HOME>/exp/stan/nmr/lists/best-nmr/user/subset/lc

<TOPSPIN_HOME>/exp/stan/nmr/lists/bsms/

<TOPSPIN_HOME>/exp/stan/nmr/lists/ds/

<TOPSPIN_HOME>/exp/stan/nmr/lists/eurotherm/corr

<TOPSPIN_HOME>/exp/stan/nmr/lists/eurotherm/tcf

<TOPSPIN_HOME>/exp/stan/nmr/lists/f1/

<TOPSPIN_HOME>/exp/stan/nmr/lists/group/

<TOPSPIN_HOME>/exp/stan/nmr/lists/scm/

<TOPSPIN_HOME>/exp/stan/nmr/lists/vc/

<TOPSPIN_HOME>/QTP/

<spect> represents the current spectrometer name or the user-specified name that was explicitly chosen when ***nmr_save*** is started.

From the following directories every file is saved that does not belong to the genuine Bruker BioSpin distribution:

<TOPSPIN_HOME>/conf/instr/servtool/bsmstool/boss

<TOPSPIN_HOME>/conf/instr/topshim/spect

<TOPSPIN_HOME>/conf/instr/topshim/probeheads

<TOPSPIN_HOME>/exp/stan/nmr/lists/gp/

<TOPSPIN_HOME>/exp/stan/nmr/lists/wave/

<TOPSPIN_HOME>/exp/stan/nmr/au/scl/

<TOPSPIN_HOME>/exp/stan/nmr/au/src/

<TOPSPIN_HOME>/exp/stan/nmr/par/

<TOPSPIN_HOME>/exp/stan/nmr/parx/preemp

```
<TOPSPIN_HOME>/plot/layouts/
<TOPSPIN_HOME>/prog/tcl/xwish3_scripts/
```

Additionally, the following files are also saved:

```
<TOPSPIN_HOME>/conf/instr/selpulse.*
<TOPSPIN_HOME>/conf/instr/probehead
<TOPSPIN_HOME>/conf/instr/<spect>/2Hlock
<TOPSPIN_HOME>/conf/instr/<spect>/19Flock
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/CurrPushSolvent
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/hardware.par
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/hardware.src
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/racks.use
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/scanner.src
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/solvents.add
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/solvents.par
<TOPSPIN_HOME>/conf/instr/<spect>/best-nmr/solvents.use
<TOPSPIN_HOME>/conf/instr/<spect>/hardware_list
<TOPSPIN_HOME>/conf/instr/<spect>/nuclei
<TOPSPIN_HOME>/conf/instr/<spect>/rs232_device/best
<TOPSPIN_HOME>/conf/instr/<spect>/rs232_device/bestscan
<TOPSPIN_HOME>/conf/instr/<spect>/specpar
<TOPSPIN_HOME>/conf/instr/<spect>/uxnmr.par
<TOPSPIN_HOME>/conf/instr/<spect>/uxnmr.info
<TOPSPIN_HOME>/conf/global/layoutsearchpath
<TOPSPIN_HOME>/exp/stan/nmr/lists/probeheads
<TOPSPIN_HOME>/exp/stan/nmr/lists/solvents
<TOPSPIN_HOME>/prog/logfiles/heliumlog
<TOPSPIN_HOME>/prog/logfiles/heliumlog.err
<TOPSPIN_HOME>/prog/server/export.conf
<LM_LICENSE_FILE>[1]
```

For safety reasons the tar-file will be saved in a directory ***nmr_backup_<date>-***

1. This is the environment variable for the license file, in a default installation this is: `/usr/local/flexlm/Bruker/licenses/license.dat`

time.tar. This file contains date and time of saving, so that overwriting the tar-file is not possible easily and the data are always available. Please note that *Overwriting existing backup file* is only possible by saving data twice in the same minute. It is recommended that all data are backuped on a different Server or CD to prevent for a motherboard-crash.

6.5.5 How to restore informations saved with nmr_save

Note that this will overwrite your complete ***TOPSPIN*** configuration plus spectrometer configuration. Restore from a backup file only if you are absolutely sure that this is necessary. If in doubt do not restore or at least create a backup of the current state before.

Start TOPSPIN and type in the command:

```
nmr_restore
```

or click

Options → Manage Configuration → Restore installation specific file

A window *NMR_Save* will appear.

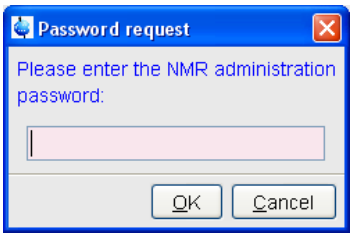
1. Enter the path where you archive file is stored in the field *Location of Backup file*

   (default is: `<TOPSPIN_HOME>\nmr_backup`).

2. Enter the location of the *restore destination*

   (default is: `<TOPSPIN_HOME>`)

3. Click on ***Restore***
   A window *Password request* will appear:



Please enter the NMR administration password and click ***OK***.

4. Execute the ***TOPSPIN*** command ***cf***

6.5.6 How to use user_save and user_restore

Similar to the function ***nmr_save*** and ***nmr_restore*** that saves and restores installation specific files, the commands ***user_save*** and ***user_restore*** save and restore user-specific data in a TAR-file. These commands save and restore all user-specific data listed in the directory
Options → Preferences → Manage source directories for edpul, edau etc.
and
<USER_HOME>/.topspin-<PC_NAME>/prop

The periodic-saving-function avilable with the command cron is also available for ***user_saved-*** and ***user_restored*** data. The TAR-file will be written in the following directory:
nmr_backup_<username>-<date>->time>.tar

For saving and restoring data with user_save and user_restore the same steps like for ***nmr_save*** and ***nmr_restore*** have to be executed.
Please note that for restoring data with user_restore the *NMR administration password* is not recommended. Furthermore all data that are restored with ***user_restore*** are archived in one central directory `user_backup`, not in the individual directories where they have been read from with ***user_save***. So user-specific configuration files can be taken from one PC to another.

6.5.7 How to read the archive file

Although the archive file created by nmr_save is a tar file, it should not be opened or read with the tar command. It is packed in a special procedure and the only correct way of extracting the file is the TopSpin command ***nmr_save***!

If you like to have a look at the content of an archive file or copy just some files from it, you should extract the archive into a temporary directory, e.g. /tmp/backup-test. Then you can check and copy the extracted files from there.

6.5.8 Is all information restored in their original places?

No, the *license* file, the *heliumlogfile* and the *heliumlog.err* file are restored in a different directory, because the current ones should not be overwritten. If you want

to reuse the restored files you can find them in the restore destination you have chosen, in the subdirectory conf/instr with the extension *.backup*

All other files are restored in their original places.

Chapter 7

Plotting and Printing with TopSpin

7.1 Printing / plotting data

7.1.1 Plotting and printing

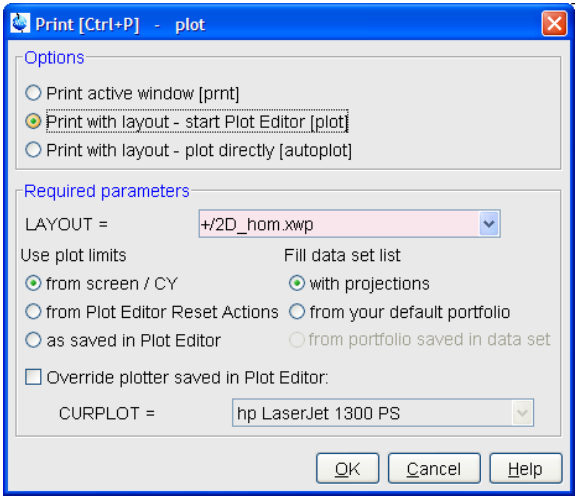
Under RED HAT ENTERPRISE LINUX WS 4, all common printer drivers can be used for plotting and printing. When a printer is installed under RED HAT ENTERPRISE LINUX WS 4, it can be used for plotting from TOPSPIN and TOPSPIN PLOT EDITOR.

7.1.2 Print/Plot from the Menu

The current data window can be printed as follows:

1. From the TOPSPIN menu:
   - Click the print button in the upper toolbar
   - or Click **File** → **Print**
   - or Enter ***print*** or ***Crtl-p***

All these actions are equivalent; they open the Print dialog box.



2. In the Print dialog box:

- Select ***Print active window [prnt]***
- Click ***OK***

Before printing starts, the operating system print dialog box will appear to select e.g. the printer and printer properties.

The Print dialog box contains two further options:

- ***Print with layout - start Plot Editor [plot]***

  If you select this option and click OK, the Plot Editor will be started. This option is equivalent to entering plot on the TOPSPIN command line.

- ***Print with layout - plot directly [autoplot]***

  Selecting this option activates the Plot Editor layout list box. Select the desired layout and click ***OK*** to print. Standard layouts are delivered with TOPSPIN. They use the Windows default printer. User defined layouts use the printer defined in the TOPSPIN PLOT EDITOR. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

For each of the last two options one of the following parameters is required.

Use plot limits:

- ***from screen/ CY***

  The processing parameter CY and the x-axis limits as they are displayed

in TOPSPIN are used

- ***from Plot Editor Reset Actions***

  The plot limits and maximum intensity are set according to the TOPSPIN PLOT EDITOR Reset Actions (right-click inside the TOPSPIN PLOT EDITOR data field and choose *Automation* to set the *Reset Actions*).

- ***as saved in Plot Editor***

  The plot limits and maximum intensity are set in the specified layout

Fill dataset list:

- ***from your default portfolio***

  The portfolio contains the current TOPSPIN dataset plus the data from the default Plot Editor portfolio

- ***from port folio saved in dataset***

  The portfolio contains the current TOPSPIN dataset plus the data from the portfolio stored in this dataset

Override plotter saved in Plot Editor:

Allows choosing a different plotter than defined in the Plot Editor layout. This is a temporary setting only, the plotter definition in the layout will stay unchanged.

7.1.3 Plot data from the Processing guide

Printing/plotting data can be done from the Processing guide by clicking the ***Plot/Print*** button. If ***Automatic mode*** is checked, the active data window will be printed as it appears in the screen. If ***Automatic mode*** is unchecked, you will get the dialog box.

7.1.4 Plot data with the TOPSPIN PLOT EDITOR

Although the ***print*** command allows you to use or start the TOPSPIN PLOT EDITOR, you can also start it from the command line (enter ***plot***). This will open the TOPSPIN PLOT EDITOR from which you can create layouts and plot data. The complete TOPSPIN PLOT EDITOR functionality is described in its online manual that can be opened from the TOPSPIN PLOT EDITOR Help menu.

7.1.5 Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type, e.g. .png, .tif, .wmf etc. To do that:

1. Click **Edit → Export**
2. Navigate to the storage folder
3. Enter the destination filename and extension
4. Click ***Export***

The resolution of such a screen dump equals the resolution of your screen. When you import a graphics file into an other program, you may loose information when resizing the graphics.

7.1.6 TOPSPIN PLOT EDITOR

1. TOPSPIN PLOT EDITOR uses the printer driver system of the operating system for any printer output. This means that any printer for which a system driver is correctly installed can be selected as print device. Note that the printer name in a layout file written by the Windows XP version is probably not known by the Linux version of TOPSPIN PLOT EDITOR because of the different printer handling. Apart from that, layout files can be freely interchanged between the two platforms.
2. Another way of exporting graphics is the menu option *File/Print* which allows you to print the complete layout into a file. The format can be choosen from a list (e.g. PostScript, Epsi, PDF, JPEG, PCX, PNG or TIFF). Most current graphical-oriented windows applications can import this format. This provides a convenient way of importing TOPSPIN PLOT EDITOR graphics into programs like Word or Powerpoint.
3. With the TOPSPIN PLOT EDITOR you can directly send your current plot as Email. Just click **File → Send** and TOPSPIN PLOT EDITOR will pop-up your default mail client and add the current plot as an EMF attachment.

Chapter 8

User Management

8.1 Adding a new user account

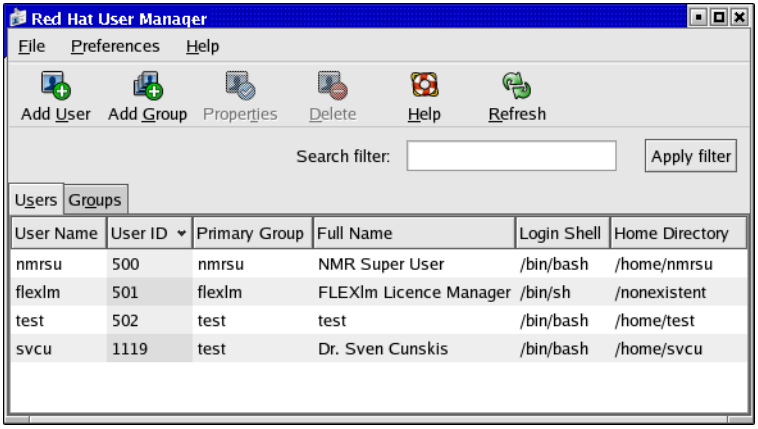
If you want to add a new user[1] and this new user already exists on other hosts in the network, make sure that you use the same *User ID* and *User Name* on all hosts in the network. It is also useful to use the same *Group ID* and *Group Name,* especially, if you want to mount directories via NFS between IRIX and Linux systems.

Perform the following steps:

1. Click **<red hat> → System Settings → User and Groups**
2. If you are not logged in as root, a window *run as root - KDE su* will appear
   - enter root password

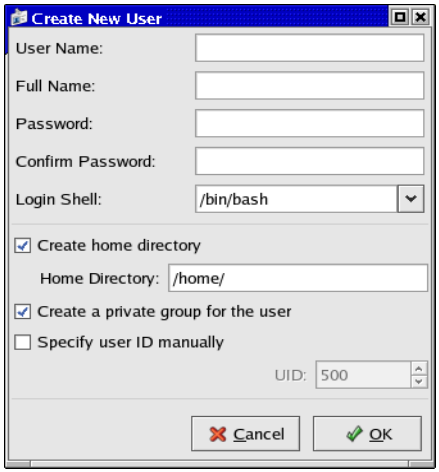
1. The default configurations of a new user are copied from `/etc/skel/` into the home directory of the new user. If you want to change the default informations, e.g. by adding an icon that starts ***TopSpin*** copy the respective file into `/etc/skel/`

3. A window *KDE User Manager* will appear:



- Click **Add User**

4. A window *Create New User* will appear



- Enter the new **User Name**
- Enter **Full Name** of the new user
- Enter and confirm the **password**
- Make sure that **Create home directory** is enabled and that a legal path is entered in the field **Home directory**. The default */home/* will create the home directory:

/home/<USER_NAME>

- The field **Create a private group of this user**:

  a) enabled (default):

  This configuration in conjunction with the default umask (002) will lead to the situation, that only the user is able to write in those files he created with the ***TopSpin***. That means no other user could work with his spectroscopic data.

  b) disabled:

  New user will be assigned to the group **users**

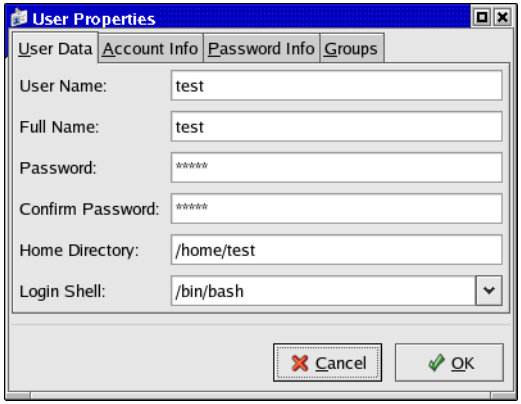
  This configuration in conjunction with the default umask (002) will lead to the situation, that the user and all members of the group *users* are able to write in those files he created with the ***TopSpin***. That means all other users of his/her group can work with his spectroscopic data.

- Enable the field *Specify user ID manually* if necessary (see introduction of this chapter) and type in the desired ID of the new user
- click **OK**

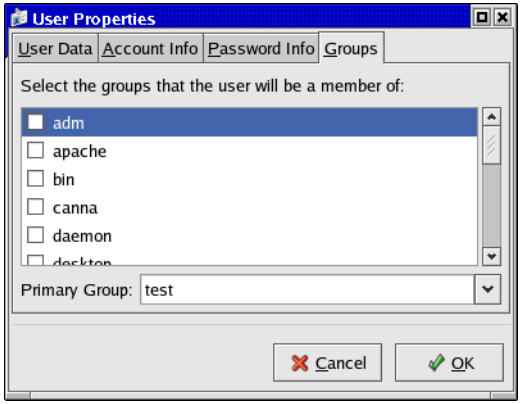
8.1.1 Change group membership of an existing user

1. Click **<red hat> → System Settings → Users and Groups**
2. If you are not logged in as root, a window *run as root - KDE su* will appear
   - enter root password
3. A window *KDE User Manager* will appear:
   - Click on an existing user and click on **Properties**

4. A window *User Properties* will appear:



- Click on **Groups**



You will see in the appearing window the field Primary Group that shows the original group of the user.

- In the field *Select the groups that the user will be a member of* you can now add the user to other groups simply by selecting the respective field of the list of group(s)
- Click **OK**

Part II

RED-HAT Enterprise Linux WS 4 Installation-Tips and Configuration

Chapter 9

RED HAT Enterprise Linux WS 4

9.1 Hints for installation of Red Hat

A Linux NMR workstation purchased from Bruker BioSpin comes with a pre-installed Linux distribution, currently RED HAT ENTERPRISE LINUX WS 4.

If you want to install Red Hat by yourself, Bruker BioSpin recommends to use the installation guide of the Red Hat Documentation CD. This offers, in different languages, a very easy and detailed description of all necessary steps. Those steps which are recommended by Bruker BioSpin are listed below, for all other configuration steps you can choose your personnel settings.

9.2 Scratch installation of Desktop computer

1. Start the installation of RED HAT ENTERPRISE LINUX WS 4 as described on the Red Hat Documentation CD
2. In the window *Mouse Configuration*:

   select your mouse (the default *generic mouse* might not support all features) (e.g

select *Microsoft Intellimouse* if you have a wheel mouse, otherwise the middle button will not work correctly)

3. In the window *Disk Partitioning Setup* choose **Manually partition with Disk Druid**
4. In the window *Partitioning*:

   Bruker BioSpin recommends to create the following partitions on a 80GB hard-disk. For all these partitions you should select the button: **Force to be a primary partition** and as **File System Type** ‚*ext3*[1]‘:

   a) a partition **/boot** with 125MB size
   b) a partition **/** with 16GB size
   c) define the swap partition **/swap** with 4GB size by selecting *swap* as **File System Type**
   d) a partition **/opt** should use the remaining space (enable **Fill to maximum allowable size**)
5. In the window *Boot Loader Configuration* accept the default *Use GRUB as the boot loader*
6. In the window *Network Configuration* disable *Active on Boot* for *eth1* if your PC does not control a spectrometer (e.g. notebook or workstation).

   If the PC is controlling a spectrometer you should select *Active on Boot* for eth1. Additionally you can click on *Edit* of eth1 and configure it for spectrometer control. For this you can type in the IP address and subnet mask:

   !

   IP-address (eth1): 149.236.99.1

   Subnet mask (eth1): 255.255.255.0

   The hostname should be created by DHCP (if available). Changing the hostname to another name can be done in the installed system, see chapter 10.2
7. In the window *Firewall*, select the firewall configuration you prefer.

   If you select other than *No Firewall* and the installation is for spectrometer control, you have to enable your spectrometer communication for full access. Click on ***eth1*** in the section:

   If you would like to allow traffic from a device, select it below

1. ext3 file system is a journaling filesystem. The advantage of a journaling filesystem is, that an accidental power off would not end in most cases to a file system check and missing data.

! Note: Bruker BioSpin does not support SElinux at the moment. Therefor it is required to choose *Disable* in the section *Enable SELinux*!

8. In the window *Timezone Selection*:

   it is necessary to configure the *Location*, but do not enable *System clock uses UTC*

9. In the window *Package Defaults*:

   we recommend to select: *Customize the set of packages to be installed*

   and in the following window *Package Group selection*

   scroll down to the end of the list and select **Everything**[1]

10. During the installation process, you will be asked to insert all four installation CDs one after the other. After finishing with the fourth CD you will be asked to insert the first CD once again.
11. The window **Congratulations** appears and informs you about a successful installation. You have to remove the CD and press **Exit**, this will reboot the PC.
12. When the system is coming up again, a window *Welcome* appears
13. You have to accept the license agreement, to adjust date and time and you will be asked for creating a non-administrative user account.
14. In the window *Red Hat Network* you can select to register at the Red Hat Network right now (**Yes, ...**) or you can choose **No...** in case you have currently no network connection etc.
15. A window *Additional CDs* appear

    On HP computers it is necessary to install the drivers/update CD that can be downloaded from the HP web side

    http://welcome.hp.com/country/us/en/support.html

    Enter there the type of your PC (e.g. xw4300 for the currently delivered HP xw 4300) and follow the instructions of the following pages.

    If you have the correct CD for your PC available or any other CD that should be installed now (e.g. a Red Hat Extras CD), you have to insert the respective CD then click on the **Install...** button right to the text *Additional CDs*

16. You will be guided trough the installation process
17. After finishing the installation process of the HP driver/update CD you will be

1. This installation requires about 4GB space on the harddisk

asked to reboot now or later. In case you want to install further CDs it is recommended to click on reboot later, because otherwise this process is stopped.

18. After finishing this installation you can start ***TopSpin*** installation (see chapter 2.2 for a brief description or chapter 4.3 for a detailed description)

9.3 Installation of additional Red Hat packages on already installed systems

If you have done the full installation of RED HAT ENTERPRISE LINUX WS 4 as it is described in chapter 9.2, the packages described in this chapter are already installed and you can skip this chapter.

If you want to prepare an already installed RED HAT ENTERPRISE LINUX WS 4 system for TOPSPIN, you have to make sure that the following packages are available:

Package	available on ...	Necessary for
acrobat reader	*https://rhn.redhat.com/network* and *RHEL WS 4 Extras CD*	documentation viewer
nfs-utils	*https://rhn.redhat.com/network* and *Operating System CD **2** of 4*	acquisition
glibc-kernheaders	*https://rhn.redhat.com/network* and *Operating System CD **3** of 4*	compiling AU programs
glibc-devel	*https://rhn.redhat.com/network* and *Operating System CD **3** of 4*	compiling AU programs
uucp	*https://rhn.redhat.com/network* and *Operating System CD **4** of 4*	acquisition

For an installation description see the following chapters. For more information about useful packages, please refer to chapter 15.3.1.

Please note that with RED HAT ENTERPRISE LINUX WS 4 there is no easy to use graphical tool for installation of individual programs (rpm-files) which are available e.g. on the operating system CD. Several different possibilities for installation of individual programs are available, in the following chapter a description of the most easy and safe procedure is given. It requires that your Linux system is connected to the internet and you have a your system already subscribed at Red Hat. For more details about this please see chapter 15.8.

If you are not connected to the internet you can install the respective rpms with the browser *nautilus*. To do this open a shell, enter the command **`nautilus`**, click on **Places → Computer → CD drive → RedHat → RPMS** and double click the respective filename. You have to enter the root password and then the installation process starts.

The installation of each of the packages listed above is described in an individual chapter. Of course you can also install all packages in one step just by selecting all of them in step 11.

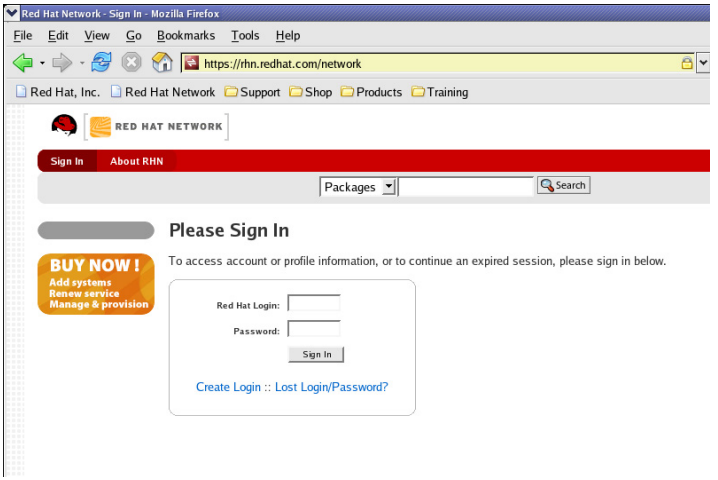
9.3.1 Additional packages for documentation view - Acrobat Reader

The software packages *acroread* is necessary if you wants to open manuals from the ***Help*** menu of TOPSPIN.

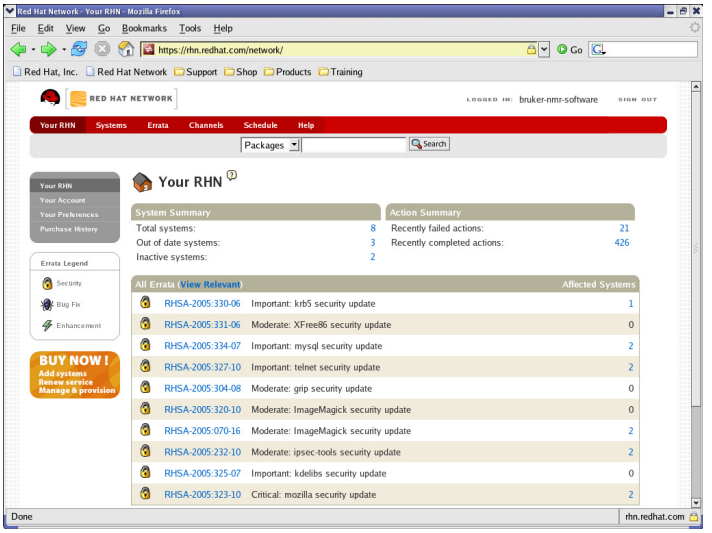
1. Check if *acroread* is installed so far
   - Open a shell and type in: **`rpm -q acroread`**
   - is the output like this: *`acroread-<version-number>`*
   - Yes? You can skip this chapter
   - No? Go to step 2.
2. Open a web browser and go to:

   https://rhn.redhat.com/network
3. A web page appears which asks you to login as registered user. Enter your Red

Hat Network user name and password.[1]

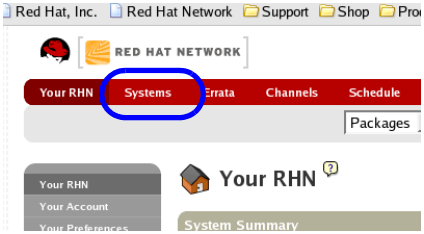


You will now enter your individual Red Hat network area



1. For details about the registration at Red Hat Network see chapter 15.8.1

4. Click on *Systems*



The list of systems which are registered for your individual Red Hat network account appears

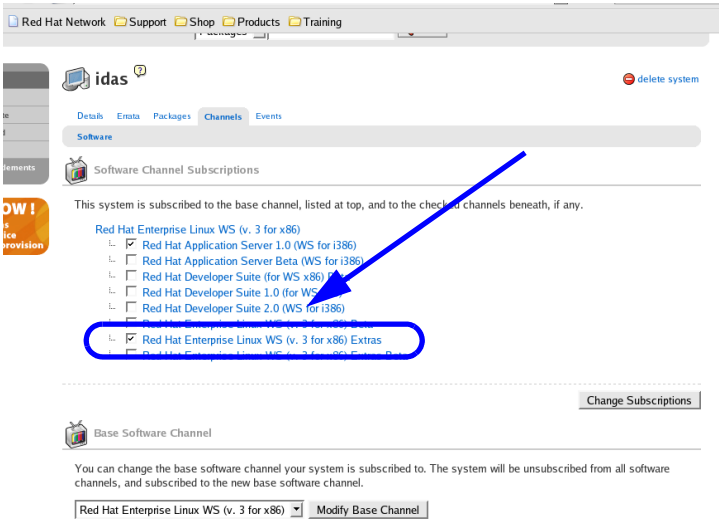
5. Click on the name of the system you want to install the acroread package

   The summary of this system appears

6. Click on *Alter Channel Subscriptions*

   The page switches to the defined *Base Software Channel* and possible *Software Channel Subscriptions*.

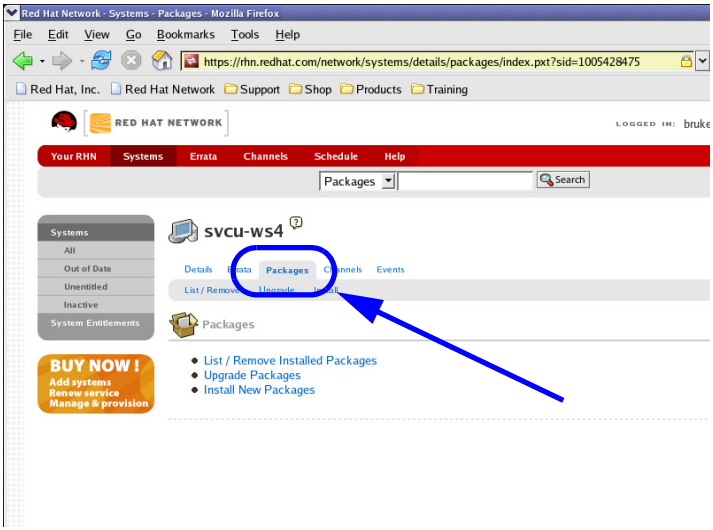
7. Make sure that *Red Hat Enterprise Linux WS (v. 4 for x86) Extra* is checked.



8. If you have checked this field for the first time you have to click on:

   Change Subscription

9. Click on *Packages*



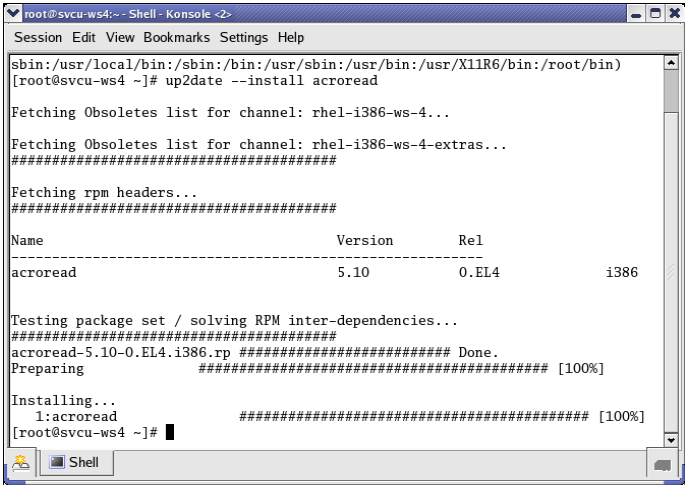
10. Click on *Install New Packages*
11. Select all packages which starts with *acroread*. In case you do not want to install any plugins select the main program *acroread-<version_number>* only.
12. Scroll down to the end of the page and click on *Install Selected packages*
13. You get a summary of all selected packages, click *Confirm* to start installation.

    Installation will need a few seconds. After it is finished you can see the word *Done* in the lower left corner of the window.
14. Go to a shell and login as root with the command

    `su -`

    enter your root password
15. Enter the command

up2date --install acroread



Acrobat reader has now been installed, you can start it from a shell with the command **acroread** or create a icon on the desktop to start the program (for details see chapter 15.7). It will automatically opened when you open a manual from within TOPSPIN.

9.3.2 nfs-utils

The software package *nfs-utils* is necessary if the PC controls a spectrometer.

1. Check if *nfs-utils* is installed so far
   - Open a shell and type in:

     rpm -q nfs-utils
   - is the output like this

     nfs-utils-<version-number>
   - Yes? You can skip this chapter
   - No? Go to step 2.
2. Open a web browser and go to:

   https://rhn.redhat.com/network
3. A web page appears which asks you to login as registered user. Enter your Red Hat Network user name and password.[1]

You will now enter your individual Red Hat network area

4. Click on *Systems*

   The list of systems which are registered for your individual Red Hat network account appears

5. Click on the name of the system you want to install the acroread package

   The summary of this system appears

6. Click on *Alter Channel Subscriptions*

   The page switches to the defined *Base Software Channel* and possible *Software Channel Subscriptions*.

7. Make sure that *Red Hat Enterprise Linux WS (v. 4 for x86) Extra* is checked.

8. If you have checked this field for the first time you have to click on:

   Change Subscription

9. Click on *Packages*

10. Click on *Install New Packages*

11. Select *nfs-utils-<version_number>*

12. Scroll down to the end of the page and click on *Install Selected packages*

13. You get a summary of all selected packages, click *Confirm* to start installation.

    Installation will need a few seconds. After it is finished you can see the word *Done* in the lower left corner of the window.

14. Go to a shell and login as root with the command

    `su -`

    enter your root password

15. Enter the command

    `up2date --install nfs-utils`

The package *nfs-utils* has now been installed.

9.3.3 Additional packages for compilation of AU programs

The packages *glibc-kernheaders* and *glibc-devel* are necessary for compilation of AU programs.

---

1. For details about the registration at Red Hat Network see chapter 15.8.1

1. Check if *glibc-kernheaders* and *glibc-devel* are installed so far
   - **rpm -q glibc-kernheaders**
   - **rpm -q glibc-devel**
   - is the output like this

     glibc-kernheaders-<version-number>

     glibc-devel-<version-number>
   - Yes? You can skip this chapter
   - No? Go to step 2.
2. Open a web browser and go to:

   https://rhn.redhat.com/network
3. A web page appears which asks you to login as registered user. Enter your Red Hat Network user name and password.[1]

   You will now enter your individual Red Hat network area
4. Click on *Systems*

   The list of systems which are registered for your individual Red Hat network account appears
5. Click on the name of the system you want to install the acroread package

   The summary of this system appears
6. Click on *Alter Channel Subscriptions*

   The page switches to the defined *Base Software Channel* and possible *Software Channel Subscriptions*.
7. Make sure that *Red Hat Enterprise Linux WS (v. 4 for x86) Extra* is checked.
8. If you have checked this field for the first time you have to click on:

   Change Subscription
9. Click on *Packages*
10. Click on *Install New Packages*
11. Select *glibc-kernheaders-<version_number>*
12. Select *glibc-devel-<version_number>*
13. Scroll down to the end of the page and click on *Install Selected packages*

1. For details about the registration at Red Hat Network see chapter 15.8.1

14. You get a summary of all selected packages, click *Confirm* to start installation.

    Installation will need a few seconds. After it is finished you can see the word *Done* in the lower left corner of the window.

15. Go to a shell and login as root with the command

    `su -`

    enter your root password

16. Enter the commands

    `up2date --install glibc-kernheaders`

    `up2date --install glibc-devel`

The packages *glibc-kernheaders* and *glibc-devel* have now been installed.

9.3.4 uucp

The software package *uucp* is necessary if the PC controls a spectrometer.

1. Check if *uucp* is installed so far
   - Open a shell and type in:

     `rpm -q uucp`
   - is the output like this

     `uucp-<version-number>`
   - Yes? You can skip this chapter
   - No? Go to step 2.
2. Open a web browser and go to:

   https://rhn.redhat.com/network
3. A web page appears which asks you to login as registered user. Enter your Red Hat Network user name and password.[1]

   You will now enter your individual Red Hat network area
4. Click on *Systems*

   The list of systems which are registered for your individual Red Hat network account appears

1. For details about the registration at Red Hat Network see chapter 15.8.1

5. Click on the name of the system you want to install the acroread package

   The summary of this system appears

6. Click on *Alter Channel Subscriptions*

   The page switches to the defined *Base Software Channel* and possible *Software Channel Subscriptions*.

7. Make sure that *Red Hat Enterprise Linux WS (v. 4 for x86) Extra* is checked.
8. If you have checked this field for the first time you have to click on:

   Change Subscription

9. Click on *Packages*
10. Click on *Install New Packages*
11. Select *uucp-<version_number>*
12. Scroll down to the end of the page and click on *Install Selected packages*
13. You get a summary of all selected packages, click *Confirm* to start installation.

    Installation will need a few seconds. After it is finished you can see the word *Done* in the lower left corner of the window.

14. Go to a shell and login as root with the command

    `su -`

    enter your root password

15. Enter the command

    `up2date --install uucp`

16. The package *uucp* has now been installed.

9.4 Check if all necessary components are installed and active

To check if all necessary components are installed and active, please type

`/sbin/chkconfig --list`

in a shell and compare the output with this example

```
nfs             0:off   1:off   2:on    3:on    4:on    5:on    6:off
nfslock         0:off   1:off   2:off   3:on    4:on    5:on    6:off
bootparamd      0:off   1:off   2:on    3:on    4:on    5:on    6:off
```

If an entry is off, you can activate it in general:

```
/sbin/chkconfig <service> on
```

If an entry is off, you can activate it for a specific runlevel:

```
/sbin/chkconfig --level <runlevel> <service> on
```

for example to start bootparamd at runlevel 5:

```
/sbin/chkconfig --level 5 bootparamd on
```

With **chkconfig** command you define (permanently) which service will be started/not started on which runlevel after the next reboot. It does NOT activate/deactivate the respective service, instantly.

For a temporary activation/deactivation of a process you have to use the command:

```
service <service> start/stop
```

There are mostly more possibilities for the different services like reload, restart ... . To get a list which possibilities are available just type in

```
service <service>
```

A service which is listed below xinet.d can be started with the chkconfig command immediately. e.g. the command

```
chkconfig smb-swat on
```

will turn on samba swat immediately, it is neither necessary to reboot nor to use the *service* command.

9.5 Dual Boot computer

It is possible to configure a PC in a dual boot mode, so that you can decide during boot time if you like to start Windows or Linux. This is not a necessary feature for spectrometer PC's and Bruker BioSpin does not recommend to configure the PC in dual boot mode.

Chapter 10

Network configuration

10.1 Configuring the laboratory network

The easiest way to add a Linux PC to a laboratory network is using *DHCP* (**D**ynamic **H**ost **C**onfiguration **P**rotocol). It allows you to go online just by defining the hostname. The IP address, name- and mailserver will be created dynamically. Please contact your network administrator to find out whether DHCP is the right choice for you, or whether a fixed TCP/IP address is to be assigned to your PC. Because the licensing of ***TopSpin*** and many other programs and operating system features needs a correct network configuration there are three ways to do this:

1. Those PC's which are configured by Bruker BioSpin Germany are set to DHCP. If this configuration can be used the PC should be connected to the network before the boot process starts. After the PC is coming up the network works correctly and ***TopSpin*** can be started.
2. If the PC should connected to the network by using a fix IP address you have to ask your system administrator for it. After the correct configuration the network works correctly and ***TopSpin*** can be started
3. If the PC should not get a network connection it is necessary to work with a neutral IP address e.g. 192.168.1.1. This address is not routed to any network computer by world-wide-agreement. If you configure this number you will not have a connection to any other computer (internet) but ***TopSpin*** can be started.

10.2 Changing the hostname of the PC

The hostname of the PC is defined within the network configuration. Because there are different possibilities how to set up a network correctly (DHCP, fix IP address or no network connection) there is no general description on how to change the hostname.

If you want to change the hostname just follow the instructions given in the chapters 10.4 - 10.6.

Changing the hostname may has an effect on programs. For the Bruker BioSpin software you might have to check these two places:

1. In case the PC is a license server the name of the PC is stored in the license.dat file that is stored in the flexlm installation directory. In a default installation this is:

   `/usr/local/flexlm/Bruker/licenses/license.dat`

   If this PC acts as a license server and you changed the license file, you have to be sure that the respective file is changed in the same way on all license clients.

2. The user specific configuration is stored in the directory:

   `<USER_HOME>/.topspin-<PC_NAME>`

   To keep the individual ***TopSpin*** configuration in case the computer name was changed, rename these directories.

10.3 Some useful commands

There are two commands that allows to easily check if network is set up correctly:

`hostname` and **`hostname -f`**

`hostname` has to show the short name of the PC, e.g. *nmrpc* and

`hostname -f` has to show the full qualified name e.g. *nmrpc.chemistry.university.com.* If the answers are not as described, something is wrong with your network configuration. Because the Linux system reacts very sensitive on wrong network configuration, you might get several problems, e.g. ***TopSpin*** does not start, spectrometer will not boot, the ***TopSpin*** license can not checked out etc..

A convenient command for checking the functionality of the ethernet cards is

`/sbin/mii-tool`

The output of this command shows a list of all ethernet cards and gives the information if the connection is working properly or not.

If a ethernet card is not able to be activated in the graphical tool, you can use the following commands (in this example for ‚eth0‘):

```
service network restart
ifdown eth0
ifup eth0
```

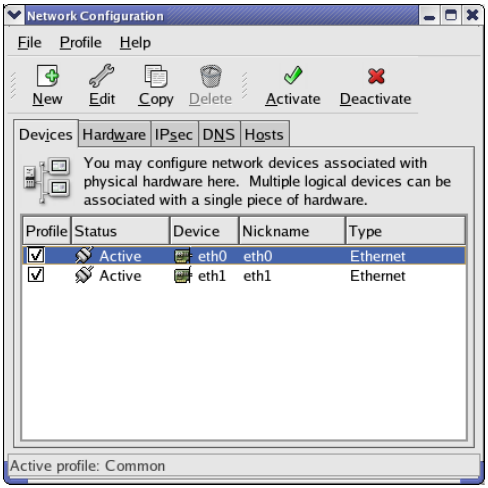
10.4 Configuring the laboratory network by DHCP

1. Click **<red hat> → System Settings → Network** [1]

   a window *Query* will appear and asks for the root password

   - enter root password

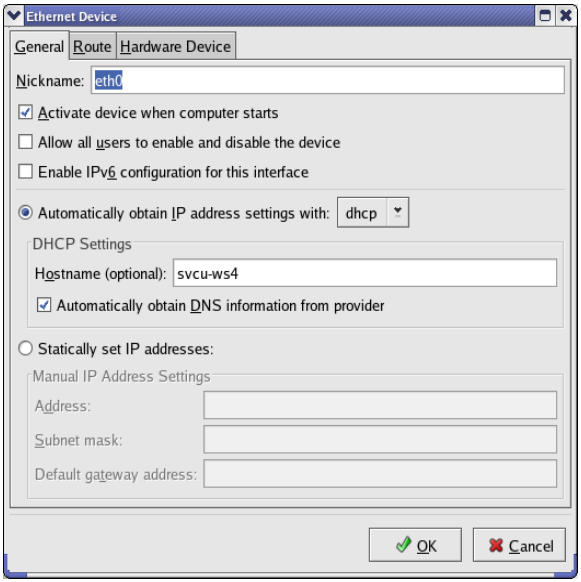
2. A window *Network Configuration* will appear



   - On the tab pane **Devices** click on *eth0* and click **Edit** . Note that it is necessary to use *eth0* for your internet connection, because *eth1* is required for your spectrometer network connection.

1. The shell command for starting the network configuration is: **system-config-network** or simply **neat**

3. A window *Ethernet Device* will appear

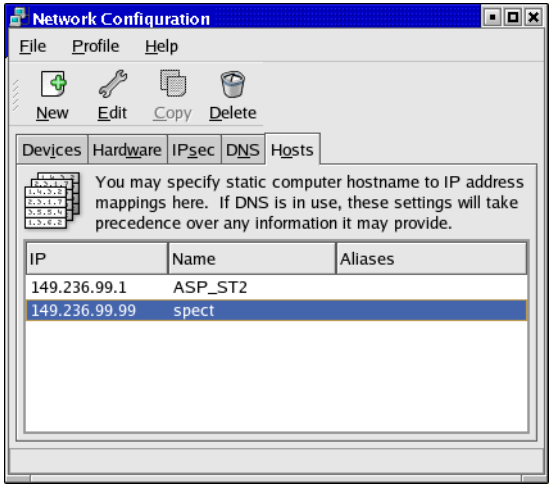


- select the field:
  Activate device when computer starts
- select the field:
  Automatically obtain IP address settings with:
  and click the little arrow to the right of this field and select:
  dhcp

!

- enter the hostname of the PC in the field *Hostname (optional)*
- Contact your network administrator to get the information if you can check the field *Automatically obtain DNS information from provider*
- click **OK**

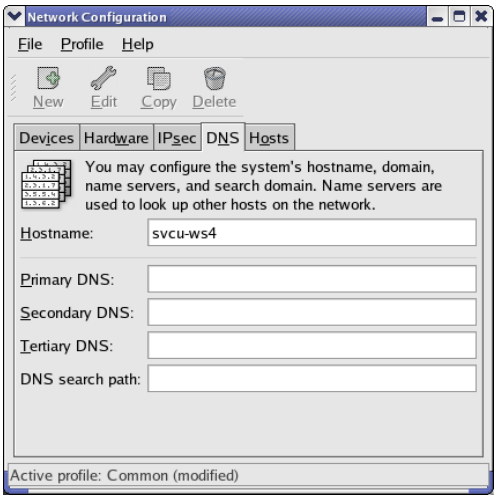
e) In the window *Network Configuration* click on the tab pane *Hosts*[1]



- Either this entry is correct and was visible in previous Linux versions, you will not see here an entry *127.0.0.1* / Name: *localhost.localdomain* / Nickname: *localhost* The operating system controls this entry and does not show it here in this interface. Nevertheless you can check the file `/etc/hosts` to get the information if this entry is there or not.
- Be sure that there is NO entry with the name of this PC. If there is one highlight it and click on **Delete**
- The two entries that can be seen in the picture are necessary for the spectrometer connection. If this PC does not control a spectrometer they are not necessary.

1. This information is stored in the file */etc/hosts*
This file contains also the line: *127.0.0.1 localhost.localdomain localhost*
This is required information and must not be deleted / modified!

f) Click on the tab pane *DNS* [1]



- enter the hostname without the domainname into the field *Hostname* [2]
- click **File → Save**
- click **File → Quit**

Note that the information given here are very important. In case wrong names/addresses are entered here network calls might end in long time-outs which can cause e.g. acquisition problems.

10.5 Configuring the laboratory network by using a fixed TCP/IP address

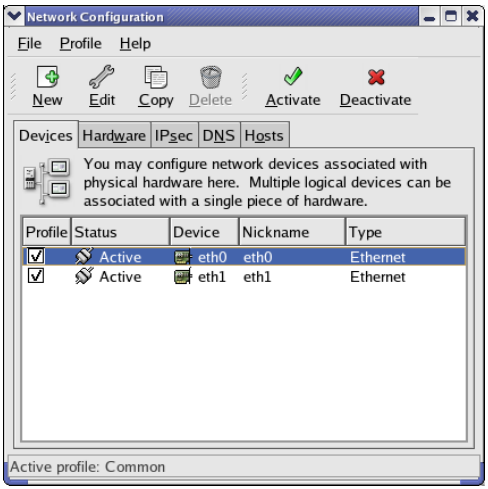
1. Click **<red hat> → System Settings → Network** [3]

a window *Query* will appear and asks for the root password

- enter root password

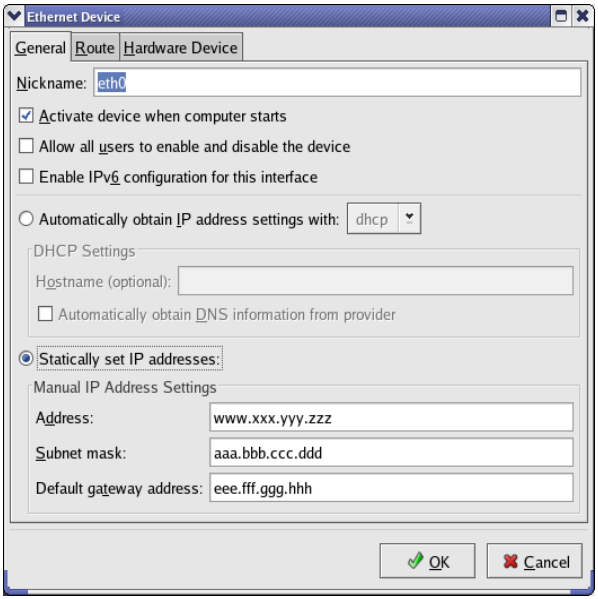
1. The information given in this tab is stored in the file */etc/resolv.conf*
2. In this field you have to enter the hostname only, without domainnames, i. e. only *nmrpc* and not *nmrpc.chemistry.university.com*
3. The shell command for starting the network configuration is: **redhat-config-network** or simply **neat**

2. A window *Network Configuration* will appear



- On the tab pane **Devices** click on *eth0* and click **Edit** . Note that it is necessary to use *eth0* for your internet connection, because *eth1* is required for your spectrometer network connection.

3. A window *Ethernet Device* will appear



- select the field:

Activate device when computer starts

- select the field:

  Statically set IP addresses

  and type in the

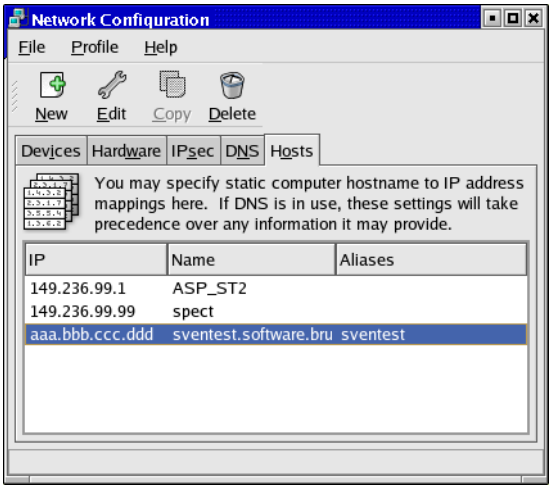
  IP address,

  Subnet mask and

  Default Gateway Address

  that should be used from this PC (if you do not know them, contact your network administrator)
- click **OK**

g) In the window *Network Configuration* click on the tab pane *Hosts*[1]



- click **Add** and create an entry for the IP address of this PC. The Name has to be the full qualified domain name like this:

  nmrpc.chemistry.university.com

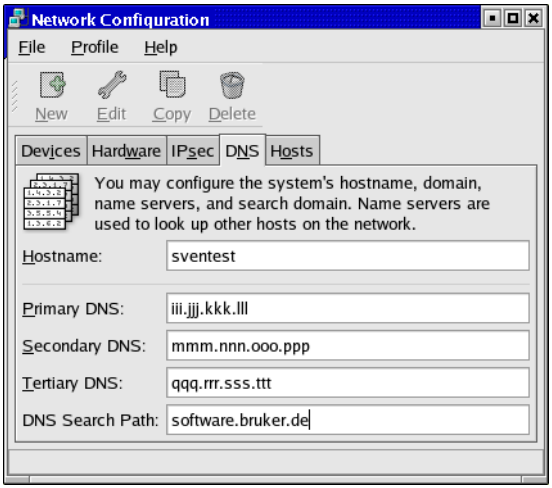
  and the Nickname:

  nmrpc

1. This information is stored in the file */etc/hosts*
This file contains also the line: *127.0.0.1 localhost.localdomain localhost*
This is required information and must not be deleted / modified!

- The two entries *ASP_ST2* and *spect* that can be seen in the picture are necessary for the spectrometer connection. If this PC does not control a spectrometer they are not necessary.

h) Click on the tab pane *DNS* [1]



- enter the hostname without the domainname into the field *Hostname* [2]
- enter the domain name in the field *DNS Search Path*
- click **File → Save**
- click **File → Quit**

Note that the information given here are very important. In case wrong names/addresses are entered here network calls might end in long time-outs which can cause e.g. acquisition problems.

Remember, that the network administrator must enter your new host on the nameserver.

1. The information given in this tab is stored in the file */etc/resolv.conf*
2. In this field you have to enter the hostname only, without domainnames, i. e. only *nmrpc* and not *nmrpc.chemistry.university.com*

10.6 Spectrometer PC that should not be connected to the laboratory network

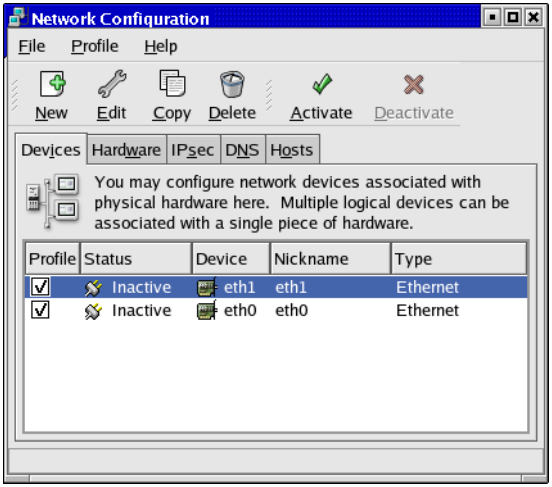
In case the spectrometer PC should not be connected to the laboratory network, it is nevertheless necessary to configure a kind of 'virtual network'.

1. Click **<red hat> → System Settings → Network** [1]

   a window *Query* will appear and asks for the root password

   - enter root password

2. A window *Network Configuration* will appear



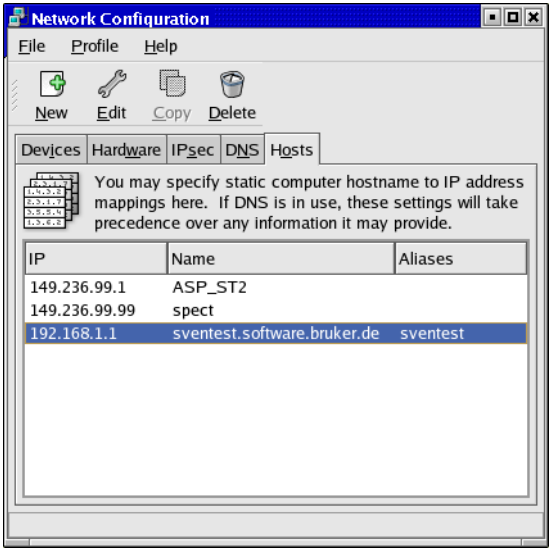
   - On the tab pane **Devices** click on *eth0* and click **Edit** . Note that it is necessary to use *eth0* for your internet connection, because *eth1* is required for your spectrometer network connection.

1. The shell command for starting the network configuration is: **redhat-config-network** or simply **neat**

3. A window *Ethernet Device* will appear

- select the field:
  Activate device when computer starts
- select the field:
  Statically set IP addresses
  and enter in the field:
  Address:
  192.168.1.1
  and in the field:
  Subnet Mask:
  255.255.255.0
- click **OK**

i) In the window *Network Configuration* click on the tab pane *Hosts*[1]



- Either this entry is correct and was visible in previous Linux versions, you will not see here an entry *127.0.0.1* / Name: *localhost.localdomain* / Nickname: *localhost* The operating system controls this entry and does not show it here in this interface. Nevertheless you can check the file `/etc/hosts` to get the information if this entry is there or not.
- click **Add** and create an entry for the IP address of this PC. The Name has to be the full qualified domain name like this:

  nmrpc.chemistry.university.com

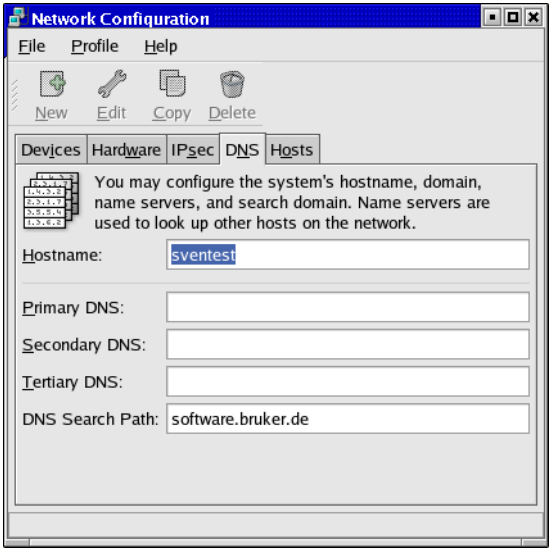
  and the Nickname:

  nmrpc
- The two entries that can be seen in the picture are necessary for the spectrometer connection. If this PC does not control a spectrometer they are not necessary.

---

1. This information is stored in the file */etc/hosts*
This file contains also the line: *127.0.0.1 localhost.localdomain localhost*
This is required information and must not be deleted / modified!

j) Click on the tab pane *DNS* [1]



- enter the hostname without the domainname into the field *Hostname* [2]
- enter the domain name in the field *DNS Search Path*
- leave the DNS fields empty
- click **File → Save**
- click **File → Quit**

Note that the information given here are very important. In case wrong names/addresses are entered here network calls might end in long time-outs which can cause e.g. acquisition problems.

10.7 Configuring the spectrometer network

! The network configuration for spectrometer control will be done automatically in case the ethernet card is not yet configured. This configuration will be done by the *Diskless* package that is part of a ***TopSpin*** installation. The description of the fol-

1. The information given in this tab is stored in the file */etc/resolv.conf*
2. In this field you have to enter the hostname only, without domainnames, i. e. only *nmrpc* and not *nmrpc.chemistry.university.com*

lowing chapter can be used for checking the configuration.

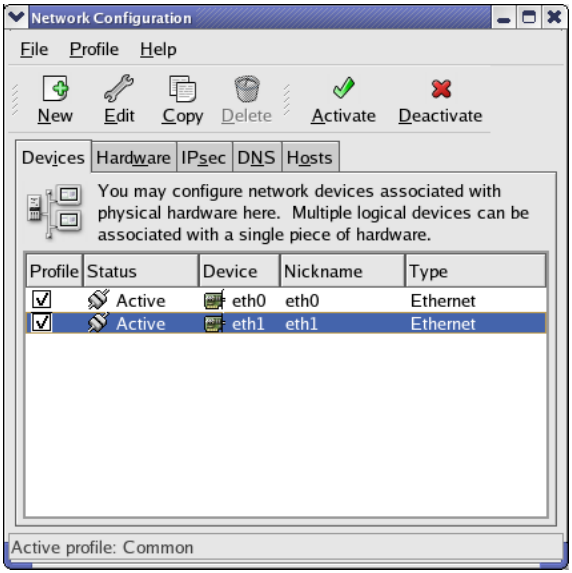
10.7.1 Configuration of the spectrometer network

1. Click **<red hat> → System Settings → Network** [1]

   a window *Query* will appear and asks for the root password

   - enter root password

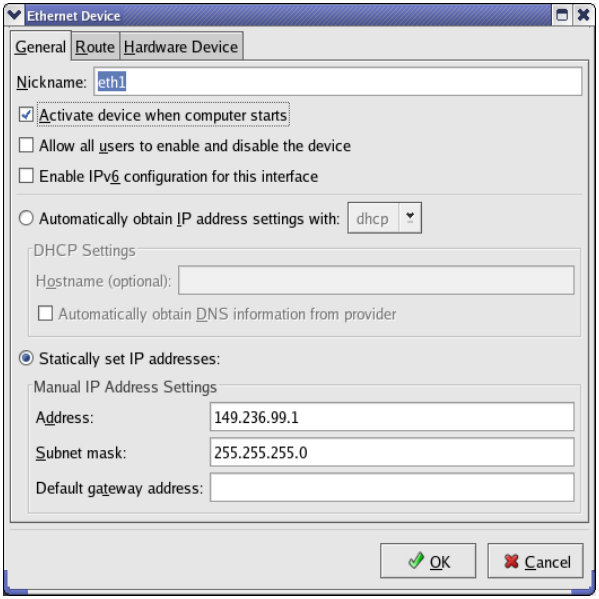
2. A window *Network Configuration* will appear



   - click on *eth1* which is the ethernet card you have to use for the spectrometer network connection and click **Edit**

1. The shell command for starting the network configuration is: **redhat-config-network** or simply **neat**

3. A window *Ethernet Device* will appear



- be sure that the field *Activate Interface at boot time* is checked[1]
- be sure that the field *Allow any user to (de)activate interface* is not checked

- select the field:

  Statically set IP address

  and enter in the field:

  Address:

  149.236.99.1

  and in the field:

  Subnet Mask:

  255.255.255.0

- click **OK**

k) In the window *Network Configuration* click on the tab pane *Hosts*[2]

1. On notebooks it might be useful to disable the *Activate Interface at boot time* function. This will avoid waiting for time outs during boot process, if there is no network connection.
2. This information is stored in the file */etc/hosts*

- be sure that there are the following entries:

IP	Name	Nickname
149.236.99.1	ASP_ST2	<whatever>
149.236.99.99	spect	<whatever>

If one of them is missing click **New → Add** and create it

- click **File → Save**
- click **File → Quit**

10.8 Nameserver configuration

In case there are some problems with the network, e.g. the name server is not available, everything on the desktop seems not to react anymore. In fact any activity takes a very long time.

The reason for this could be that DNS resolver does not work anymore due to network problems. To check this press the buttons *Ctrl-Alt-F1*, login as *root* and enter the command **`host <ENTER_NAME_OF_YOUR_PC>`**. If the answer is something like:

;;connection timed out no servers could be reached

the PC has lost the name server connection.

To make sure that the PC will not as easily run again into such trouble enable caching name services. *‚nscd‘* is the necessary package is which is typically installed. To enable *nscd* do the following:

1. Open a Linux shell

2. Type in **`su -`** to become superuser

3. Enter the command: **`chkconfig nscd on`**

If this does not work you have to install the *nscd* package, this can be done either with the command *up2date nscd* or by installing it from the Red Hat CD. For more details about installing packages see chapter 9.3.

After installing the package you should configure the caching delay. For this edit

the file */etc/nscd.conf* and search for the line:

positive-time-to-life hosts 3600

Change the value to:

positive-time-to-life hosts 260000

This will remember the name for about three days (~a weekend).

This information is also available form the Bruker Knowledge Base item 5762:

http://www.bruker-biospin.de/shell/bkb/show_bug.cgi?id=5762

10.9 Network diagnostic commands

Here is a list of the most important network diagnostic commands as they can be entered from the shell:

- **`arp`** - displays or modifies the IP to physical address translation tables
- **`hostname`** - displays the short name of the current host
- **`hostname -f`** - displays the full qualified name of the current host
- **`host IP`** - displays the name that is connected with this IP
- **`ifconfig`** - displays information about the current TCP/IP configuration
- **`netstat`** - displays protocol statistics and current TCP/IP connections
- **`ping`** - checks if a destination host is receiving TCP/IP packets
- **`route`** - maintains and displays routing tables
- **`traceroute`** - displays the route, packets take to a destination host
- **`mii-tool`** - list all ethernet cards and show if they work or not

For more details about commands you can enter either:

```
man <command>
```

or

```
<command> --help
```

10.10 Accessing remote files and directories

10.10.1 Necessary Samba packages and configurations

To use samba it is necessary to install at the package *smb* and for the graphical configuration the package *smb-swat*. To allow access and configuration both packages must be enabled. To check this open a shell, login as root with the command ‚**su -**‘ and enter:

```
chkconfig --list smb
```

Typically the service is off and the answer is something like this:

smb 0:off 1:off 2:off 3:off 4:off 5:off 6:off

```
chkconfig --list swat
```

Typically the service is off and the answer is something like this:

swat off

To turn on these services enter

```
chkconfig smb on
```

and

```
service smb start
```

and

```
chkconfig swat on
```

For more details about the commands *chkconfig* and *service* see chapter 9.4

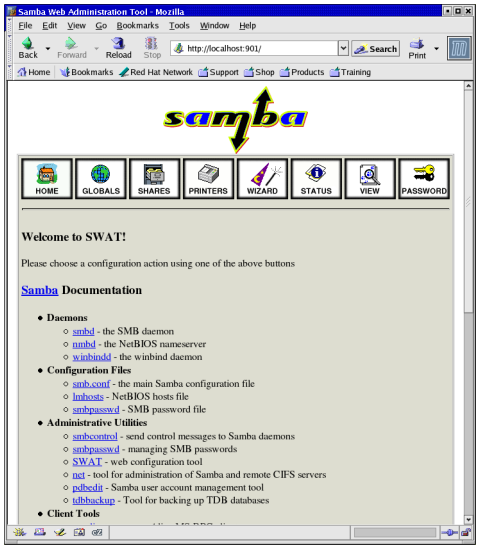
10.10.2 Sharing directories from a Linux host using Samba

If you are logged in on a Windows 2000/XP host, you can access data which reside on a Linux host, using the sharing mechanism. This, however, only works if the Samba package is installed on the Linux host (see chapter 15.3).
After installation of Samba is done, you can configure it with SWAT (Samba Web Administration). This tool can be started from your Web Browser, e.g.:

<red hat> → Internet → Firefox Web Browser

by entering the address: *http://localhost:901*/

You will be asked for username and password. For configuration of SWAT it is necessary to login as root. Other users are neither able to see the whole information nor can change it!



There you have to define:

- the **password** and the **user** for configuration in the **Password** section
- the **workgroup** in the **GLOBALS** section
- the **directories** you want to share in the **SHARES** section

After configuration reboot the PC

10.10.3 Mounting Windows 2000/XP partitions on a Linux host using Samba

This is more convenient than mounting via NFS because you do not need to have a NFS package installed on the Windows PC. The only thing that you need is the Samba package for the Linux PC, which is available on the Red Hat CDs.

To define a mounted directory you have to gather the following information:

1. Check a valid user and the name of the Windows PC and get the information which directories are available (=shared), enter the command:

   `smbclient -L <WIN_PVC_NAME> -U <WIN_PC_USER>`

   for example for the Windows PC *nmrpc.chemistry.university.com* and the user

Administrator the command looks like this:

smbclient -L nmrpc.chemistry.university.com -U Administrator

You will be asked to enter the users password. The answer of the command is a list of all shared directories on the Windows PC, e.g.:

```
Sharename      Type           Coment
----------     -----          -------
E$             Disk           Default share
tmp            Disk
```

now you have four information available

a) <WIN_PC_NAME>

b) <WIN_PC_USER_NAME>

c) <WIN_PC_USER_NAME_PASSWORD>

d) <WIN_PC_SHARE>

2. Create a group called *nmruser* and add those user who should get access into the shared directory. To get information how to create a group please refer to chapter 8.1

3. As a second step you have to define the directory wherein the contents of the shared Windows directory should appear. It is recommended to create therefor a new directory:

mkdir <WIN_PC_DATA_DIR>

4. To allow an automatic mount of the directory of the Windows PC during boot of the Linux PC you have to create a text file (= <FILEX>) with the information of the user name and corresponding password. The syntax of the file has to be:

```
username = <WIN_PC_USER_NAME>
password = <WIN_PC_USER_NAME_PASSWORD>
```

Because the file contains a plain password, you have to make sure that it is only readable by root. You can do this as root on a LINUX shell with the two commands:

chown root.root <FILEX>

chmod 600 <FILEX>

Now you can put together the information and add a new line in the file `/etc/fstab`:

```
//<WIN_PC_NAME>/<WIN_PC_SHARE>   /<WIN_PC_DATA_DIR>   smbfs
rw,gid=nmruser,dmask=775,credentials=<FILEX>,user 1 2
```

This is one line between `smbfs` and `rw` is a space. The option `gid=nmruser,dmask=775` gives full control to the user and the group, others get read and execute.

10.10.4 Mounting Windows 2000/XP partitions from a Linux host using NFS

This requires that the NFS server is installed on the Windows PC. If this PC is controlling a spectrometer, the Hummingbird NFS Server is already installed. The partition `C:\Bruker\Diskless\clients\spect` is mounted via NFS by the spectrometer CCU (which is a UNIX host). In the same way, you can mount any Windows 2000/XP partition or directory on any UNIX or Linux host. Proceed as follows:

1. Export the Windows 2000/XP partition as described in *Installation Guide for Windows XP*.
2. On the Linux host:
   a) Open a shell
   b) Type **`su`** to become superuser
   c) Create a mount directory, e.g. **`mkdir /ntdata`**
   d) mount the partition, e.g.:

      `mount nthost:/c/data /ntdata`

      Note that if the pathname on the Windows 2000/XP host contains upper case letters, these must also be specified with the mount command.

10.10.5 FTP and Telnet

The security level of ftp and telnet are not very high. Because of this, these services are not installed on a typical RED HAT ENTERPRISE LINUX WS 4 installation. The modern and secure alternative is SSH.

If you want to install ftp and telnet services see chapter 15.3

Chapter 11

Installing a Printer

11.1 Introduction

In the following you can found the description of the print system ‚CUPS'. In RED HAT ENTERPRISE LINUX WS 4 CUPS is the only print system, the older ‚LPRng' is not available anymore.

11.2 Print system ‚CUPS' [1]

11.2.1 Installation of a Local printer

In order to install a Local printer on a Linux PC, you have to take the following steps:

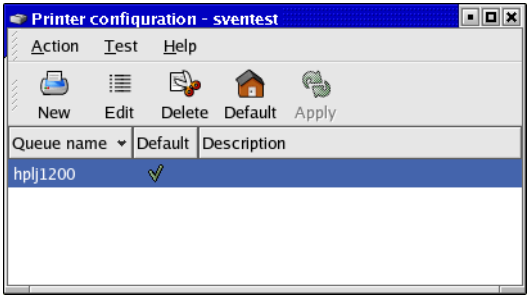
1. Click **<red hat> → System Settings → Printing**

   A window *Query* will appear and asks for the root password

1. To define the default printer of the system root can also execute the command:
lpadmin -d <printer_name>
To define a user specific default printer the user has to execute the command:
lpoptions -d <printer_name>

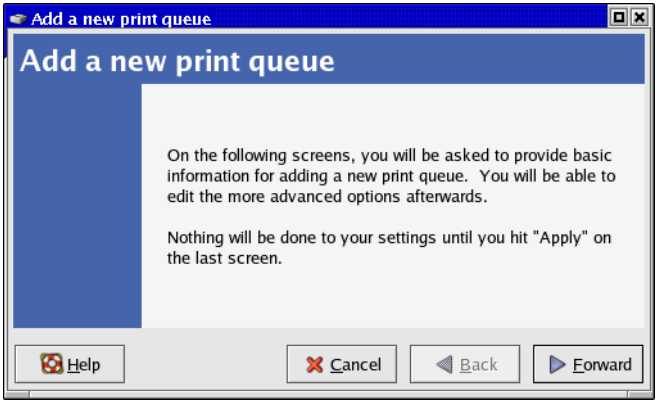
- enter root password

2. The window *Printer configuration* will appear



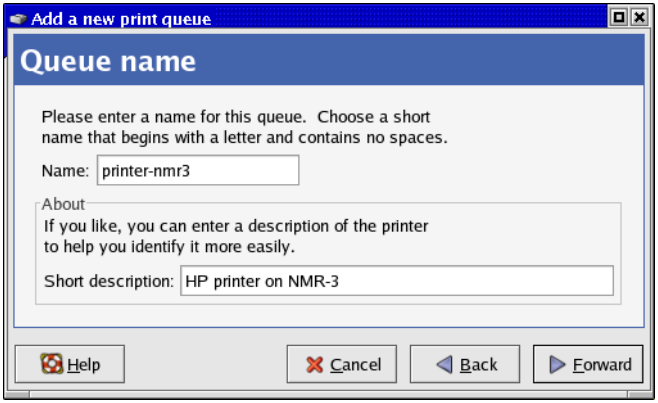
- Click **New**

3. A window *Add a new Print Queue* will appear



- Click **Forward**

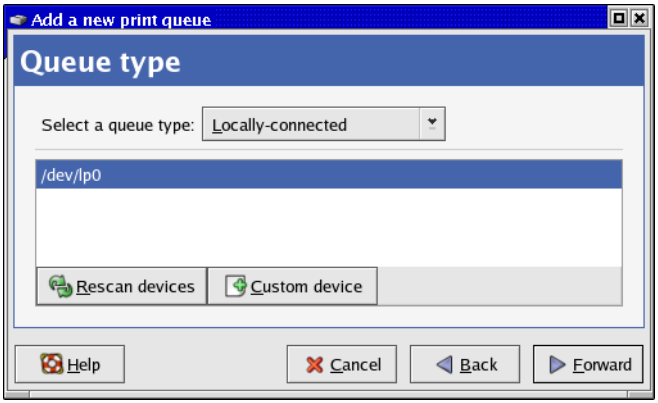
4. The window changes to *Queue name*



Enter name and short description of the printer (in this example *printer-nmr3* and *HP printer on NMR-3*)

- Click **Forward**

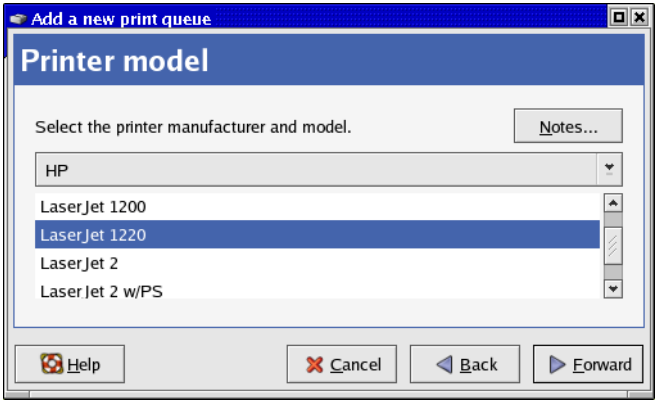
5. The window changes to *Queue type*



Select *Locally-connected* and the port where the printer is connected (in this example */dev/lp0*)

- Click **Forward**

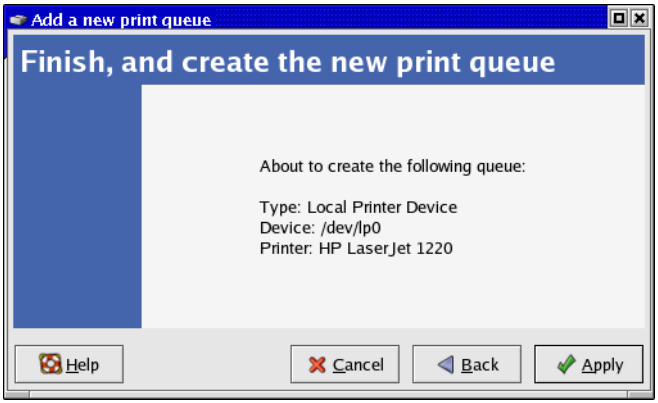
6. The window changes to *Printer model*



Select the manufacturer and the model of the printer in this example *HP Laser Jet 1220*)

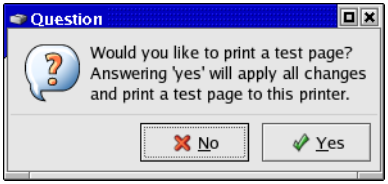
- Click **Forward**

7. The window changes to *Finish, and create the new print queue*



- Click **Apply**

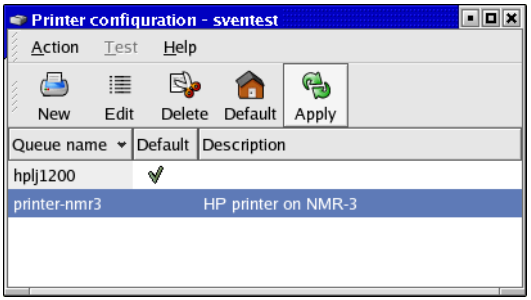
8. The new window *Question* appears



In case the printer is already connected it is recommended to print a test page

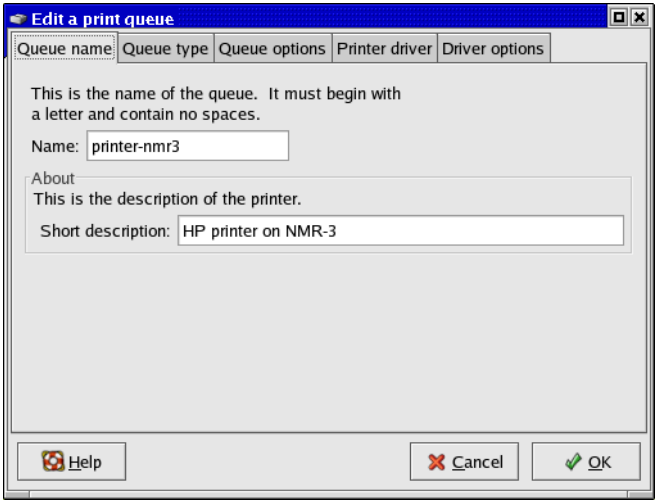
- Click **Yes**

If it is not connected so far, click on **No** and back in the window *Printer configuration* on **Apply**

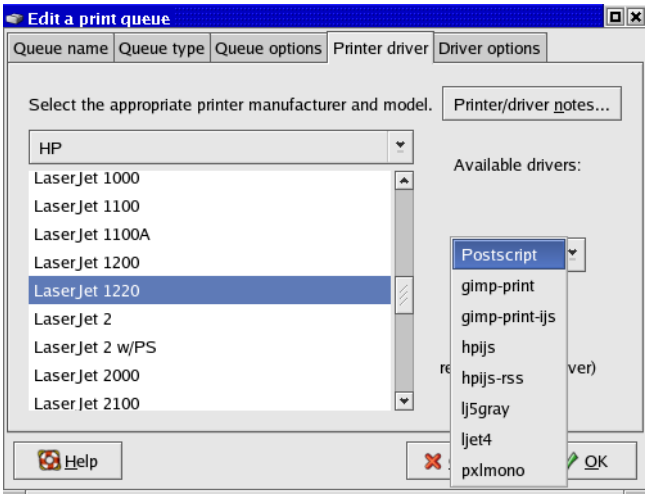


9. To configure the printer click on its name and on **Edit**

10. The new window *Edit a print queue* appears



11. To change the driver click on the tab pane **Printer driver**



If there are several printer drivers, ‚Postscript‘ is always a good choice, and the old ‚ljet4‘ works also in most cases very well)

12. Click **OK** and back in the window *Printer configuration* on **Apply**

13. The printer is ready to use

11.2.2 Installation of a Unix network printer

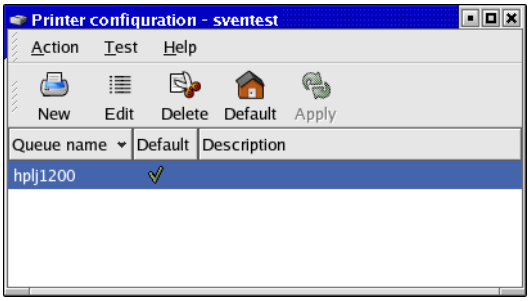
In order to install a Unix network printer on a Linux PC, you have to take the following steps:

1. Click **<red hat> → System Settings → Printing**

   A window *Query* will appear and asks for the root password

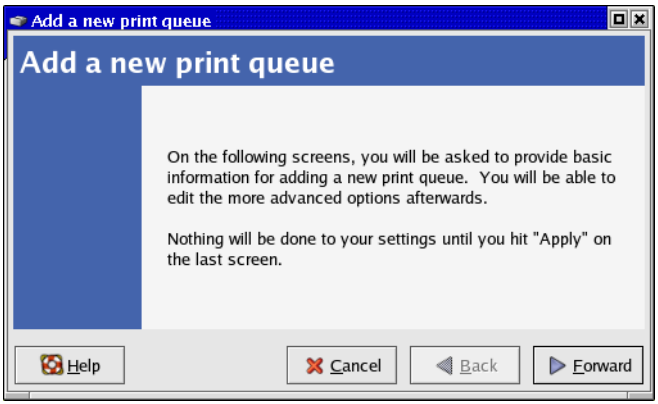
   - enter root password

2. The window *Printer configuration* will appear



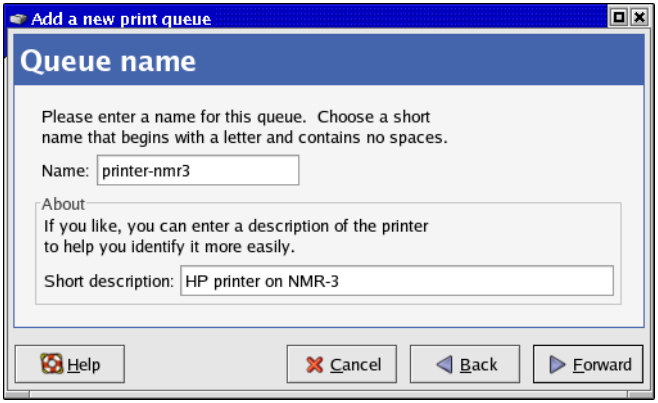
   - Click **New**

3. A window *Add a new Print Queue* will appear



   - Click **Forward**

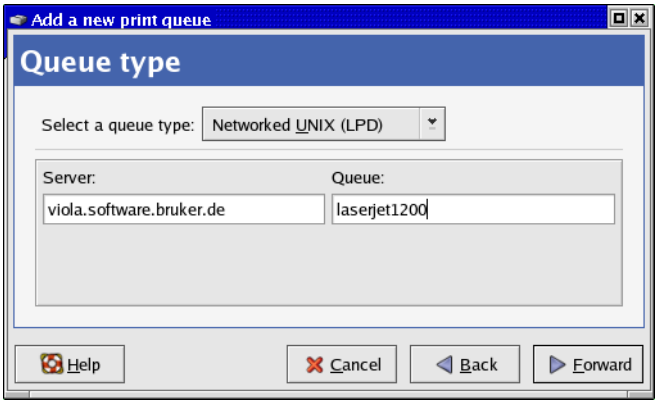
4. The window changes to *Queue name*



Enter name and short description of the printer (in this example *printer-nmr3* and *HP printer on NMR-3*)

- Click **Forward**

5. The window changes to *Queue type*

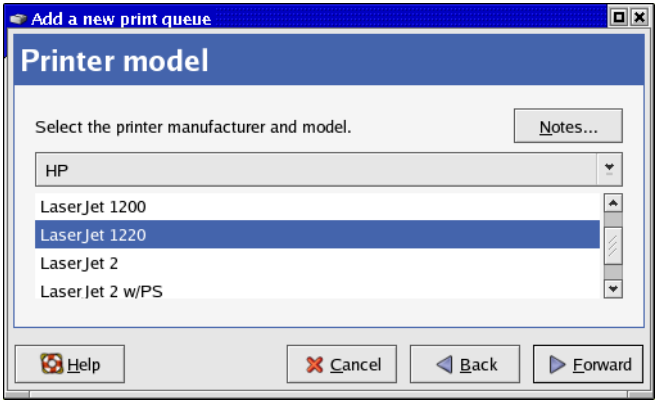


Select *Networked UNIX (LPD)* and enter the hostname/IP address[1] and the queue of the printer (in this example *viola.software.bruker.de* and *laserjet1200)*

- Click **Forward**

1. You can enter either a name or a IP address of the printer. Everything will work what can be used for a successfully **`ping`** to the respective PC

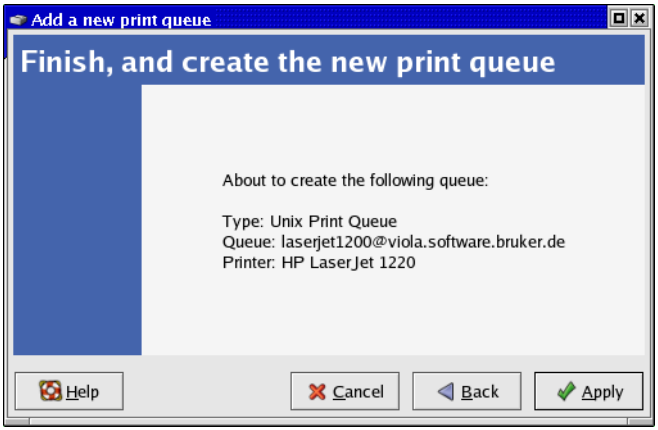
6. The window changes to *Printer model*



Select the manufacturer and the model of the printer in this example *HP Laser Jet 1220*)

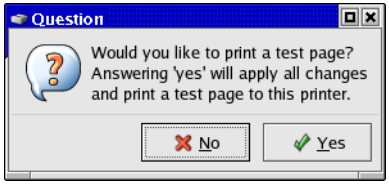
- Click **Forward**

7. The window changes to *Finish, and create the new print queue*



- Click **Apply**

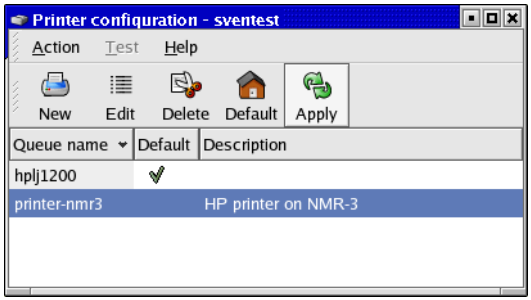
8. The new window *Question* appears



In case the printer is already connected it is recommended to print a test page

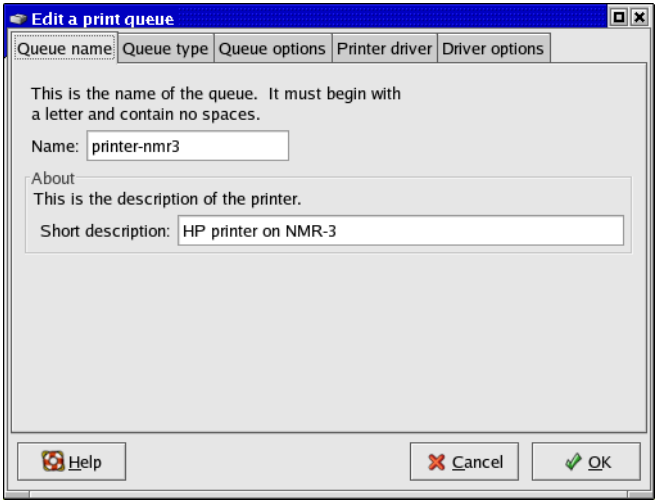
- Click **Yes**

If it is not connected so far, click on **No** and back in the window *Printer configuration* on **Apply**

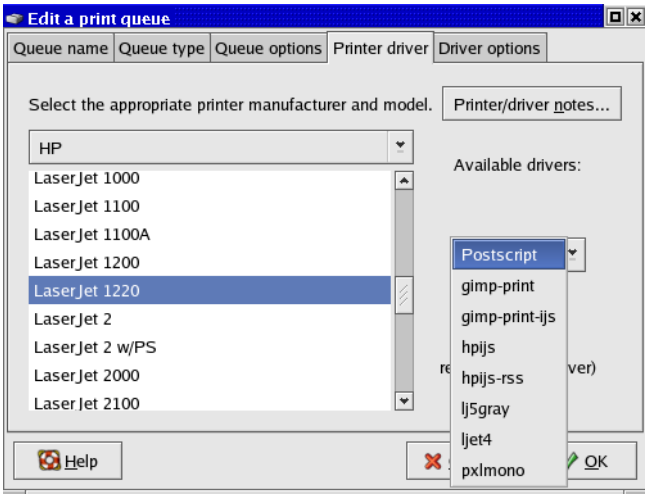


9. To configure the printer click on its name and on **Edit**

10. The new window *Edit a print queue* appears



11. To change the driver click on the tab pane **Printer driver**



If there are several printer drivers, ‚Postscript‘ is always a good choice, and the old ‚ljet4‘ works also in most cases very well)

12. Click **OK** and back in the window *Printer configuration* on **Apply**

13. The printer is ready to use

11.2.3 Installation of a Windows network printer

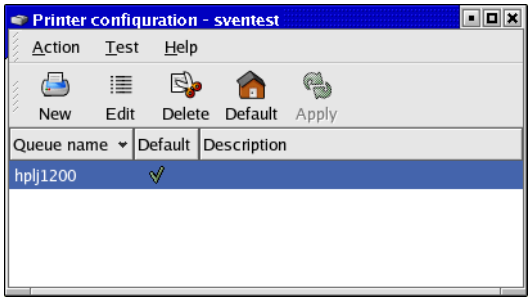
In order to install a Windows network printer on a Linux PC, you have to take the following steps:

1. Click **<red hat> → System Settings → Printing**

   A window *Query* will appear and asks for the root password

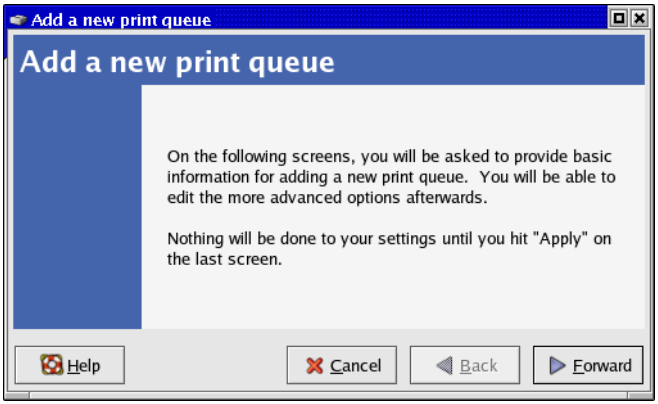
   - enter root password

2. The window *Printer configuration* will appear



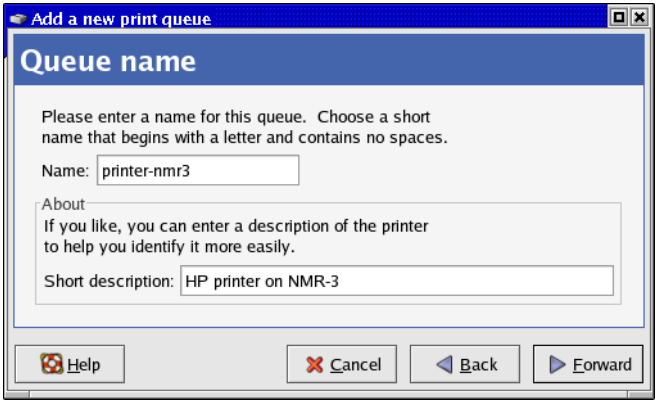
   - Click **New**

3. A window *Add a new Print Queue* will appear



   - Click **Forward**

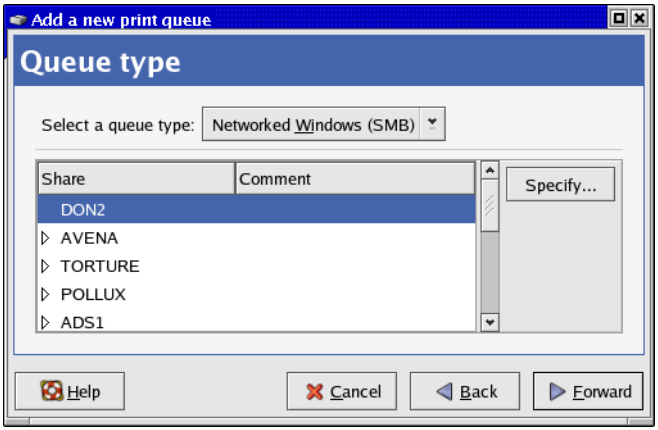
4. The window changes to *Queue name*



Enter name and short description of the printer (in this example *printer-nmr3* and *HP printer on NMR-3*)

- Click **Forward**

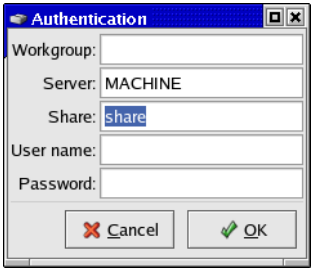
5. The window changes to *Queue type*



Select *Networked Windows (SMB)* and the required shared printer from the list. You will see all printers that are reachable without username and password. If the required printer is not in the list, ...

- Click **Specify**

The window Authentication appears, enter all entries manually

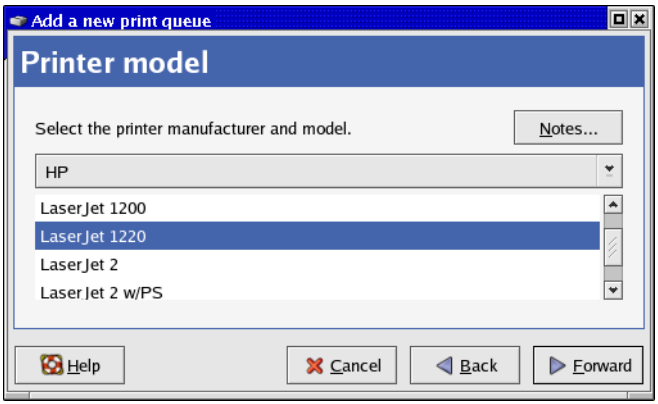


.. if it is on the list, click on the entry and the window Authentication will appear with those information that are available. Fill in the missing information about the user name and password.

- Click **Forward**

6. The window changes to *Printer model*

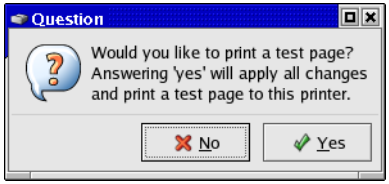
   Select the manufacturer and the model of the printer



- Click **Forward**

7. The window changes to *Finish, and create the new print queue*
   - Click **Apply**

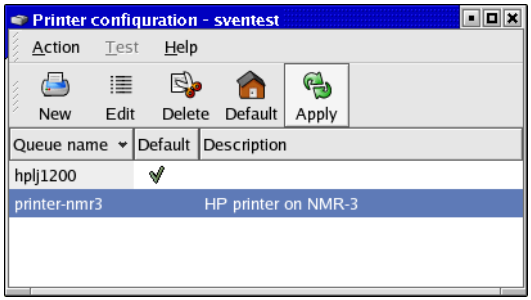
8. The new window *Question* appears



In case the printer is already connected it is recommended to print a test page

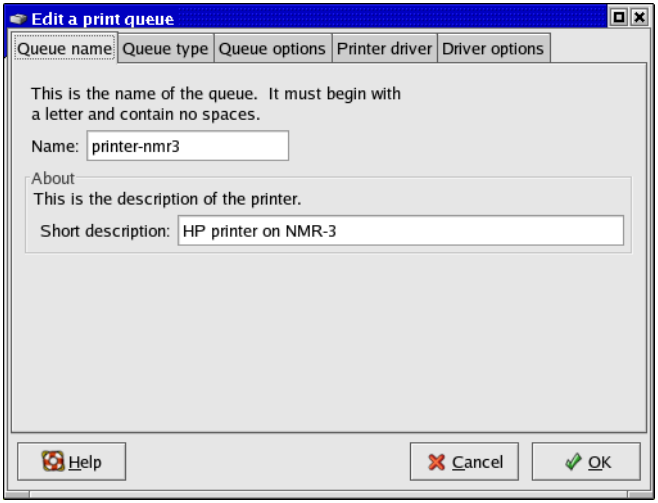
- Click **Yes**

If it is not connected so far, click on **No** and back in the window *Printer configuration* on **Apply**

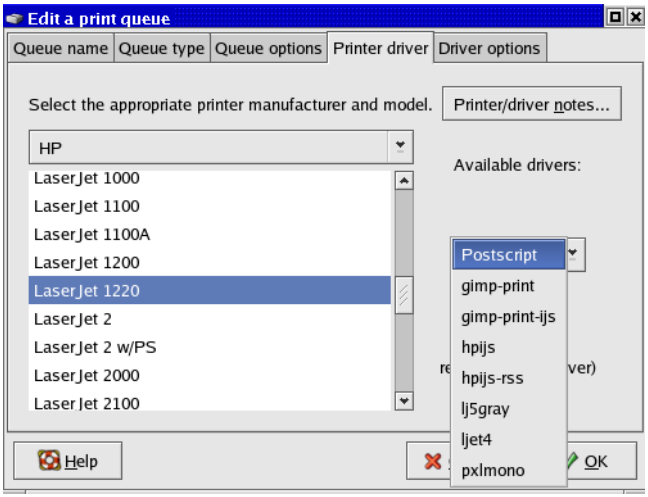


9. To configure the printer click on its name and on **Edit**

10. The new window *Edit a print queue* appears



11. To change the driver click on the tab pane **Printer driver**



If there are several printer drivers, ‚Postscript‘ is always a good choice, and the old ‚ljet4‘ works also in most cases very well)

12. Click **OK** and back in the window *Printer configuration* on **Apply**

13. The printer is ready to use

11.2.4 Installation of a Jet Direct printer

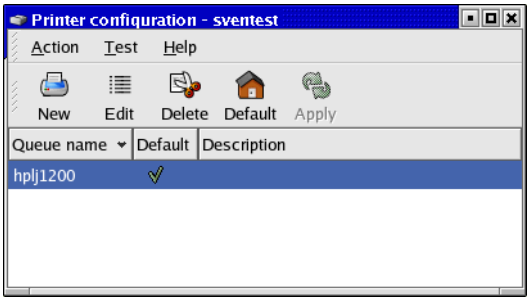
In order to install a Jet Direct printer on a Linux PC, you have to take the following steps:

1. Click **<red hat> → System Settings → Printing**

   A window *Query* will appear and asks for the root password

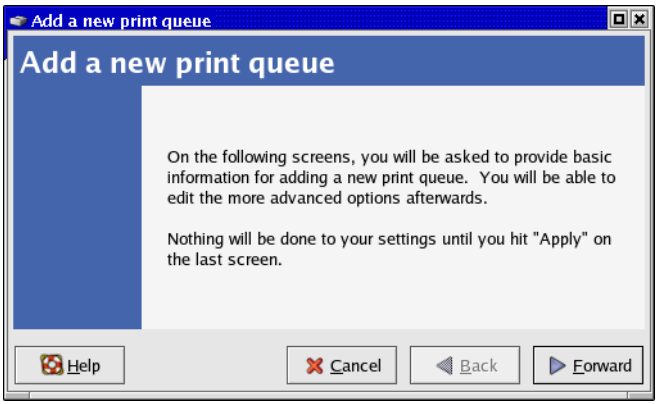
   - enter root password

2. The window *Printer configuration* will appear



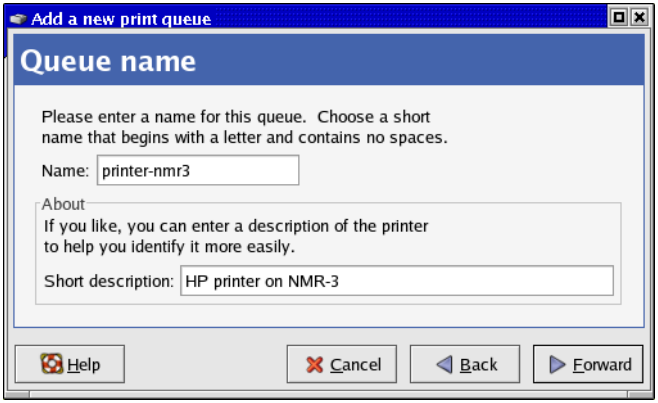
   - Click **New**

3. A window *Add a new Print Queue* will appear



   - Click **Forward**

4. The window changes to *Queue name*

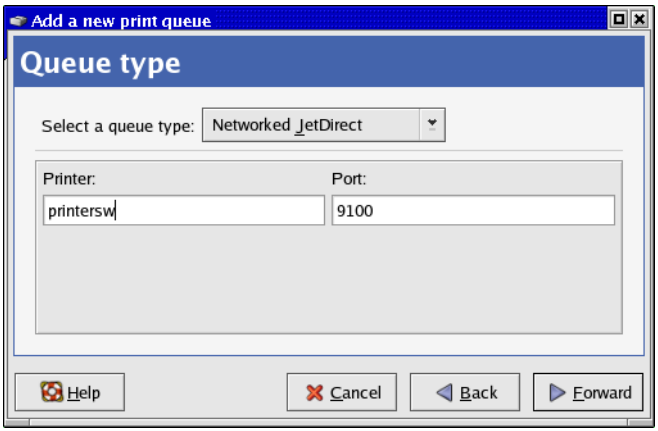


Enter name and short description of the printer (in this example *printer-nmr3* and *HP printer on NMR-3*)

- Click **Forward**

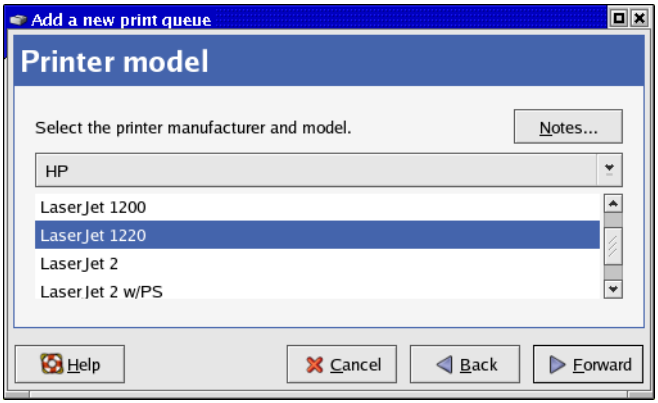
5. The window changes to *Queue type*

Select *Networked JetDirect* and enter name and port of the printer (in this example *printersw* and *9100*



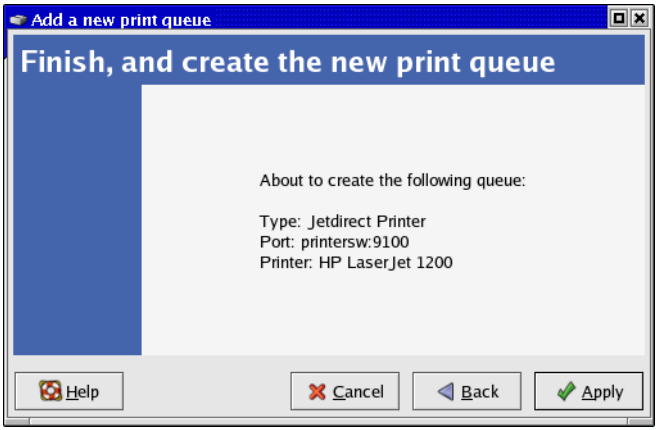
- Click **Forward**

6. The window changes to *Printer model*
   Select the manufacturer and the model of the printer in this example *HP Laser Jet 1220*)



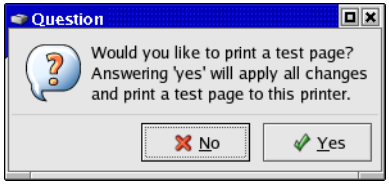
- Click **Forward**

7. The window changes to *Finish, and create the new print queue*



- Click **Apply**

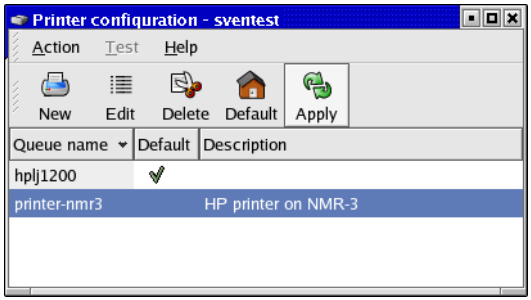
8. The new window *Question* appears



In case the printer is already connected it is recommended to print a test page

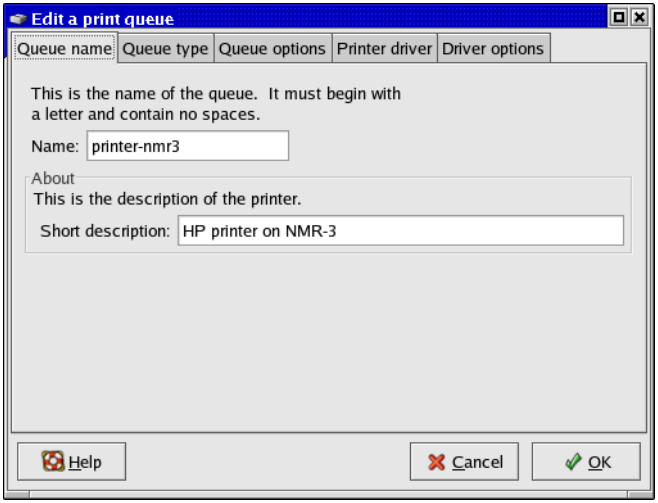
- Click **Yes**

If it is not connected so far, click on **No** and back in the window *Printer configuration* on **Apply**

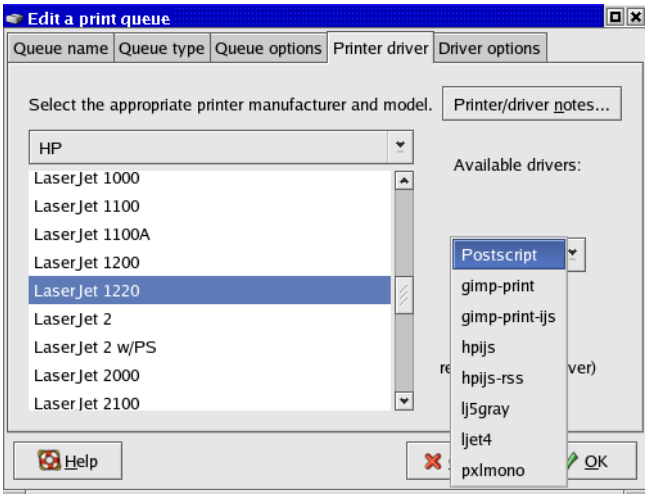


9. To configure the printer click on its name and on **Edit**

10. The new window *Edit a print queue* appears



11. To change the driver click on the tab pane **Printer driver**



If there are several printer drivers, ‚Postscript‘ is always a good choice, and the old ‚ljet4‘ works also in most cases very well)

12. Click **OK** and back in the window *Printer configuration* on **Apply**

13. The printer is ready to use

Part III

Tips, Tricks and Troubleshooting

Chapter 12

Troubleshooting TopSpin

12.1 TopSpin does not start

If ***TopSpin*** does not start, you should first look for an error message in the window where the ***TopSpin*** startup messages appear. Then check if you have one of the following problems:

- A window *Choose Server or File* appears:

  The file `license.dat` was not found. You might have one of the following problems:

  `license.dat` has been deleted or renamed

  → Setup the file `license.dat` as described in chapter 5.2.

- *Invalid license key (inconsistent license key)*

  The file `license.dat` might contain one of the following errors:

  - The FEATURE line contains the wrong license key, the wrong date and/or the wrong number of licenses
  - The hostid is appended at the end of the FEATURE line

- *Invalid host*

- The file `license.dat` contains additional characters at the end of the FEATURE line (after ““)
- For some more information about license problems see chapter 5.2.
- If you do not get the license to run:

  Open a shell and execute:

  `/bin/sh flexlm_diagnostic /tmp/flexlm_diagnostic-out.txt`

  The scripts may require 1 minute to execute.

  Please send the whole output of the TOPSPIN start window using copy&paste and the file */tmp/flexlm_diagnostic-out.txt* to:

  nmr-software-support@bruker.de

12.2 TopSpin troubleshooting

If your current ***TopSpin*** session has a problem, you can find in this chapter some instructions how to get rid of this situation.

In order to stop ***TopSpin*** in case of any problems, the first thing to know is, that it is using a client / server structure. It is possible to start more than one client. This feature is used for the remote control but can also be very useful for troubleshooting!

- The client can be stopped without touching a running acquisition.

To get rid of a ***TopSpin*** problems follow the description below. These steps are increasingly drastic. Please note that this procedure is only necessary in case of any problems as TopSpin does not react anymore.

1. Create debug information and send it to Bruker. For this follow the instructions in chapter 12.2.1
2. Open a Linux shell and start a second **TopSpin** graphical user interface with the command:

   `<TOPSPIN_HOME>/topspin -client`

   <TOPSPIN_HOME> is the ***TopSpin*** installation directory, in a default installation this is `/opt/topspin`

   Does the second ***TopSpin*** graphical user interface works fine?

   - Yes? The problem is solved you can go ahead with TopSpin.

Although you can now work with TopSpin you should restart the program as soon as possible. Typically wait until the current acquisition is finished, then exit and restart TopSpin.

- No? go ahead with next step

3. To kill the current ***TopSpin*** session completely, execute the shell command:

   killtopspin

*Note, that this will stop your **TopSpin** session and therefore also a running acquisition.*

4. Start ***TopSpin*** and go on working.

12.2.1 Send debug information to Bruker BioSpin

If you are in a situation, that ***TopSpin*** problems appear periodically please send information about this to Bruker BioSpin. For a successful and fast processing of incoming emails please make sure that the following information is given:

1. Use ***TopSpin*** command ***about*** to get the information about:
   - version number
   - Server patchlevel
   - GUI build number
2. Operating system information
   - kernel version (shell command **uname -r**)
   - operating system version

     (shell command **more /etc/redhat-release**)
3. If the PC is sued for acquisition control add the Bruker BioSpin order number of the spectrometer.
4. A detailed description how to reproduce the problem
5. ***TopSpin*** internal debug files. To get these files do the following:

   Go into the Linux shell where TopSpin was started, maximize the window and then press the keys **Ctrl** and **Backslash** (‚\‘) simultaneously. This will create a debug output within the shell. To mark the whole text, click with the left mouse button at the end of the text, keep the mouse pressed and move it up until you reached the beginning of the text. Click on Edit - Copy. Now enter the command:

```
nedit <TOPSPIN_HOME>/prog/curdir/<USER_NAME>/stack.txt
```

   <TOPSPIN_HOME> is the ***TopSpin*** installation directory, in a default installation

this is `/opt/topspin`

The *nedit* window will appear and you will be asked if you want to create a new file. Select **New File** and in the main *nedit* window:

- click on **File → Paste**
- click on **File → Save**
- click on **File → Exit**

Now it is necessary to pack all available information which Bruker needs to analyze your problem. For this open a shell and execute the following two commands:

```
cd <TOPSPIN_HOME>/prog/curdir/<USER_NAME>
tar cvzf /tmp/bug.tar.gz * ~/.topspin-<NAME_of_PC>/prop/protocol*
```

Please attach the file */tmp/bug.tar.gz* into an email and send it to this address:

nmr-software-support@bruker.de

If the filesize is too big you can also put it on the german Bruker BioSpin ftp server:

ftp://ftp.bruker.de

You have to login with the user name *ftp* and your email address as password. Now you are authorized to put files into the directory ‚*incoming*' (or to get files from the directory ‚*outgoing*'). When you have uploaded files into ‚*incoming*' send an email to

nmr-software-support@bruker.de

with the information described above and a list of files you have uploaded onto the ftp server.

12.3 Communication problems between PC and Spectrometer

If the acquisition (***zg***, ***gs***, ***wobb***) and/or configuration (***cf***) fails, you might have a communication problem between the Linux PC and the spectrometer.

Different spectrometer hardware requires different troubleshooting procedures. To find out which spectrometer do you have, check which combination of the follow-

ing boards are present in your spectrometer.

name	specific boards	Troubleshooting information
AVANCE (AV)	CCU-RCU	chapter 12.3.1
AVANVCE-II	CCU-DRU	chapter 12.3.1
AVANCE-III	IPSO-DRU	chapter 12.3.2

For a convenient classification the respective boards are shown below. Note, the pictures are just an example, e.g. the EC level can be different.

Do I have an **AV** type spectrometer?

Yes, if you have the two boards:

CCU *and* *RCU*

For troubleshooting information go to chapter 12.3.1

Do I have an **AV-II** type spectrometer?

Yes, if you have the two boards:

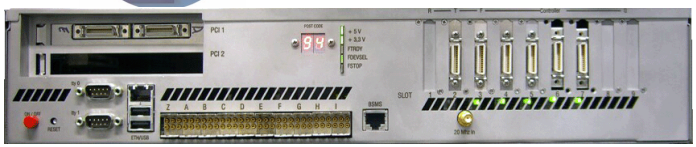
CCU *and* *DRU*

For troubleshooting information go to chapter 12.3.1

Do I have an **AV-III** type spectrometer?

if you have the two boards:

IPSO *and* *DRU*



For troubleshooting information go to chapter 12.3.2

Note that CCU, RCU and DRU have an upright orientation while the Ipso board is typically horizontally orientated.

In all cases the first step of troubleshooting should be to check if the spectrometer is on power and there is a physical network connection between the Linux PC and the spectrometer.

12.3.1 Troubleshooting for AV and AV-II type of spectrometer

First of all it is necessary to check the communication between the PC and the CCU. This can be done in the following way:

a) Open a shell

b) Type **`telnet spect`**

Depending on whether **`telnet spect`** works (you get a login prompt) or not, continue with paragraph 12.3.1.1 or 12.3.1.2.

12.3.1.1 Communication problems but telnet spect works

If **`telnet spect`** works, the CCU has booted. This means that the spectrometer network software is installed and running. The communication problems obviously have other causes. Two of the most common causes are mentioned below.

In each of the following steps you must be logged in on the PC as root and type the indicated commands in a shell.

1. Check if the process *startd* is running on the CCU:

a) Type **`telnet spect`** and log in on the CCU as root

b) Type **`ps -efw| grep startd`**

Does this command show you 2 processes `/etc/startd`?

YES? Then *startd* is running, type **`exit`**, go to step 2

NO? Then you found the problem, go to step 1c.

c) Type **`/etc/startd`**

Trying to start *startd* in this way might show you the reason why *startd* was not started automatically. You might have a hardware problem and starting the *startd* manually indicates which board has a failure. Run the corresponding hardware test (see chapter 12.7.1).

2. Check the list of PC names in the file `/etc/resolv.conf`.

Every entry in this file must be correct, otherwise there will be time-outs in network traffic which interfere with the connection to the spectrometer.

3. Check if the spectrometer has an alias name which is not specified in `/etc/hosts`:

   a) Type **`cd /<TOPSPIN_HOME>/conf/instr`**

   <TOPSPIN_HOME> is the directory where ***TopSpin*** is installed (default is `/opt/topspin`)

   b) Type **`more curinst`**

   What is the output of this command?

   - `spect?` Then the spectrometer does not have an alias name
   - different from `spect`, e.g. `av600`? Then do the following:

     type **`grep spect /etc/hosts`**

     What is the output of this command?

     `149.236.99.99 spect av600`? Then the alias name is specified

     `149.236.99.99 spect`? Then you found the problem, go to c)

   c) Edit the file `/etc/hosts`:

   append the alias name, e.g. `av600` after `spect`

If these two steps did not solve your problem, copy the contents of the two history files into an email to your local Bruker BioSpin office. Where do you can find the files, can be seen by entering the command ***hist*** in ***TopSpin***. These files contain the necessary information:

`<TOPSPIN_HOME>/prog/curdir/<USER_NAME>/history`

`<TOPSPIN_HOME>/prog/curdir/<USER_NAME>/history_j.txt`

12.3.1.2 Communication problems and telnet spect does not work

If **`telnet spect`** does not work, the CCU has probably not booted up completely. This can have several causes, either software or hardware related. The following information describe software related problems.

In each of the following steps you must be logged in on the PC as root and type the indicated commands in a shell. After each step, type **`telnet spect`** and see if you get a login prompt.

1. Open a Linux shell and become superuser; type **`su -`**

2. Check if there are firewall rules that prohibit to contact the spectrometer

a) go to the directory */etc/sysconfig*

- **`cd /etc/sysconfig`**

b) what is the configuration of *iptables*[1]

- **`iptables -L`**

  Did you get a information that contains three times *`(policy ACCEPT)`*?

  - Yes ? No problem, go to step 3
  - No, the answer is at great length? go to step c

c) to check if this is the problem it is the best to stop the firewall temporarily. Note that this can cause security problems. If in doubt please contact your system administrator. To stop the firewall type in (for more details about the firewall see chapter 15.2):

- **`service iptables stop`**

  Check the spectrometer connection once again. Does it work now?

  - No ? No problem, go to step 3
  - Yes ? You might have found the problem. The system administrator has to make sure that the ethernet card for spectometer control gets full access or he has to disable firewall package in general. This can be done by the command:

    `chkconfig iptables off`

    Note: You have to reboot the PC.

3. Reboot the PC and CCU using *reviveccu*[2]:

type **`reviveccu`**

→ follow the instructions:

a) You will be asked to switch off the acquisition rack

b) *reviveccu* will automatically reboot the PC

---

1. If you use the firewall package *iptables*, you have to make sure that it allows the ethernet card for spectrometer control full access (see chapter 15.2.1)
2. The command **`reviveccu`** executes a shell script which will first remove the two files: `/usr/diskless/clients/spect/root/etc/mtab` and `.../utmp` and then reboot spectrometer-CCU and Linux-PC.

c) Switch on the acquisition rack after the PC has rebooted

4. Check the nameserver configuration:

a) Type **`grep hosts /etc/nsswitch.conf`**

What is the output of this command?

Nothing? No problem, go to step 5.

- *Cannot open nsswitch.conf*? No problem, no nameserver; go to step 5.
- *hosts: files dns nisplus*? No problem, this entry is correct; go to step 5
- *hosts dns....* or *hosts nisplus....*? You found the problem: go to step b.

b) Edit the file `/etc/nsswitch.conf` and check if the line *hosts* looks like this: *hosts: files dns nisplus*

where *files* refers to the local `/etc/hosts` file and *dns* to the DNS (bind) and *nisplus* refer to nameservers.

This specifies that network commands like **`telnet`** should first check the local file `/etc/hosts` then, if the host was not found, contact the Domain Name System (*dns*) and finally the Network Information System (*nisplus*). The entries *dns* and *nisplus* are only useful if you have the corresponding network systems. Make sure the entry *files* comes first, the existence and the order of entries *nisplus* and *dns* depends on your network.

5. Check the list of PC names in the file `/etc/resolv.conf`.

Every entry in this file must be correct, otherwise there will be time-outs in network traffic which interfere with the connection to the spectrometer.

6. Check if NFS is running:

a) Type **`ps -efw| grep nfsd`**

Does the output of this command show you 8 processes */usr/etc/nfsd* ?

YES? Then NFS is running, continue with step 8
NO? Then you found the problem, continue with step c

b) Check the file

- `/etc/sysconfig/network`

Does the file contain the entry

```
NETWORKING=yes
```

YES? Then NFS can be started, continue with step 8
NO? Then you found the problem, change the entry to yes and restart NFS manually. Open a shell and type in:

service nfs restart

c) Type **/sbin/chkconfig nfs on**

d) Type **reviveccu**

e) Run step 5a again and if NFS is still not running continue with step 7

7. Check if NFS is installed:

a) Type **rpm -q nfs-utils**

Does the output of this command show you the package *nfs-utils*?

YES? Then NFS is installed, go to step 8
NO? Then you found the problem, install the package *nfs-utils*. For a installation description please refer to chapter 9.3.2

8. Check if the process *bfsd* is running:

a) Type **ps -fC bfsd.linux**

Does the output of this command show you the process

/usr/diskless/bfsd.linux

YES? Then *bfsd* is running, continue with step 9

NO? Then you found the problem, continue with step 8b

b) Check the configuration of bfsd. Correct it if it is wrong.

- type in **/sbin/chkconfig --list bfsd** and check if the output show *on* in runlevel 5, e.g.[1]:

bfsd 0:off 1:off 2:on 3:on 4:on 5:on 6:off

c) Start the bfsd manually.

- type in **service bfsd start**

and check if the output of step 8a is correct now. If it is not, go ahead.

d) Check the output of the command ***hostname***

Is the output of this command:

a plain **hostname**? No problem, continue with step 9.
a **hostname.domainname**? You found the problem. Change the hostname as described in chapter 10.2. Then continue with step 7h.

1. If a process like this is not started, start it on a shell by typing **service <process> start**

e) Check the output of the command ***hostname -f***

Is the output of this command:

a **hostname.domainname**? No problem, continue with step 9.
a plain **hostname**? You found the problem. Change the hostname as described in chapter 10.3. Then continue with step 7h.

f) Check the file `/etc/hosts`[1] - at least the following entries have to exist for spectrometer control:

127.0.0.1 localhost.localdomain localhost

149.236.99.1 ASP_ST2

149.236.99.99 spect

If the ethernet card for the laboratory network is not configured as DHCP, also the name of the own PC has to be listed

xyz.xyz.xyz.xyz name_of_own_pc.domain name_of_own_pc

Does this entry exists?

Yes? No problem, continue with step 9.
No? You found the problem. Add the name of the PC as described in chapter 10.5. Then continue with step 8h.

g) Check if the ethernet card for the laboratory network is configured as DHCP (see chapter 10.4). If so check if the DHCP server is still active:

- open a Linux shell
- type in **`su -`** to become superuser
- type in **`ifconfig`**

  you will get a description of the configurations of the ethernet cards. Check the IP address of the PC, this is the number behind *inet addr:* , typically of *eth0*
- take the IP address and type in **`host <IP-address>`**

  is the answer like this:

`<IP-address>.in.addr.arpa. domain name pointer <PC-Name.domainname>`

Yes? No problem, continue with step 9.
No? You found the problem. Contact your network administrator to check

1. It is also possible to use the graphical tool for checking / configuring the entry, see chapter10.5

the nameserver and DHCP server.

h) Type **reviveccu**

9. Check if the `/usr/diskless` partitions are exported:

a) Type **/usr/sbin/exportfs -v**

Does the output of this command show you both partitions with correct options :

`/usr/diskless/dl_usr`

spect (ro,async,wdelay,root_squash)

and

`/usr/diskless/clients/spect`

spect (rw,async,wdelay,no_root_squash)

YES? Then the partitions are exported, continue with step 10

NO? Then you found the problem, continue with step 9b

b) Check the file `/etc/exports` and correct it if it is wrong (see chapter 12.3.1.3)

c) Type **reviveccu**

10. Check if the spectrometer network is correctly configured:

Please refer to chapter 10.7.1

11. Reconfigure the spectrometer network:

- You can use the automatic procedure which will be started by typing:

  /<TOPSPIN_HOME>/prog/bin/install.net/install.net

  where **<TOPSPIN_HOME>** is the directory where ***TopSpin*** is installed (default `/opt/topspin`). This command reconfigures the entire spectrometer network.

- You can check it manually, see chapter 10.7

12. Reconfigure the spectrometer network by re-installing the DISKLESS package:

Insert the ***TopSpin*** DVD into the DVD drive, select the Diskless package and deselect all other packages. For more details see installation description in chapter 10.7.1

To check if hardware related problems causes the CCU not to boot do the following:

1. Check if the ethernet cable between PC and CCU is properly connected.
   → Remove and re-connect the ethernet cable and the transceiver or minihub.
2. Check if the ethernet interface is broken.
   a) Physically connect the CCU to the first ethernet interface (*eth0)* [1]
   b) Become superuser; type **`su -`**
   c) Change the configurations between eth0 and eth1 as described in chapter 10.5 and 10.7.1.

! Note: Write down all configuration parameters like IP addresses, nameserver etc.

3. Replace the ethernet cable, transceiver or minihub between the PC and CCU to find out if either of these components is broken.
4. If a new CCU was installed:
   a) login as root
   b) Type **`arp -d spect`**
   c) Type **`reviveccu`**

12.3.1.3 File entries made for the spectrometer network

- `/etc/hosts`

```
149.236.99.1    ASP_ST2
149.236.99.99   spect
```

- `/etc/bootparams`

```
spect root=ASP_ST2:/usr/diskless/clients/spect/root
swap =ASP_ST2:/usr/diskless/clients/spect/swapfile
dump= ASP_ST2:/usr/diskless/clients/spect/dump
```

Note that this is one line with a blank between the three entries.

- `/etc/exports`

```
/usr/diskless/dl_usr spect(ro)
/usr/diskless/clients/spect spect(rw,no_root_squash)
```

- `/etc/sysconfig/network`

```
NETWORKING=yes
HOSTNAME=hosttest
```

1. assuming that the CCU is currently connected to the second ethernet interface.

```
GATEWAYDEV=
GATEWAY=
```

- /etc/sysconfig/network-scripts/ifcfg-lo

```
DEVICE=lo
IPADDR=127.0.0.1
NETMASK=255.0.0.0
NETWORK=127.0.0.0
# If you're having problems with gated making 127.0.0.0/8
# a martian, you can change this to something else
# (255.255.255.255, for example)
BROADCAST=127.255.255.255
ONBOOT=yes
NAME=loopback
BOOTPROTO=none
```

- /etc/sysconfig/network-scripts/ifcfg-eth1

```
BROADCAST=149.236.99.255
NETWORK=149.236.99.0
NETMASK=255.255.255.0
IPADDR=149.236.99.1
DEVICE=eth1
ONBOOT=yes
BOOTPROTO=none
USERCTL=no
```

- /usr/diskless/clients/spect/root/etc/fstab

```
ASP_ST2:/usr/diskless/clients/spect/root / nfs rw,bg,hard,retry=3,timeo=20 0 0
ASP_ST2:/usr/diskless/dl_usr /usr nfs ro,bg,hard,retry=3,timeo=20 0 0
ASP_ST2:/usr/diskless/clients/spect/var /var nfs rw,bg,hard,retry=3,timeo=20 0 0
```

- /etc/xinetd.d/bootparamd[1]

```
service bootparamd
{
type= RPC
```

1. If the file is modified you can reload it with the shell command: **service xinetd reload**

```
socket_type= dgram
user= root
server= /usr/sbin/rpc.bootparamd
wait= yes
protocol= udp
rpc_version= 1
disable= no
instances= 1
log_type= FILE /usr/diskless/bootparamd.log
}
```

12.3.1.4 Files created for the spectrometer network

- `/usr/diskless/clients/spect/swapfile`

  This file can also be created manually with the command:

  `dd if=/dev/zero of=/usr/diskless/clients/spect/swapfile bs=8000000 count=1`

- `/etc/rc2.d/S95bfsd`

  This file is a symbolic link to the file `/etc/init.d/bfsd`. From this file the *bfsd* daemon `/usr/diskless/bfsd` is started.

- `/usr/diskless/clients/spect/root/dev`

  This directory contains a large number of special files such as `tty00`, `tty01`, `tty02`, etc. These files are created during the installation of the DISKLESS package from the ***TopSpin*** DVD. They can also be created manually:

  a) Become superuser: type **`su -`**

  b) `cd /usr/diskless/clients/spect/root/dev`

  c) `./MKDEV -m RS3330`

12.3.1.5 View the output of the CCU console

In order to view the output of the CCU you must connect serial port 2[1] of the PC with tty00 of the CCU, you need a cable with a round rs232 plug on the CCU side (order number HZ04161/A). The program *cu* can be used to make the output of the

1. If you connect the cable with serial port 1, you have to use *ttyS0* instead of *ttyS1*

CCU visible in a shell on the PC.

Check if *cu* is installed:

`rpm -q uucp`

if it is installed and active the answer should be:

uucp-<versions-no>

If it is not installed yet, please refer to the installation description in chapter 9.3.2

In case of any problems with this package check the permissions of the program.

1. Each user who should be able to use the `cu` command has to be a member of the group `uucp`

To add a user into this group proceed as follows:

a) Click **<red hat> → System Settings → Users and Groups**

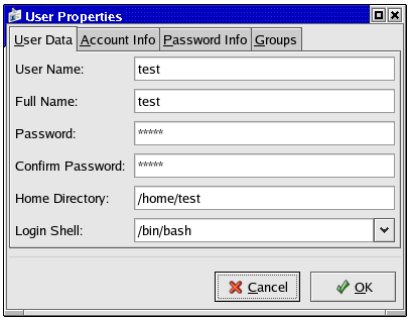
b) If you are not logged in as root, a window *run as root - KDE su* will appear

- enter root password

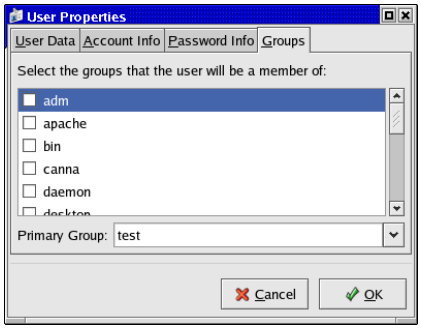
c) A window *KDE User Manager* will appear:

- Click on an existing user and click on **Properties**

d) A window *User Properties* will appear:



- Click on **Groups**



You will see in the appearing window the field Primary Group that shows the original group of the user. Leave this entry unchanged, it is not necessary to modify the primary group, it is enough to define the uucp-group membership additionally.

- In the field *Select the groups that the user will be a member of* you can now scroll to the group `uucp` and selecting the respective field
- Click **OK**

2. Type **`ls -l /dev/ttyS1`**

   The permissions, owner, and group of this file must be: *crw-rw-rw-*, *root* and *uucp* respectively. If they are different, change them as follows:

   ```
   chmod a+rw /dev/ttyS1
   chown root.uucp /dev/ttyS1
   ```

3. Type **`ls -l /var`**

   The group of the directory `lock` must be *uucp* and has to have write permissions. If they are different, change them as follows:

   - login as root
   - type in:

     `chgrp uucp /var/lock`

   - type in:

     `chmod g+rwx /var/lock`

Type **`/sbin/reboot`**

12.3.1.6 View/change the prom parameters

1. Open a shell and become root
2. Type **`cu -lttyS1`**

→ You will get the prompt *`connected`* and you can see the CCU output messages:

a) Push the reset button of the CCU

b) Press **`Control-C`** to interrupt the boot process

The CCU will be in Monitor Mode now, the prompt will change to >>, type:

>> **`printenv`**

You will get a list of environment variables, the most important are:

```
netaddr=149.236.99.99
netmask=0xffffff00
bootfile=bfs()/usr/diskless/clients/spect/root/unix.r4600_std[1]
bootmode=c
```

These values must be shown as specified above[2]. You can set the environment variables as follows:

>> **`setenv netaddr 149.236.99.99`**

>> **`setenv netmask 0xffffff00`**

To boot the CCU again, type:

>> **`u`**

c) To exit the *cu* program type:

>> **`~.Enter`** (press the keys: tilde, dot, Enter)

12.3.1.7 Viewing the boot process

When all environment parameters are correct, you can view the boot process and see where it hangs. This might give you an indication as to what the problem is.

---

1. For CCU 4-7 the bootfile entry is:
`bootfile=bfs()/usr/diskless/clients/spect/root/unix.r3004_std`
2. If the *`netaddr`* is different, the spectrometer network files must be adjusted. However, when you install the DISKLESS package the entries are set back to *149.236.99.99* and your CCU will not boot anymore. Therefore we strongly recommend not to change the *`netaddr`*.

1. Open a shell and become root
2. Type **`cu -lttyS1`**

   → you will get the prompt *`connected`* and after typing **`Enter`** you can see the CCU output
3. Push the reset button of the CCU

   The CCU will try to boot now. The output of the boot process is listed below. The marks '---?---' indicate positions where the boot process possibly hangs or goes into an endless loop:

   Autoboot: Waiting to load
   bfs()/usr/diskless/clients/spect/root/unix.r4600_std
   (CTRL-C to abort)
   loading

   ---1---

   Obtaining /usr/diskless/clients/spect/root/unix.r4600_std from server c85
   851056+115728+824448 entry: 0x80021000
   CPU: MIPS R4700 Processor Chip Revision: 1.0
   FPU: MIPS R4700 Floating Point Unit [CP1] Revision: 1.0
   RISC/os Release 4_52 mips Version UMIPS
   Total real memory = 16777216
   Available memory = 14356480

   ---2---

   Root on nfs file : Swap on nfs file :

   ---3---

   hostname: spect
   domainname: dummy

   ---4---

   Root fstype nfs
   Available memory = 12705792

   ---5---

   Root on nfs file : Swap on nfs file :

   ---6---

   The system is coming up. Please wait.
   ASP_ST2:/usr/diskless/clients/spect/var mounted on /var
   ASP_ST2:/usr/diskless/dl_usr mounted on /usr

Internet daemons: portmap inetd.
NFS daemons: nfsd biod lockd statd.
The system is ready.

Booting might hang, stop (and print an error message) or go into an endless loop at one of the positions 1 through 5. This might be caused by one of the problems mentioned below. Check the indicated files and correct them if necessary or perform the indicated steps.

a) If booting stops at position ---1--- you might have one of the following problems:

- the *bfsd* is not running; go to 12.3.1.2, step 8
- the DISKLESS packages is not installed; see chapter 12.3.1.2, step 12
- the network is not set up correctly; check the configuration (see chapter 10.7.1)

If the problems above do not exist, please enter the following command in a shell:

`/sbin/arp -a`

The output should contain a line like:

spect (149.236.99.99) at a.b.c.d.e.f [ether] on eth1

where *a.b.c.d.e.f* is a hexadecimal hardware ethernet address of the CCU. The command **`arp -a`** displays all active connections, if there is no `spect` entry available, check the network configuration and the ethernet cable.

b) If booting stops at position ---2--- please try the following:

- push the CCU reset button
- type Ctrl-C to interrupt the boot process and enter:

  >> **`setenv bootmode m`**
  >> **`setenv bootmode c`**

- push the CCU reset button

c) If booting stops at position ---3--- one of the following problems exist:

- the CCU (hostname spect) is searched for on a nameserver first:

  The search order is determined by *hosts*:

  `/etc/nsswitch.conf: hosts: files dns nisplus`

  Make sure the first location to be searched is the local `/etc/hosts` file

as specified by the entry *files* as specified above.

- the network is not set up correctly; check `/etc/hosts`, `/etc/bootparams`
- the swapfile does not exist; check the file

  `/usr/diskless/clients/spect/swapfile`

  If the file does not exist please refer to chapter 12.3.1.4
- start of bootparam fails; check if *bootparamd* is active right now[1]:

  `ps -ef | grep bootparamd`

  Does the answer show the two processes *rpc.bootparamd* and *grep bootparamd*?:

  Yes? Continue with the troubleshooting list

  No? Do the following:

  start *bootparamd* right now:

  `service bootparamd start`

  and check what is the general configuration for bootparamd:

  `/sbin/chkconfig --list bootparamd`

  If the entry for 5 is off, activate it in general:

  `/sbin/chkconfig --level 5 bootparamd on`
- edit the file `/etc/hosts.allow` and add the line

  ALL: spect

d) If booting stops at position ---4--- one of the following problems exist:

- NFS is not running; see chapter 12.3.1.2, step 5
- diskless partitions are not exported; see chapter 12.3.1.2, step 9
- the network is not set up correctly; check the file `/etc/hosts`

e) If booting stops at position ---5--- or ---6--- with the following error message please do like described:

`mount root ASP_ST2:/usr/diskless/clients/spect/root`

1. Note that in case the laboratory network is not active, starting of the bootparamd might fail. For checking the network you can use the command **/sbin/mii-tool**. The output shows if the ethernet cards are connected and working properly

```
failed, rpc status 15
PANIC: vfs_mountroot: cannot mount root'
```

you had to check the file (see chapter 12.3.1.3)

```
/etc/xinetd.d/bootparamd
```

f) If booting is very slow or hangs at an arbitrary point you might have a hardware problem (see chapter).

4. To exit the *cu* program type:

>> **~.Enter** (press the keys: tilde, dot, Enter)

12.3.1.8 Running CCU diagnostic tests

1. Open a shell and become root

2. Type **cu -lttyS1**

→ you will get the prompt *connected* and you can see the CCU output:

a) Push the reset button of the CCU

b) Press **Control-C** to interrupt the boot process

The CCU will be in monitor mode now, the prompt will change to >>

>> **setenv bootmode m**

c) Push the CCU reset button

The CCU diagnostic tests will start automatically. If one or more diagnostic tests fail, the CCU could be broken. If they are all passed successfully, your CCU seems to be okay. The bootmode is automatically set back to its normal value **c**.

d) To exit the *cu* program press:

>> **~.Enter** (press the keys: tilde, dot, Enter)

12.3.2 Troubleshooting for AV-III type of spectrometer

There are some differences in troubleshooting AV/AV-II and AV-III type of spectrometers. An important difference is, that on AV-III spectrometer is neither **telnet spect** available nor a nfs server necessary. Several hardware units are connected via ethernet devices and controlled via a DHCP Server. This server comes with the Diskless installation of the ***TopSpin*** DVD. The process is called *dhcpd*.

To find out what are the IP addresses of the different (via ethernet connected) hardware units there are two different possibilities:

- the ***TOPSPIN*** command ***ha*** (for ***h***ardware ***a***ddresses)
- the shell command **ethernet-service-tools**

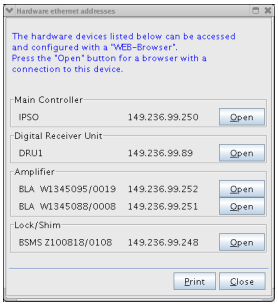
Both commands offer a list of available (via ethernet connected) hardware units and their IP addresses. A mouse click on the name of a module opens the start page of the respective module in a web browser. From there it is easy possible to reset, test and configure the hardware unit. The firmware download can also be started from there.

Note that the web pages of the hardware units are optimised for the web browser *Mozilla*. Usage of *Konqueror* might cause problems, especially with firmware downloads!

12.3.2.1 Communication problems with an AV-III spectrometer

To check if an AV-III is booted correctly you can use the following tests:

1. To check which ethernet connected hardware is available you can use either the TOPSPIN command ***ha*** or the shell command **ethernet-service-tools**
   - ***TOPSPIN*** command ***ha***



   A window appears that shows several hardware modules. Does the window offers an entry ‚IPSO‘?

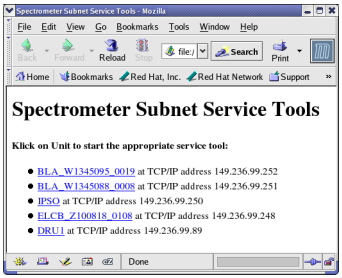
   Yes? The AV-III is booted correctly, go on with the ***TOPSPIN*** command ***cf***

   No? Go to step 2

   - Open a shell and enter the command:

     ethernet-service-tools

A window appears that shows several hardware modules. Does the window offers an entry ‚IPSO‘?



Yes? The AV-III is booted correctly, go on with the ***TopSpin*** command ***cf***

No? Go to step 2

2. Check the network configuration with the following commands:

a) Check the output of the command ***hostname***

- open a Linux shell
- type in **`su -`** to become superuser
- enter ***`hostname`***

Is the output of this command:

- a plain **hostname** like ‚**`nmrpc`**‘? No problem, continue with the next step.
- anything else, e.g. ‚**`nmrpc.chemistry.university.com`**‘? You found the problem. Change the hostname as described in chapter 10, reboot the PC and check if the spectrometer now boots correctly.

b) Check the output of the command ***`hostname -f`***

- open a Linux shell
- type in **`su -`** to become superuser
- enter ***`hostname -f`***

Is the output of this command:

- a **hostname.domainname** like ‚**`nmrpc.chemistry.university.com`**‘? No problem, continue with the next step.
- anything else, e.g. ‚**`nmrpc`**‘? You found the problem. Change the hostname as described in chapter 10, reboot the PC and check if the spectrometer now boots correctly.

c) Check the file `/etc/hosts`[1] - at least the following entries have to exist for spectrometer control:

127.0.0.1 localhost.localdomain localhost

149.236.99.1 ASP_ST2

149.236.99.99 spect

If the ethernet card for the laboratory network is not configured as DHCP, also the name of the own PC has to be listed

xyz.xyz.xyz.xyz name_of_own_pc.domain name_of_own_pc

Does this entry exists?

Yes? No problem, continue with the next step.
No? You found the problem. Add the name of the PC as described in chapter 10.5. Then reboot the PC and check if the spectrometer now boots correctly.

d) Check if the hostname and IP address of the PC is correctly available in the nameserver.

- open a Linux shell
- type in **`su -`** to become superuser
- type in **`hostname -fv`**

  You will get an answer like this:

  ```
  gethostname()='name_of_own_pc'
  Resolving 'name_of_own_pc' ...
  Result: h_name='name_of_own_pc.domain'
  Result: h_addr_list=149.236.13.65
  'name_of_own_pc.domain'
  ```

- take the IP address listed at *`h_addr_list`* and type in the command:

  `host <IP-address>`

  is the answer like this:

```
<IP-address>.in.addr.arpa. domain name pointer <name_of_own_pc.domain>
```

The answer contains only one line and this line shows the same name

1. It is also possible to use the graphical tool for checking / configuring the entry, see chapter 10.5

which is the answer of the above command **`hostname -fv`**

Yes? No problem, continue with the next step.
No? You found the problem. Contact your network administrator to correct the nameserver settings.

3. The firewall may prevent the spectrometer booting. To check this:

- open a Linux shell
- type in **`su -`** to become superuser and check what is the configuration of *iptables*[1] with the command

  `service iptables status`

  Did you get a information that contains three times *`(policy ACCEPT)`*?

  Yes ? No problem, go to next step

  No, the answer is at great length? You may have found the problem. To check this it is the best to stop the firewall temporarily. Note that this can cause security problems. If in doubt please contact your system administrator. To stop the firewall type in (for more details about the firewall see chapter 15.2):

  `service iptables stop`

  Check the spectrometer connection once again. Does it work now?

  - No ? No problem, go to next step
  - Yes ? You might have found the problem. The system administrator has to make sure that the ethernet card for spectometer control gets full access or the firewall has to disable in general. This can be done by the command:

    `chkconfig iptables off`

    Note: You have to reboot the PC.

4. The DISKLESS package is not installed. Insert the ***TopSpin*** DVD into the DVD drive, select the Diskless package and deselect all other packages. For more details see installation description in chapter 10.7.1. After installation of Diskless reboot the spectrometer.

5. Check if the DHCP service is running[2]. Open a shell and enter the command

1. If you use the firewall package *iptables*, you have to make sure that it allows the ethernet card for spectrometer control full access (see chapter 15.2.1)

/sbin/service dhcpd status

Is the answer like this:

dhcpd (pid <xxxx>) is running

Yes? The DHCP service is running, go to the next step

No? You may have found the problem, the DHCP is not running, start it with the command

service dhcpd start

To make sure that it will automatically started with the next boot, enter the command

chkconfig --level 2345 dhcpd on

Now you have to reboot the spectrometer.

6. Did the spectrometer booted successfully?

Yes? You have fixed the problem, the DHCP service is now working correctly.

No? Check the status of the DHCP service once again

/sbin/service dhcpd status

Is the answer like this:

dhcpd (pid <xxxx>) is running

Yes? The DHCP service is running, go to the next step

No? You may have found the problem, the DHCP cannot be started.

Check the files /var/log/messages* for any messages like this:

```
AUG 16 11:34:50 <name_of_PC> dhcpd:      No subnet declaration for eth1 (150.205.205.72).
AUG 16 11:34:50 <name_of_PC> dhcpd:      You must write a subnet declaration for this
AUG 16 11:34:50 <name_of_PC> dhcpd:      subnet. You cannot prevent the DHCP server
AUG 16 11:34:50 <name_of_PC> dhcpd:      from listening on this subnet because your
AUG 16 11:34:50 <name_of_PC> dhcpd:      operating system does not support this capability.
```

This information shows, that the DHCP server listened to the wrong network card, because the listed IP address is not the spectrometer IP address (149.236.99.1). To change this do the following:

2. The DHCP service is a standard Linux package. Configuration and if necessary installation is automatically done with installation of DISKLESS. Only DHCP requests from eth1, the spectrometer network card are managed by the DHCP process. This configuration is defined in the file `/etc/sysconfig/dhcpd`

- execute /sbin/ifconfig -a
- check what is the name of the network adapter which has the IP address *149.236.99.1*
- Edit the file `/etc/sysconfig/dhcpd` and replace the line:

  DHCPDARGS=eth1

  with

  DHCPDARGS=<NAME_OF_THE_ADAPTER>
- Save and exit the file
- Start the DHCP server

  `/sbin/service dhcpd start`

Does the spectrometer is able to boot now?

Yes? You have fixed the problem, the DHCP service is now working correctly. Please note that this fix has to be redone after every DISKLESS installation

No? No problem, go to next step.

7. Check if the *tftpd* service is running. Open a shell and enter the command

- open a Linux shell
- type in **`su -`** to become superuser
- type in **`chkconfig --list tftp`**

Is the answer like this:

```
tftp  on
```

No? You may have found the problem, the tftpd is not running, start it with the command

`chkconfig tftp on`

Now you have to reboot the spectrometer.

Yes? The tftpd service is configured to run, go to the next step

8. Check if the *xinetd* service is running. Open a shell and enter the command

- open a Linux shell
- type in **`su -`** to become superuser
- type in **`service xinetd status`**

Is the answer like this:

xinetd (pid <xxxx>) is running ...

No? You may have found the problem, the xinetd is not running, start it with the command

service xinetd start

To make sure that it will automatically started with the next boot, enter the command

chkconfig --level 345 xinetd on

Now you have to reboot the spectrometer.

Yes? The xinetd service is running, go to the next step

If for whatever reasons the xinetd service can not be started or you are not allowed to start it then start the tftpd manually. This can be done with the command:

/usr/sbin/in.tftpd -l -s /tftpboot

To check if this process is active use the command:

ps -fC in.tftpd

The way you have started this process will keep it running until the next reboot, then it must be started manually once again.

If these troubleshooting steps do not give any hint on an existing problem, you might have a hardware problem. Please get in contact with your local Bruker BioSpin office. Addresses of several offices can be found in chapter 17, for contact information about all Bruker BioSpin office please go to our web server:

http://www.bruker-biospin.de/NMR/about/offices

12.4 General steps that you can try to locate or solve problems

12.4.1 The Bruker BioSpin web server

The Bruker BioSpin web pages contain a large amount of information about known errors and problems. An easy and powerful tool for everybody is the Bruker BioSpin Knowledge Base:

http://www.bruker-biospin.de/shell/bkb/index.cgi

For some pages you need an account to enter them. If you do not have one, go to *www.bruker.de* and click on **Register Now**. Fill out the form to get a free account.

12.4.2 RED HAT help

- Click **<red hat>** → **Documentation**
- Type **`man <command>`**, e.g. **`man find`**

12.4.3 Checking the history of *TopSpin*

The history function keeps track of all the commands you have entered in ***TopSpin*** and of all error messages. This can be very useful if you discuss a problem with your Bruker BioSpin service or support person.

- Enter **hist** in ***TopSpin***

you will get a window with the information about the two history files and the contents of these files. You can use this window to copy-and-paste error messages into your email to Bruker BioSpin.

The history files are automatically re-initialized (overwritten) when ***TopSpin*** is started and the previous one is store with the extension `.old`

12.4.4 Rebooting the PC

Rebooting the PC workstation is a quick and efficient way to kill and restart any hanging processes. Perform the following steps:

1. Check who is logged in; type **`who`**

   → warn all users who are logged in that you are going to shutdown the system
2. Shutdown the computer; type **`/sbin/shutdown`**[1]
3. When the computer is down, switch it off; push the power button
4. Switch the computer on, it will boot automatically

12.4.5 Rebooting the PC and the CCU with 'reviveccu'

If you have any kind of communication problem between the PC and the spectrometer CCU, it is always a good idea to reboot both.

1. To force a file system check after the reboot you can use the command **shutdown -r -F now**

1. Check who is logged in; type **who**

   → warn all users who are logged in that you are going to shutdown the system
2. Become superuser: type **su -**
3. Type **reviveccu**

   → follow the instructions:

   a) You will be asked to switch off the acquisition rack

   b) reviveccu will automatically reboot the PC

   c) Switch on the acquisition rack after the PC has rebooted

12.5 Various problems in Linux

12.5.1 The entire screen is frozen

If you have lost mouse control on the entire screen, there are several things you can do. The following steps are increasingly drastic; perform the next higher step only if the previous one didn't help.

1. Press the Escape key: **Esc**
2. Press the three keys: `Ctrl-Alt-F1` simultaneously
   - this will open a text console, you may login as root and enter **init 3** and then **init 5**, if this does not work ...
   - ... press the three keys: `Ctrl-Alt-Delete` simultaneously

   → this will reboot the system
3. If the system is connected to the network, log in as root via ssh from a different host and type **/sbin/reboot**

   → this will reboot the PC
4. Push the power button, this is not dangerous in case the Linux system uses an ext3 file system

Important: before you reboot or shutdown the system, first check who is logged in if this is still possible: type **who.** Warn all users who are logged in that you are going to shutdown the system.

12.5.2 Programs like killtopspin, reviveccu and touser are not found

These programs are delivered with ***TopSpin*** and are executed by the superuser from a shell. However, if you become superuser with the command **su**, the programs may not be found. You can solve this problem in two different ways:

1. Become superuser with the command '**su -**' or
2. Log out and log in as root

   Now the programs **shmrm**, **reviveccu**, **touser** etc. can be typed in from any directory and will always be found.

12.5.3 Xserver does not start after reboot / not enough disk space available

In case the Xserver does not start after a reboot of the Linux PC, the cause could be that the harddisk is 100% full. In every user's home directory there is a file called

`.xsession-errors`

that could contain a lot of error messages and become very big (xGB!). It is possible to delete this file with the shell command:

```
rm -rf .xsession-errors
```

Note: After deleting this file you have to log out to free the reserved disk space.

It is helpful to check these files and of course the core file which are named as core.<pid> under Linux. To find them, you can use the command:

```
find / -name core.* -print
```

12.5.4 You cannot log in as normal user

There are several possible reasons why you cannot login as normal user. First find out if other normal users can log in. If they can, the problem is user specific:

1. Your password is wrong
2. The hard disk is full. Login in single user mode and remove unwanted files
3. One of your personal setup files is corrupt. Check the files:
   - `/home/<user>/.desktop-<hostname>/log`
   - `/var/log/messages`

12.6 Useful configuration hints

In this chapter you can find some useful configurations of the xorg.conf file.

12.6.1 Definition of the font path

In the file `/etc/X11/xorg.conf` you can add an information about the location of the fontpath, which make it easier for programs to find the necessary fonts. E.g. if you have fonts available in */usr/X11R6/lib/X11/rgb*

```
...
Section "Files"
   RgbPath"/usr/X11R6/lib/X11/rgb"
   FontPath   "unix/:7100"
EndSection
...
```

12.6.2 Increase the swap space

With the description below you can create a second swap file in case you want to increase the swap size of your system:

1. Open a linux shell
2. Login as root with the command **`su -`**
3. Enter the command:

   `dd if=/dev/zero of=/swapfile bs=2097445888 count=1`
4. Enter the command:

   `mkswap /swapfile`
5. Enter the command:

   `swapon /swapfile`
6. Check if the creation of the swapfile was successful:

   `cat /proc/swaps`

   You should get a three-line answer, e.g.:

```
Filename      Type           Size      Used      Priority
/dev/hda5     partition      2048720   <xxx>     -1
```

```
/swapfile    file          2048726  0        -2
```

7. To activate the swap file during boot time enter the command:

   nedit /etc/fstab

   and duplicate the line that describes the original swap entry. Change the second column from swap into /swapfile. Save and close this file.

8. Enter the command:

   reboot

12.7 Spectrometer hardware tests

The ***TopSpin*** DVD contains various programs to test the spectrometer hardware components.

12.7.1 Spectrometer internal boards

Test programs for spectrometer internal boards like RCU, TCU, FCU etc. are started on the CCU.

1. Type **telnet spect** and log in as root
2. Type **/u/systest/rcu/rcutest** (to test the rcu)

After starting a test, type `h` to get help or type `auto` to run a complete test. The tests for the other boards are started in the same way, just replace the names accordingly.

Chapter 13

Important Linux features

13.1 Important Commands

13.1.1 rpm

calls the Red Hat package manager which manage the installation of software packages.

- **`rpm -q ABC`** → list version of installed package *ABC*
- **`rpm --help`** → list options and their description for the rpm command
- **`rpm -qa`** → list all installed programs
- **`rpm -Uvh abc`** → install or upgrade the rpm package *abc*. This action is silent and shows #-marks as display of progress
- **`rpm -Fvh abc`** → upgrade the rpm package *abc*. Does not install any new packages. This action is silent and shows #-marks as display of progress
- **`rpm -Va`** → list all files of the default installation which are modified since the installation
- **`rpm -qi ABC`** → list informations of version and installation of package *ABC*
- **`rpm -ql ABC`** → list informations of installed files of package *ABC*

13.1.2 cd

cd: "change directory"

- **`cd`** → change to your home directory
- **`cd dira`** → change to directory *dira*
- **`cd /u/data/guest/nmr`** → change to directory */u/data/guest/nmr*
- **`cd dataseta`** → change to directory */u/data/guest/nmr/dataseta*
- **`cd ..`** → change to directory */u/data/guest/nmr*
- **`cd ../../usera/nmr`** → change to directory */u/data/usera/nmr*

13.1.3 ls

`ls`: list the contents of a directory

- **`ls`** → list files and subdirectories in current directory
- **`ls -l`** → list complete file information
- **`ls -al`** → also list files starting with '.'
- **`ls -Rl`** → also list the contents of all subdirectories
- **`ls -lt`** or **`ls -lrt`** → sort by time of last modification

13.1.4 chmod

chmod: change the permissions of a file or directory

(To understand the permissions and type of access please refer to chapter 14.1)

1. using the character representation: **`chmod [ugo][+-][rwx] filename`**
   - **`chmod a+r fila`**
     make fila readable for all users
     `-r--r--r-- user group 102 Apr 10 12.20 fila`
   - **`chmod a+w fila`**

make fila writable for all users

```
-rw-rw-rw- user group 102 Apr 10 12.20 fila
```

- **chmod ug+x fila**

  make fila executable for the owner and the group

  ```
  -rwxrwxrw- user group 102 Apr 10 12.20 fila
  ```

- **chmod o-w fila**

  make fila not writable for others

  ```
  -rwxrwxr-- user group 102 Apr 10 12.20 fila
  ```

- **chmod -R +w dira**

  make the directory tree dira, including all files and sub directories, writable for all users

2. using the numerical representation: **chmod xxx filename**

   - **chmod 444 fila**

     make fila readable for all users

     ```
     -r--r--r-- user group 102 Apr 10 12.20 fila
     ```

   - **chmod 222 fila**

     make fila writable for all users

     ```
     --w--w--w- user group 102 Apr 10 12.20 fila
     ```

   - **chmod 640 fila**

     make fila read/write for the owner, read for the group

     ```
     -rw-r----- user group 102 Apr 10 12.20 fila
     ```

   - **chmod 751 fila**

make fila read/write/execute for the owner, read/execute for the group and execute for others

```
-rwxr-x--x user group 102 Apr 10 12.20 fila
```

- **chmod -R 222 dira**

  make the directory tree dira, including all files and sub directories, writable for all users

13.1.5 chown / chgrp

chown /chgrp: change the owner/group of a file or directory. The output of:

ls -l filea or

ls -ld dira shows the result.

- change the owner of the file *fila* to *usera*

  chown usera fila

  ```
  -r--r--r-- usera system 102 Apr 10 12.20 fila
  ```

- change the group of the file *fila* to *grpa*

  chgrp grpa fila

  ```
  -r--r--r-- usera grpa 102 Apr 10 12.20 fila
  ```

- change the owner of directory *dira* to usera

  chown usera dira

- change the owner of directory tree *dira* to *usera*, including all files and subdirectories

  chown -R usera dira

- change the group of directory tree *dira* to *grpa*

  chgrp -R grpa dira

- set the owner and group of the directory tree *dira* to *usera* and *grpa*

```
chown usera.grpa dira
-rwxr-xr-x usera grpa 102 Apr 10 12.20 dira
```

13.1.6 grep

grep: search for a string in a text file and show the lines containing this string

- search for string *stringa* in the file *fila*

```
grep stringa fila
```

- search for *stringa* in all files in the current directory

```
grep stringa *
```

- search for *stringa* in all files AND directories in the current directory

```
grep -r stringa *
```

- search for *stringa* in all files which starts with *a*, *b*,*c* or *d*

```
grep stringa [a-d] *
```

- print the lines in fila not containing *stringa*

```
grep -v stringa fila
```

- ignore upper/lower case in *stringa*

```
grep -i stringa fila
```

- search for *stringa* or *stringb* in the file *filea*

```
grep -i "stringa|stringa" fila
```

- search for *stringa* in the output of a command, e.g. **`ps -ef`**
  `ps -efw| grep stringa`

13.1.7 find

`find`: search for files and directories in a directory tree

- search for entries (files and directories) called *fila* in the directory tree *dira*
  `find dira -name fila -print`

- search for *fila* on all local partitions, not on NFS mounted partitions
  `find / -local -name fila -print`

- search for entries that start with *a*
  `find dira -name "a*" -print`

- search for entries not called *fila*
  `find dira ! -name fila -print`

- search for entries newer than the file *fila*
  `find dira -newer fila -print`

- search for files bigger than 1000 blocks
  `find dira -size +1000 -print`

- run a Linux command (e.g. *rm*, *lp*) on all entries *fila*
  `find dira -name fila -exec lp {} \;`

  for example to delete 2D processed data: *2rr*, *2ri*, *2ir* and *2ii* in */opt/topspin:*
  `find /opt/topspin -name "2[ir][ri]" -exec rm {} \;`

13.1.8 ps

ps: show the Linux process table

- show all processes

  ps -efw

```
UID PID PPID C STIME TTY TIME COMD
root 0 0 0 14:01:12 ? 0:01 sched
root 1 0 0 14:01:12 ? 0:00 /etc/init
root 164 1 0 14:01:48 ? 0:00 /usr/etc/nfsd 4
root 270 1 0 14:01:56 ? 0:00 /sbin/cron
lp 254 1 0 14:01:54 ? 0:00 /usr/lib/lpsched
root 308 1 0 14:01:58 ? 0:00 /opt/topspin/prog/topspin/bfsd
guest 312 309 0 14:01:59 pts/2 0:00 /opt/topspin/prog/top-
spin/cpr/cpr
```

- show all ***TopSpin*** processes

  ps -efw | grep prog

```
UID   PID  PPID  C STIME TTY TIME COMD
guest 1143 686 0 17:07:14pts/1 0:00 /opt/topspin/prog/cpr/cpr
guest 1151 1143 0 17:07:24 pts/1 0:00 /opt/topspin/prog/mod/go
guest 1149 1143 0 17:07:15 pts/1 0:01 /opt/topspin/prog/cpr/xcpu
guest 1170 1168 0 17:09:42 pts/0 0:00 grep prog
```

13.1.9 kill

kill: terminate a Linux process

(for a graphic tool use **<red hat> → System → KDE System Guard**)

- kill processes with PID 1149, 1151 and 1143

  kill 1149 1151 1143

- kill directly processes with PID 1149, 1151 and 1143
  `kill -9 1149 1151 1143`

Use **`kill -9 PID`** only if **`kill PID`** does not kill the process!

13.1.10 compress, gzip

`compress`, **`gzip, bzip`**: compression to reduce the size of a file

File compression can be used to:

- save disk space on rarely used files
- reduce network traffic (e.g. **`rcp`**, **`ftp`**, E-mail)

- compress a file, *fila* is replaced by *fila.Z*
  `compress fila`

- uncompress a file, *fila.Z* is replaced by *fila*
  `uncompress fila`

- compress a file, *fila* is replaced by *fila.gz*
  `gzip fila`

- uncompress a file, *fila.gz* is replaced by *fila*
  `gunzip fila`

- compress a file, *fila* is replaced by *fila.gz*
  `bzip2 fila`

- uncompress a file, *fila.gz* is replaced by *fila*

```
bunzip2 fila
```

Some remarks:

- Uncompression does not require the suffix *.Z* or *.gz*
- compression factor depends on the file type (20-70%)
- **gzip** gives a better reduction in size than **compress**

13.1.11 tar

tar: This command allows to convert a directory (tree) into a file. This is a convenient tool for attaching many files to an email or transferring them via ftp

- copy the directory-tree *dira* into the file *dira.tar*

```
tar cvf dira.tar dira
```

- extract *fila* from *dira.tar*

```
tar xvf dira.tar fila
```

- copy the directory-tree *dira* into the file *dira.tar* and compresses (gzip) the file

```
tar cvzf dira.tar.gz dira
```

- copy the directory-tree *dira* into the file *dira.tar* and compresses (bzip2) the file

```
tar cvjf dira.tar.bz2 dira
```

- extract *fila* from compressed file *dira.tar.gz*

```
tar xvzf dira.tar fila
```

- list the occurrences of *fila* in *dira.tar*

```
tar tvf dira.tar fila
```

- append *filb* to the end of the archive

  tar rvf dira.tar filb

- append if *fila* does not exist in *fila.tar* or if it exists but has been modified

  tar uvf dira.tar fila

- you can copy with relative pathnames e.g.

  cd /u/data/guest/nmr

  tar cvf dataseta

- or with absolute pathnames e.g.

  tar cvf /u/data/guest/nmr/dataseta

13.2 Important Files

13.2.1 /etc/shadow

the file `/etc/shadow`:

- contains the complete password information
- has one line for each user (account) on the system, each line contains 9 fields separated by colons
- example

```
root:$1$Oz.sVA5j$yMP3jpXgNTIjLTo6CZ7QK1:11432:0:99999:7:::
bin:*:11432:0:99999:7:::
daemon:*:11432:0:99999:7:::
adm:*:11432:0:99999:7:::
lp:*:11432:0:99999:7:::
sync:*:11432:0:99999:7:::
shutdown:*:11432:0:99999:7:::
halt:*:11432:0:99999:7:::
```

```
mail:*:11432:0:99999:7:::
news:*:11432:0:99999:7:::
uucp:*:11432:0:99999:7:::
operator:*:11432:0:99999:7:::
games:*:11432:0:99999:7:::
gopher:*:11432:0:99999:7:::
ftp:*:11432:0:99999:7:::
nobody:*:11432:0:99999:7:::
nscd:!!:11432:0:99999:7:::
mailnull:!!:11432:0:99999:7:::
ident:!!:11432:0:99999:7:::
rpc:!!:11432:0:99999:7:::
rpcuser:!!:11432:0:99999:7:::
xfs:!!:11432:0:99999:7:::
gdm:!!:11432:0:99999:7:::
apache:!!:11535:0:99999:7:::
testuser:oaHKvUemEH3TE:11561:0::7:::0
```

meaning of the fields:

1. *Login name*
2. *Encrypted password*
3. *Days since Jan 1, 1970 that password was last changed*
4. *Days before password may be changed*
5. *Days after password must be changed*
6. *Days before password is to expire that user is warned*
7. *Days after password expires that account is disabled*
8. *Days since Jan 1, 1970 that accoumt is disabled*
9. *A reserved field*

13.2.2 /etc/passwd

the file `/etc/passwd`:

- contains the complete login account information

- has one line for each user (account) on the system, each line contains 7 fields separated by colons

example

```
root:x:0:0:root:/root:/bin/bash
bin:x:1:1:bin:/bin:
daemon:x:2:2:daemon:/sbin:
adm:x:3:4:adm:/var/adm:
lp:x:4:7:lp:/var/spool/lpd:
sync:x:5:0:sync:/sbin:/bin/sync
shutdown:x:6:0:shutdown:/sbin:/sbin/shutdown
halt:x:7:0:halt:/sbin:/sbin/halt
mail:x:8:12:mail:/var/spool/mail:
news:x:9:13:news:/var/spool/news:
uucp:x:10:14:uucp:/var/spool/uucp:
operator:x:11:0:operator:/root:
games:x:12:100:games:/usr/games:
gopher:x:13:30:gopher:/usr/lib/gopher-data:
ftp:x:14:50:FTP User:/home/ftp:
nobody:x:99:99:Nobody:/:
nscd:x:28:28:NSCD Daemon:/:/bin/false
mailnull:x:47:47::/var/spool/mqueue:/dev/null
ident:x:98:98:pident user:/:/bin/false
rpc:x:32:32:Portmapper RPC user:/:/bin/false
rpcuser:x:29:29:RPC Service User:/var/lib/nfs:/bin/false
xfs:x:43:43:X Font Server:/etc/X11/fs:/bin/false
gdm:x:42:42::/home/gdm:/bin/bash
apache:x:48:48:Apache:/var/www:/bin/false
```

```
testuser:x:1001:1003:testuser:/home/testuser:/bin/bash
```

meaning of the fields:

1: *Login name*

2: *password*

3: *User Id*; must be a unique number for each user

4: *Group Id*; must be a unique number for each group

5: *Full Name*; the users full name, may contain blanks

6: *home directory*; usually /home/"user", but can be different

7: *shell*; must contain full pathname e.g. /bin/sh or /bin/bash

In the field *password* there are several entries possible:

- the field is empty

  Security leak: the user has no password, everybody is able to login on this account
- the field contains an encrypted password

  Security leak: the user has a password, everybody is able to read and probably able to decrypt this password
- the field contains: *****

  There is no password which translates to the encrypted password: *****

  Nobody is able to login on this account
- the field contains: *x* (default configuration)

  The account has a shadow password. The encrypted password is written in the file `/etc/shadow` that is only readable for root (see chapter 13.2.1). This is the default setting on Red Hat Enterprise Linux WS 3

13.2.3 /etc/group

The file `/etc/group`

- contains the complete information for groups of login accounts

- has one line for each group on the system

Each line contains 4 fields separated by colons:

example

```
root::0:root
users::100:guest,jim
```

meaning of the fields:

1. *the Group Name*
2. *encrypted group password; usually empty*
3. *group Id; must be unique for a group and the same on each host*
4. *the list of users who belong to this group, separated by commas*

Why are users divided into groups?

You can share your files with users within your group and protect them from all other users.

The file `/etc/group` can only be changed by root.

13.2.4 .bashrc

The file `.bashrc`:

- sets your personal Linux environment
- is executed every time you log in
- resides in your home directory
- is used in connection with the shells *sh* and *bash*

You can edit the file `.bashrc` and add your personal preferences, e.g.:

- *umask 002*

- *PATH=$PATH:/home/guest*
- *NMR=/opt/topspin/data/guest/nmr*
- *export PATH NMR*
- *1r() { find $@ -name 1r -ls }*
- *alias ts=topspin*

Now open a new shell:

- *umask* will be set to 002
- guests home directory is part of the Linux search path
- you can type **`cd $NMR`** instead of

  `cd /opt/topspin/data/guest/nmr`
- you can type **`1r <dirA> <dirB>`** for searching all files called *1r* in the in the directory trees *dirA* and *dirB*
- you can type **`ts`** instead of **`topspin`**

Note the difference between *NMR*, an environment variable and *xw*, a Linux function.

For *csh* and *tcsh* the file `.cshrc` is used. Note that the setting of environment variables is handled differently.

13.2.5 umask

umask: set the initial permissions for file creation

The initial permissions of a file are set according to:

permission = creation permission - umask

- the creation permissions are:

  666 for files created by an editor (e.g. vi, emacs)

  777 for an executable program, created by a compiler

- each user can set his own umask, e.g in his `.profile` or `.bashrc` [1]. For this it is necessary to add a line like this:

  ```
  umask 0002
  ```

  The 4-digit number must start with zero. The following three digits describe the permissions for the user, group and others.

examples

1. create a file *fila*, e.g. with vi, for different values of umask
2. show the output of **`ls -l fila`**

- umask 000 → permissions 666

  ```
  -rw-rw-rw- 1 owner group 10 Jun 7 12:20 fila
  ```

- umask 002 → permissions 664

  ```
  -rw-rw-r-- 1 owner group 10 Jun 7 12:20 fila
  ```

- umask 024 → permissions 642

  ```
  -rw-r---w- 1 owner group 10 Jun 7 12:20 fila
  ```

- umask 666 → permissions 000

  ```
  ----------  1 owner group 10 Jun 7 12:20 fila
  ```

13.3 Linux shells

A Linux shell:

- is a layer between the operating system and the user.

1. umask can be set for all users in the file `/etc/profile` and `/etc/csh.login` (*sh* and bash) or `/etc/csh.cshrc` (csh and tcsh)

- offers the user a way to communicate with the OS.
- is selected upon installation of a new user

Type echo $SHELL to find out which shell you use!

different Linux shells and the files executed during login:

- `.profile`
  sh and *bash* (also executes `.bashrc` if it exists)
- `.cshrc`
  csh and *tcsh*

Important differences between shells [1]:

- How do you set environment variables
  sh and *bash*:
  1. `export variable=value`

  csh and *tcsh*:
  `1.setenv variable value`

- *tcsh* and *bash* offer history substitution
  you can use the arrow keys to repeat and modify previously entered commands.

13.3.1 How to use the bash

- Open a shell and type in commands

- How to repeat a previously entered command
  1. use the *arrow keys* to get a command back
  2. hit the *Enter key* to execute the command again

1. type **`man sh`** or **`man csh`** for more information on these shells

- How to repeat and change a previously entered command
  1. use the *arrow keys* to get a command back
  2. use the *arrow keys* to move around in the line
     use **`Control-a`** to move to the beginning of the line
     use **`Control-e`** to move to the end of the line
  3. change the command according to your needs
  4. hit the *Enter key* to execute the command

- How to search for previously entered commands:
  type **`Control-r`** and enter a string or keyword to search for the last command containing that string by typing **`Control-r`** again, you can search for earlier commands containing the same string

- Use <TAB> key for filename/command completition:
  Not sure how File or command is written? Just enter the first characters and press <TAB> key, e.g. :
  vi /etc/X11/xo<TAB> -> vi /etc/X11/xorg.conf

- How to set the prompt in the bash
  The prompt can be changed by defining the environment variable PS1.
  1. type **`cd`** to change to your home directory
  2. edit (e.g. with vi) the file `.profile` and set PS1; you can include several items into the prompt, e.g.:
     a) the hostname of the computer:
        `PS1='\h'`
     b) the logname of the user:
        `PS1='\u'`
     c) the current directory:
        `PS1='\w'`
     d) the last part of the current directory:

```
PS1='\W'
```

e) certain characters, e.g.:

```
PS1=hello or PS1=% or PS1='>'
```
[1]

f) a combinations of the items above, e.g.:

```
PS1='\h:\w>'
```

in case of the last example the prompt will look like:
<hostname> : /u/data/guest >

3. save the file and leave the editor
4. log out and log in again to see the effect of the change

The second prompt can be set be defining the variable *PS2*.

If you want to read the manual pages for the *bash*, type: **`man bash`**

13.4 How to avoid much typing in Linux

13.4.1 General

1. use environment variables, e.g.:

   `NMR=/opt/topspin/data/usera/nmr`
   `export NMR`

   these 2 lines can be entered in your file `.bashrc`

   Open a new shell and type **`cd $NMR`** to go to the corresponding directory.
2. use Linux functions, e.g.:

   `data()`
   `{`
   `cd /opt/topspin/data/usera/nmr`
   `}`

1. characters which have a special meaning in Linux, e.g. < , >, \ , and *;* must be quoted

this line can be defined in your file `.bashrc`

Open a new shell and type **`data`** to execute the function.

3. use copy and paste

   mark text by holding the left mouse button down

   paste this text somewhere by clicking the middle mouse button

4. use the Linux shells bash or tcsh
   - use the arrow keys up/down to repeat and/or modify previously entered commands
   - use the Tab key to complete commands and paths

5. use a Linux shell script

   They are described in the next chapter 13.4.2.

13.4.2 Linux shell scripts

A shell script executes (a series of) Linux commands:

- is an executable text file
- can contain a series of Linux commands
- can contain control loops and variables

example

1. *scripta* displays the date, current directory and contents:

   edit a file *scripta* and enter:

   `date`

   `pwd`

   `ls`

   make scripta executable: **`chmod a+x scripta`**

   execute the script by typing **`./scripta`** [1]

When executing scripta a possible output is:

Wed Jan 3 03:51:07 PST 1996

/home/guest

scripta

fila

Note: the first line of the script should be:

```
#! /bin/sh
```

2. *scriptb* displays the contents of a pulse program:

- edit the file *scriptb* and enter:

  dir=/opt/topspin/exp/stan/nmr/lists/pp

  cd $dir

  cat $1

  $dir = the value of a parameter which is set in the script

  $1 = an argument given to the script when it is executed
- make the file executable: **chmod +x scriptb**
- execute the script by typing its name and argument: **./scriptb zg30**

3. Example of a control and loop structure in a shell script: [1]

```
for i in `ls *.c`                (for all files with the extension .c)
do
  if grep strn $i                (if the file contains the string strn)
  then
  rm $i                          (remove the file)
  fi
done
```

1. "./" means: the command resides in the current directory. You can skip the "./" if the current directory is part of the Linux search path. Type `echo $PATH` to see the Linux search path.
1. For more information on control and loop structures type **man sh** or **man test**.

13.4.3 cron - crontab

Any Linux command or program can be executed automatically on a regular basis.

check if crond is running: **`ps -efw| grep crond`**

if crond is not running: **`service crond start`**

create a crontab file using the following syntax:

min hour daymo month daywk command

min: minute (0-59)

hour: hour (0-23)

daymo: day of the month (1-31)

month: month of the year (1-12)

daywk: day of the week (0-6 with 0=Sunday)

command: the command or program to be executed

Suppose you want to:

- backup your data at 4.30 am on Tuesday to Friday
- delete all core files at 2 am on Sunday

Note that the second task needs root permissions.

a) type **`cd`** to go to your home directory
b) type **`su`** to become root
c) edit the file `fila` and enter the following lines:

```
30 04 * * 2-5 tar cv /u/data/<user>/nmr
00 02 * * 0 find / -name core -exec rm {} \;
```

d) type crontab fila

You can skip step b) if all tasks in your crontab file can be done as normal user. Type **`man crontab`** for more information.

Chapter 14

File and directory handling

14.1 Permissions and Type of Access

14.1.1 Permissions of a file

The permissions of a file:

- determine what each user can do with the file
- are represented :
  - by a set of characters -, *r*, *w* and *x* or
  - by a set of numbers between *0* and *7*

1 = *x* = file is *executable*

2 = *w*= file is *writable*

4 = *r* = file is *readable*

The numbers *3*, *5*, *6* and *7* are combinations of *1*,*2* and *4*:

e.g. *7* = *4* + *2* + *1*= *rwx*

14.1.2 Permissions of a directory

The permissions of a directory are represented as follows:

1 = x = search

2 = w= write

4 = r = read

14.1.3 Types of Access

Each file has 3 sets of permissions for 3 categories of users:

- the actual *owner* (shortened '*u*' like *user*)
- users who have the *same group* ID as the owner [1] (shortened '*g*' like *group*)
- users who have a *different group* ID than the owner (shortened '*o*' like *other*)

14.1.4 Example

- Type **`ls -l filename`** to see the 3 sets of file permission
  e.g. **`ls -l fila`**

```
-rwxrw-r-- 1 jim sys 987 Sep 15 15:08 fila
```

  The permissions of the file *fila* are *764*:
  7 = rwx for the *user jim*
  6 = rw- for all users of the *group sys*
  4 = r- - for *other* users

- Use the command ***`ls -ld`*** to see the directory permissions.
  e.g. **`ls -dl dira`**

```
drwxr-xr-- 1 jim sys 987 Sep 15 15:08 dira
```

1. the group attribute of a file can be changed with **`chgrp`**, the permissions of a file always refer to the group ID which is shown with **`ls -l filename`**

The permissions of the directory *dira* are *754*:

- everybody can read (= see) the directory *dira*, e.g. use **`ls`** on *dira*
- only the owner *jim* and members of the group sys can read and search e.g. use **`cd`**, **`pwd`**, **`ls`**, **`cat`**, **`more`**, **`du`**, **`file`** on or in *dira*
- only the owner *jim* can also write or remove files in *dira*, e.g. use **`rm`**, **`cp`**, **`mv`**, **`touch`** on files in *dira*

- In the following example the directories *dira*, *dirb* and *dirc* are assumed to be *readable* and *searchable*.
  - creating files

    If the user guest wants to create the file `fila`, e.g. :

    `touch /dira/dirb/dirc/fila`

    the directory *dirc* must be *writable* for *guest*, the parent directories *dirb* and *dira* do not have to be *writable* for *guest*

  - removing files

    If the user guest wants to remove the file `fila`, e.g. :

    `rm /dira/dirb/dirc/fila`

    the directory *dirc* must be *writeable* for *guest,* the parent directories *dirb* and *dira* do not have to be *writable* for *guest.* The file *fila* can have any permissions, even 000, and any owner or group, you can always remove it if its directory is writable !

Chapter 15

Useful tools for Red Hat Enterprise Linux WS 4

This chapter contains a description of some tools we found useful. We realize that many other tools are available for various purposes and we are very interested in your experiences. Just send your comments to:

`nmr-software-support@bruker.de`

15.1 How to use a memory stick under Linux

In previous Red Hat versions it was not easy to use a USB-memory stick. Under RED HAT ENTERPRISE LINUX WS 4 this became much more convenient. In this chapter you can find a description how to add a functionality which identifies one and also more than one USB stick and pops up a short-cut icon on the desktop for each device when it is plugged in.

Each Linux PC delivered by Bruker BioSpin Germany is already configured in this way.

15.1.1 Add an additional Panel

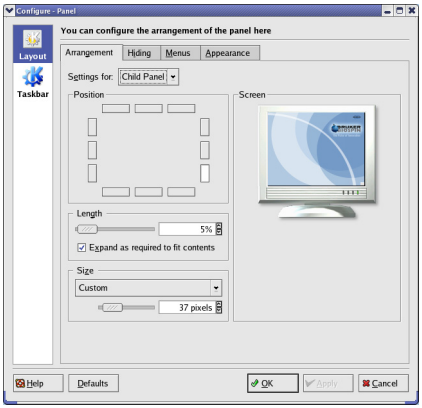
1. Click right on an empty place on the panel (task bar) and select

Add → Panel → Child Panel

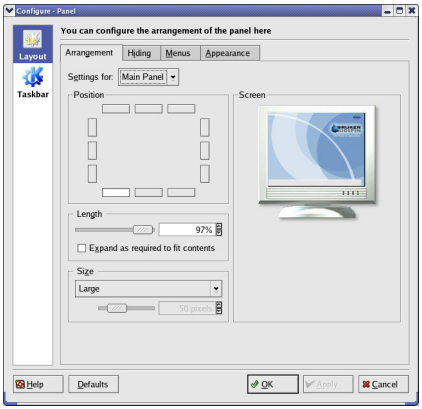
2. Click right on the main panel and select

   Configure Panel

3. In the window Configure Panel go to the tab *Arrangement* and select **Child Panel** in the field *Settings For*
4. Define as *Position* the lower rectangle on the right side, set *Length* to **5%** and *Size* to **37** pixels (see picture)



5. Select **Main Panel** in the field *Settings For*
6. Define as *Position* the left rectangle on the bottom, set *Length* to **97%** and *Size* to **Large** and deselect *Expand as required to fit content*



7. Go to the tab *Hiding* and select **Main Panel** in the field *Settings For*

8. Enable:
   Allow other windows to cover the panel and
   Raise when the pointers touches the screen's: **Bottom Edge**
9. Select **Child Panel** in the field *Settings For*
10. Enable:
    Allow other windows to cover the panel and
    Raise when the pointers touches the screen's: **Bottom Right Corner**
11. Click **OK**
12. Click right on the top of the new panel and select:
    Add → Applet → Devices
13. Click right on the top of the new panel and select:
    Configure Devices
    (Note that the respective entry in the context menu only appears if you click on the top side of the new panel)
14. A window *Devices Applet Preferences - Devices* will appear
15. In the tab *Device Types* uncheck all entries and select only:
    Mounted Hard Disk Partition and
    Unmounted Hard Disk Partition
16. In the tab *Devices* deselect all entries
    (Note that no memory stick should be connected at this time)
17. Now connect your memory stick
    → a hard disk icon appears in the new panel
18. Click left on the icon and select Open
    → a konqueror window will appear and shows the content of the memory stick

Any sticks which will be connected to the system will appear as seperate icon.

To free a memory stick click left on its icon and select **Unmount**

15.2 Firewall configuration

RED HAT ENTERPRISE LINUX WS 4 has a firewall package inside. You can activate and configure it during installation (see chapter 9.1) or in the running system.

Note that for acquisition the ethernet card for spectrometer control has not to be restricted by the firewall! For this it is strongly recommended to free the ethernet card after activating the firewall (see below)!

The rules for the firewall, checked and executed during boot time, are stored in the file[1]: `/etc/sysconfig/iptables-config`

The rules in this file are:

- defined during installation (see chapter 9.1)
- added manually (see troubleshooting, chapter 12.3.1.2)
- added manually by using a graphical user interface (see the next chapter)

15.2.1 Firewall configuration

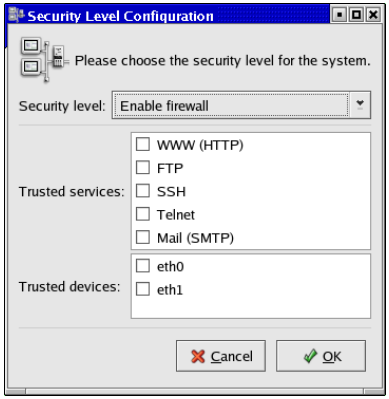
RED HAT ENTERPRISE LINUX WS 4 offers a graphical user interface that allows you to define some firewall configurations. The following example describes a firewall configuration that allows *SSH* traffic on *eth0* and frees *eth1* completely.

1. Open a Linux shell
2. Become superuser
   - **`su -`**
   - enter superuser password
3. Type in
   - **`redhat-config-securitylevel`**

     or click on
   - **SystemSettings → Security level**

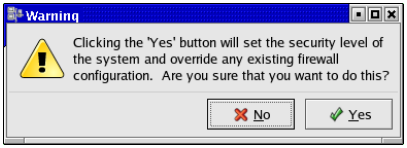
1. In RED HAT ENTERPRISE LINUX WS 4 there is also another possibility for the firewall settings: `/etc/sysconfig/iptables`

a window *Security Level Configuration* will appear



4. Select under *Security level* the entry **Enable firewall**
5. Select under *Trusted Services* the entry **SSH**
6. Select under *Trusted devices* the entry **eth1**
7. The window now looks like this, click on **OK**

8. The window *Warning* will appear



Click on **Yes**

Now the configuration of the Firewall is finished and your system is protected right now.

Note that this tool described here allows not a very specific configuration, but it is useful for a quick and secure setting. In case you like to free another service like smb you can use the start command

```
redhat-config-securitylevel-tui
```

(note that the securitylevel-tui is one word and contains no space)

A window appears wherein you can define the same rules as above described but you get an additional field called ‚Other ports'.

Another useful tool is the freeware guarddog that can be downloaded from:

http://www.simonzone.com/software/guarddog/

All these three ways that were described in this chapter uses the firewall tool of RED HAT ENTERPRISE LINUX WS 4 *iptables*. With *iptables* it is possible to define a very complex firewall installation.

15.3 Tools for internal communication

If the Linux NMR workstation should be used as server, the following packages should be installed:

Package	on CD	Necessary for
xinetd	RED HAT ENTERPRISE LINUX WS 4 *Operating System CD **2** of 4*	"superserver" for several servers
telnet-server	RED HAT ENTERPRISE LINUX WS 4 *Operating System CD **3** of 4*	for telnet logins
vsftpd	*on TopSpin 2.1 Linux CD in /linux/rpm*	for ftp sessions
rsh-server	RED HAT ENTERPRISE LINUX WS 4 *Operating System CD **3** of 4*	for rlogin and rsh
samba	RED HAT ENTERPRISE LINUX WS 4 *Operating System CD **2** of 4*	to export directories to Windows
samba-swat	RED HAT ENTERPRISE LINUX WS 4 *Operating System CD **2** of 4*	graphical configuration toll for samba

15.3.1 Installation description of an additional package: xinetd[1]

Other packages are installed similarly

1. Check if *xinetd* is installed so far
   - **`rpm -q xinetd`**
   - is the output like this

     xinetd-<version-number>
   - Yes? You can skip this chapter
   - No? Go to step 2.
2. Insert RED HAT ENTERPRISE LINUX WS 4 *Operating System CD 2 of 4*
3. Click **<red hat> → System Tools → More System Tools → File Manager - Super User Mode**
4. A window *run as root - KDE su* will appear
   - enter root password
5. A window *file:/root - Konqueror* will appear
   - go to **file:/mnt/cdrom/RedHat/RPMS**
6. Search for the entry *xinetd-<version-number>.i386.rpm*
7. Double click **xinetd<version-number>.i386.rpm**
8. A window *Completed System Preparation* will appear
   - click **Continue**
9. Close the *Konqueror* window *file:/mnt/cdrom/RedHat/RPMS*
10. To eject the CD click right on the CD icon on the desktop and choose **`eject`**

15.3.2 Check if all necessary components are installed

To check if all necessary components are installed, please type

```
/sbin/chkconfig --list
```

on a shell and if these lines are exists[2]

1. A detailed description of a software installation is described in chapter 9.3.2
2. If a process like this is not started, start it on a shell by typing **`/sbin/chkconfig <process> on`**

```
xinetd          0:off  1:off  2:off  3:on   4:on   5:on   6:off
smb             0:off  1:off  2:off  3:on   4:on   5:on   6:off
xinetd          based services:
                rexec:          on
                rlogin:         on
                rsh:            on
                telnet:         on
                vsftpd:         on
                swat:           on
```

15.4 Configure a second monitor

The NVidia graphics cards which are part of the PC equipment delivered by Bruker BioSpin Germany have two ports (DVI and VGA). Because of this it is possible to add a second monitor to the system.

The default nvidia config file `/etc/X11/xorg.conf` contains already the necessary configuration settings as part of the section '*Screen*'. You have just to remove the '#' at the beginning of the respective lines:

```
### TWINVIEW SETUP ###
# Option "TwinView"
# Option "TwinViewOrientation" "LeftOf"
# Option "MetaModes" "1280x1024, 1280x1024"
# Option "SecondMonitorHorizSync" "31.0 - 82.0"
# Option "SecondMonitorVertRefresh" "56.0 - 76.0"
# Option "ConnectedMonitor" "CRT, CRT"
```

If you want to add the same monitor as you have it already, you can just remove the '#' on the first two lines:

```
Option "TwinView"
Option "TwinViewOrientation" "LeftOf"
```

In case of different monitors you have to configure the second one with the available configuration lines.

After you have add the second monitor you can work with the two monitors as it

would be only one with a double width. You can either

- stretch the ***TopSpin*** window over the two monitors simply by clicking on the border of the ***TopSpin*** window and move the mouse until the window has the desired size

  or

- work with e.g. ***TopSpin*** on one Monitor and e.g. ICON-NMR on the second one. Just open the respective windows and move them with mouse to the desired position.

15.5 Setting up permissions for rsh, rlogin and rcp

The commands **rcp**, **rlogin** and **rsh**[1] require special access permissions. There are two ways to set up these permission.

1. The system administrator can setup up these permission for all users:

a) Open a shell

b) Type **su** to become superuser

c) **cd /etc**

d) Edit the file `hosts.allow`

Make two entries for every remote host from which access is allowed, e.g.:

```
sunflower
sunflower.netx.lab.com
```

2. As a normal user, you can allow remote access from a remote host for yourself:

a) Open a shell

b) Go to your home directory; type **cd**

c) Edit the file `.rhosts`

Make two entries for every remote host from which access is allowed, e.g.:

```
sunflower
sunflower.netx.lab.com
```

d) **chmod 644 .rhosts**

1. For installation please see chapter 15.3

In both examples *sunflower* is the hostname and *netx.lab.com* is the domainname of the remote host.

To allow **`rcp`**, **`rsh`** and **`rlogin`** network wide in all directions, you must setup the file `/etc/hosts.allow` or `.rhosts` on each host.

15.6 Creating a screenshot of the desktop

There are several programs that offer the possibility for creating a screenshot of the desktop or of individual windows.

- Click on **<red hat> → Graphics → KSnapshot**

or the program *Gimp*:

- Open a Linux shell and type in **gimp**

  Inside *gimp* you has to go to **File → Acquire → Screen Shot ...**

15.7 Creating an icon on the desktop

For a more convenient using of Red Hat, it is recommended to create icons of frequently used commands on the desktop

15.7.1 Create an icon for opening a pdf file with Acrobat Reader[1]

1. Click right mouse button on the desktop
   - a popup window appears
   - choose **Create New → File → Link To Application**
   - a window *Properties for Program.desktop* will appear
   - in section *General*:
     - choose a name for the new icon, e.g. Installation Guide
     - click on the icon symbol, in the upcoming window you can choose one that you enjoy
   - in section *Application*:

1. Note that Acrobat reader might not installed by default on your system. For installation see chapter **9.3.1**

- type in the command for opening the manual in a shell:

```
acroread /opt/topspin/prog/docu/english/xwinproc/pdf/install_guide_linux.pdf
```

(if case you have installed TOPSPIN in the default directory `/opt/top-spin`)

15.8 Register your Linux system with Red Hat

The license agreement of RED HAT ENTERPRISE LINUX WS 4 demanded to register the PC to the Red Hat Network service. A description how to register and how to use the Red Hat Network can be found in the following chapters.

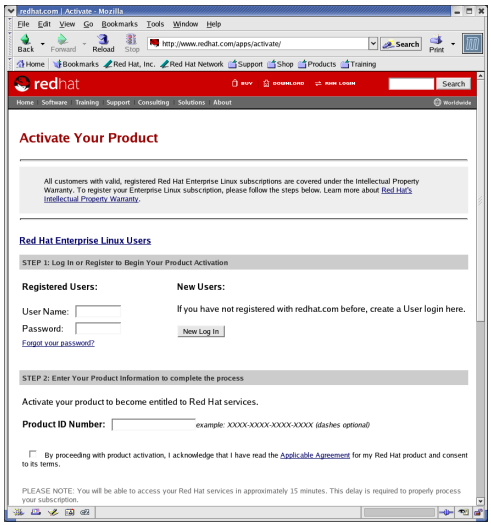
You have to do the activation of the license key first and the registration at Red Hat Network as a second step!

15.8.1 Activate your Linux license at Red Hat Network

1. Start you web browser
2. Enter the URL

   http://redhat.com/now

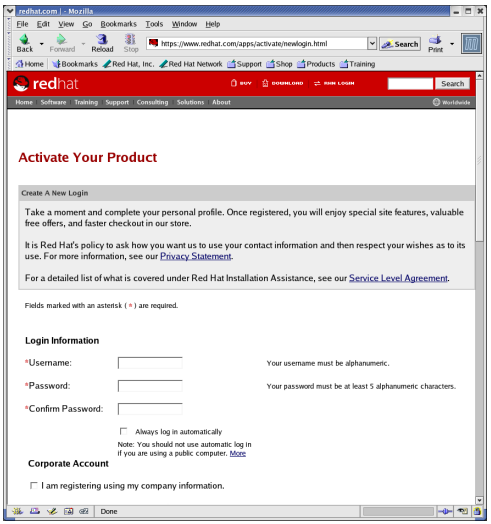
   you will see the following web side



3. If you are not registered so far or you want to use an additional account, click on

- **`New Log In`**

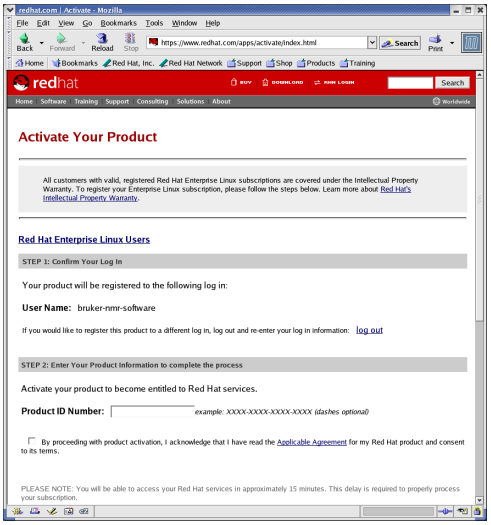
4. The window changes to



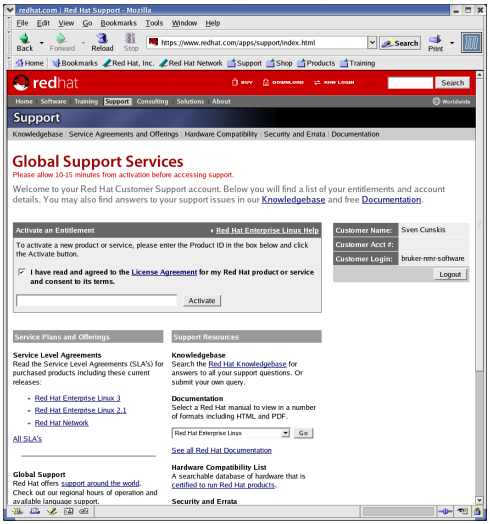
Enter all required information (fields marked with a small red asterisk). At the bottom of the window click on

- **`Create Login`**

5. The window changes to



6. In the field Product ID Number enter your license key for RED HAT ENTERPRISE LINUX WS 4
7. The window changes to



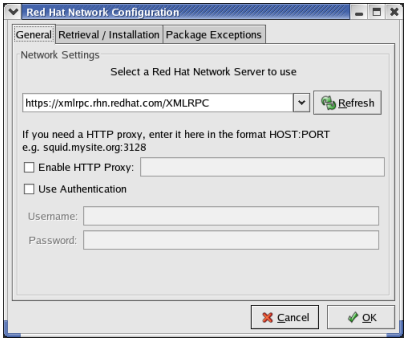
8. you have successfully activated your license code, you can now go to next chapter and register the PC to the Red Hat Network

15.8.2 Register the PC to the Red Hat Network

1. Log in as root
2. Open a Linux shell and enter **`up2date`**
3. If you are not registered to Red Hat Network so far, the window *Red Hat Network Registration* will appear

- Click **`Register with RHN`**

4. The window *Red Hat Network Configuration* will appear

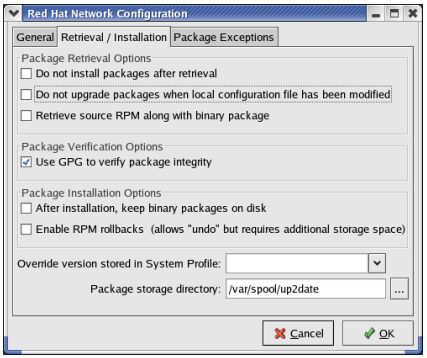


   - Click on the tab pane **`Retrieval / Installation`**

5. The window changes to *Retrieval / Installation*

   - Disable the entry

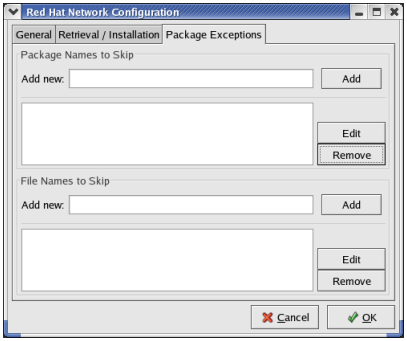
     Do not upgrade packages when local configuration file has been modified



   - Click on the tab pane **`Package Exceptions`**

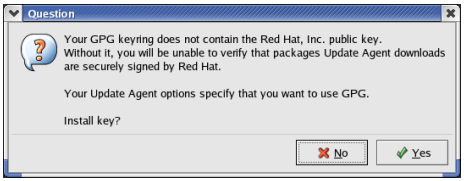
6. The window changes to *Package Exceptions*

- Click on the entry *kernel* and click on *Remove*



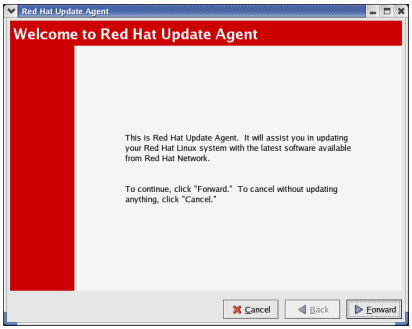
- Click **`OK`**

7. The window *Question* will appear



- Click **`Yes`**

8. The window *Welcome to Red Hat Update Agent* will appear

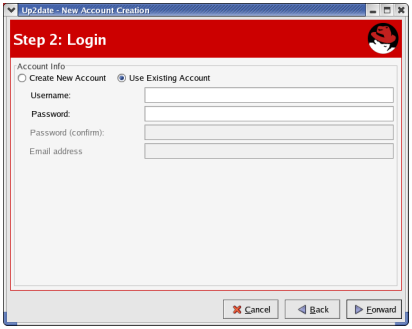


- Click **`Forward`**

9. The window will change to *Review the Red Hat Privacy Statement*

- Click **`Forward`**

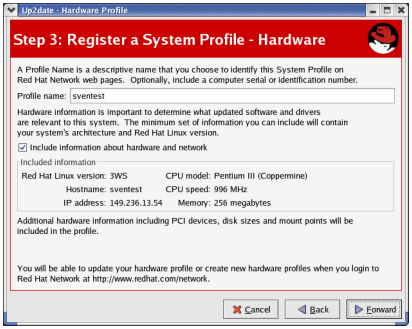
10. The window will change to *Login*



Enable *Use Existing Account* and enter the username and password that you have specified in chapter 15.8.1

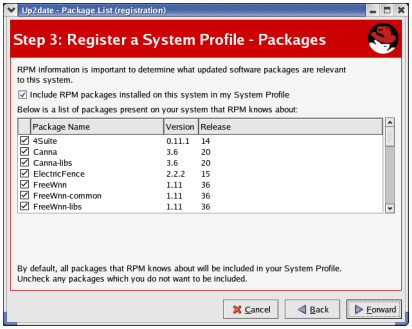
- Click **`Forward`**

11. The window will change to *Register a System Profile - Hardware*



- Click **`Forward`**

12. The window will change to *Register a System Profile - Packages*

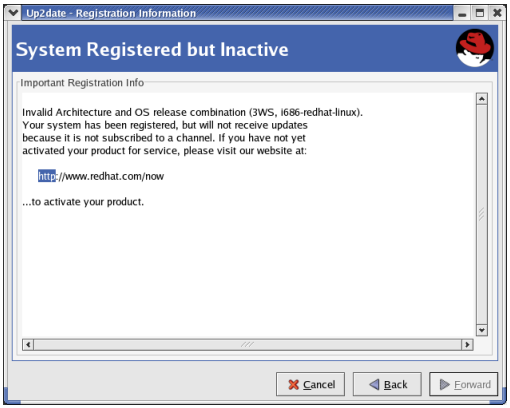


- Click **`Forward`**

13. The window will change to *Send Profile Information to Red Hat Network*

- Click **`Forward`**

If you have already activeted your license code as it is described in chapter 15.8.1, the process will go on with updating your system. Just follow the instructions given. If you have not done the activation so far, the following information window would appear.



15.8.3 Activate the Red Hat Alert Notification Tool

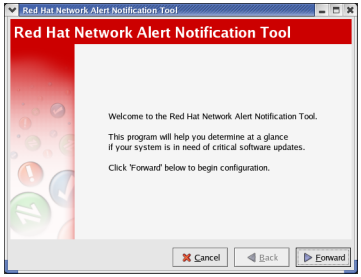
RED HAT ENTERPRISE LINUX WS 4 offers a convenient tool that checks automatically the available security fixes that can be downloaded. If there are any of those packages available or if the connection to Red Hat Network not working, he shows a blinking, red exclamation mark at the lower right side of the desktop.

If the system is up-to-date and the connection to the Red Hat Network is fine, it shows a friendly white hook in a green circle

To activate this tool proceed as follows:

1. Log in as root
2. Click on the Icon at the lower right side of the desktop

3. The window *Red Hat Network Alert Notification Tool* will appear

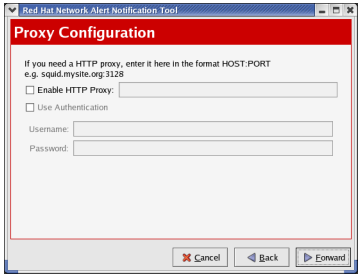


   - Click **`Forward`**

4. The window *Terms of Service* will appear

   - Click **`Forward`**

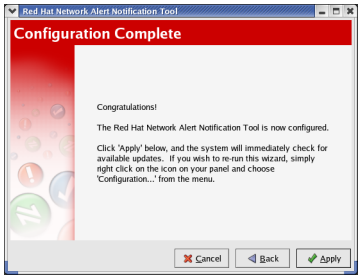
5. The window *Proxy Configuration* will appear



If you use a proxy server enter the required information, if not just leave the fields empty

- Click **Forward**

6. The window *Configuration Complete* will appear



- Click **Apply**

15.9 The Emergency Recovery DVD

Each PC which is delivered from Bruker BioSpin Germany comes with a Emergency Recovery DVD. This DVD contains an image of the PC and can be used for restoring the PC. The image contains the installed and preconfigured operating system and all necessary programs like ***TopSpin***. It does not contain any user specific data, like spectrometer configuration, NMR datasets or network configuration.

In case of a harddisk crash, a hacked system, or even a stolen PC it is possible to get back on a new PC hardware a well working system within 20 minutes. After restoring the image the last `nmr_backup` file must be restored and the ***TopSpin*** command ***cf*** must be executed.

More information about `nmr_backup` and the ***TopSpin*** command ***nmr_save*** file are available in chapter 6.5

15.9.1 Using the Emergency Recovery CD

Note: This should be done by experienced people only! All data currently on the disk will be destroyed!

If in doubt please contact your system administrator, maybe it is still possible to get data from the old disk. New harddisk are not expensive therefore using a new harddisk for restoring an image might be the best solution!

1. Insert the *Bruker Emergency Recovery DVD* and boot the PC. The window *Image Boot DVD Bruker Biospin* will appear.

   → Press **F1**

2. The *Acronis True Image* selection window appears

   Select *Acronis True Image (full version)*

   Acronis True Image will be started. This will take about 2 minutes.

3. The window *Acronis True Image* appears.

   → Click on **Recovery**

4. The window *Welcome to the Restore Image Wizard* appears.

   → Click on **Next**

5. In the window *Image Archive Selection* click on the plus sign left to *CD Drive*. Typically this is (D:) or (E:). You will see some directory and disk icons.

   → Click on the first disk icon below the directory icons.

   On the right side a short description of the image DVD will appear. Please read this carefully and make sure that this is the image you like to install on this PC.

6. Click **Next** in the window *Restored Hard Disk Drive Location*

7. Select the hard disk on which you want to restore the image. In general you will have only one hard disk available, so click on this line and then click **Next**.

8. In the window *Verify Archive Before Restoring* you can verify the image before it is used. This would need the same time which is necessary for restoring the image.

9. In the window *Partition or Disk to Restore* check the box left to *Disk 1* to restore the complete image.

10. In the window *Restore Partitions Resize* you now have the possibility to change the size of individual partitions. This is only necessary e.g. if you use a smaller hard disk that on which the image was created. So if you use the same disk size you can check *No, I do not want to resize partitions*.

    → Click on **Next**

11. In case the hard disk which you have selected contains already partitions you must select *Yes, I want to delete all the partitions on the destination hard disk drive before restoring.*

    → Click on **Next**

12. In the window *Next Selection* select *No, I do not* because you only want to restore the image on one hard disk.

    → Click on **Next**

13. In the last window you will get a summary of the choosen operations. Check if everything is defined correctly.

    → Click on **Proceed**

14. Restoring image will then be started. This process will take about 20 minutes. When it is finished a window will appear with information *Image was successfully created.*

15.10 An image of the PC

Each PC which is delivered from Bruker BioSpin Germany has a license for the backup tool *Acronis True Image*. With this software it is possible to create a one-to-one backup of the harddisk of the system.

It is recommended to periodically create a backup of the harddisk. In case of any problems (harddisk crash, virus, hacker attack ...) you are able to rebuild the situation of your last backup within a few minutes.

In chapter 15.9 it is described how to use the Bruker Emergency Recovery DVD. This DVD contains the first image of the PC. If you create periodically a new image of your PC you will be able to restore a system which is much more up-to-date and contain all your individual settings like network configuration, user management, spectrometer configuration etc.

15.10.1 Creating an image

You need a boot-CD to start Acronis True Image, if there is no such CD, you can install Acronis True Image on a Windows system and create the *Bootable Rescue Media* from there. The original *Acronis True Image installation CD* is usually bootable.

1. Insert a bootable Acronis True Image CD and boot the PC. The window *Acronis True Image* appears.

   → Click on **Create Image**

2. The window *Create Image Wizard - Welcome to the Create Image Wizard* appears.

   → Click on **Next**

3. In the window *Create Image Wizard - Selecting Partitions to Image* select the partitions you want to image.

   → Click on **Next**

4. A window *Information* appears that informs about the possibility of an incremental image

   → Click on **OK**

5. The window *Create Image Wizard - Image Archive Creation* appears. Select the partition, drive or network drive where you want to store the image. The following steps describe archiving on a network drive

   → Click on **Next**

   Please note that Acronis True Image is able to burn images to DVD with version 9.0 3.633 and higher. Previous versions can only store on CD, harddisks and network drives.

6. The window *Create Image Wizard - Creating Image Mode* appears. Select either a full backup or an incremental one. The following steps describe the creation of a full backup.

   → Click on **Next**

7. The window *Create Image Wizard - Image Archive Splitting* appears. It is recommended to choose *Fixed Size* and specify 650 MB. With this size you can afterwards burn the image files on CD if necessary.

   → Click on **Next**

8. The window *Create Image Wizard - Compression Level* appears, select *Maximum*.

   → Click on **Next**

9. The window *Create Image Wizard - Image Archive Protection* appears. You can enter a password to protect your image. If in doubt do not choose a password, this makes it more save for the restoring of the image.

   → Click on **Next**

10. The window *Create Image Wizard - Image Archive Comments* appears. Enter important information about the current image. This makes it easy in the future to identify this image.

    → Click on **Next**

11. The window *Create Image Wizard - Imaging operation summary* appears. Check if everything is correct.

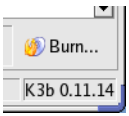
    → Click on **Proceed**

12. Creation of the image will start. This process will take about 20 minutes. When it is finished a window will appear with information *Image was successfully created.*

15.11 Using the DVD/CD-Writer

On the desktop of the Linux PCs delivered by Bruker BioSpin Germany is an icon called Burn CD/DVD. This icon starts internally the program `/usr/bin/K3b`

1. Double click the icon starts K3b. You can open one of the projects **New Audio CD**, **New Data CD**, **New Data DVD** and **Copy CD** in the lower part of the window.
2. When you have choosen a project you can define the files which should be burned on CD/DVD just by drag&drop from the upper part of the K3b window to the lower part.
3. When finished click on **Burn...** button at the lower right corner of the window.



4. A window will open where you can define several settings like verify, speed, multisession, permissions, name of the disk etc. Make sure that everything is correct configured then click on **Burn**

5. When the burning process is finished an information window will appear.

15.12 Add a new harddisk

NOTE: Using the command fdisk is recommended only for seasoned persons, because formatting the old harddisk will destroy all data on this disk!

To buy a new harddisk on the Linux PC is quite easy because you can buy a usual harddisk in a PC store. After installing the new disk you have to do the following:

1. Start the PC
2. Open a shell and become root
3. If the new harddisk is a scsi-disk, type in the command

   `cat /proc/scsi/scsi`

   If it is a ide-disk use the command

   `cat /proc/ide/hdX/model` (the *X* in *hdX* have to be replaced with the correct number of the disk, which is *a*, *b*, *c* or *d*)
4. Does the command show the harddisk which was built in?
   - Yes? Go to step 5
   - No? There was something wrong during build in, or the harddisk is damaged.
5. Type in the command **`fdisk -l`**

   the output looks like this :

Device	*Boot*	*Start*	*End*	*Blocks*	*Id*	*System*
/dev/sda1	*	*1*	*3*	*24066*	*4*	*FAT16 <32M*
...						

   A second harddisk would show upas device '*sdbx*', where x is a number. All Devices *sdax* are part of harddisk number 1, *sdbx* of number two and so on.
6. Does the output show the new disk?
   - Yes and the partitioning is OK? Go to step 9
   - Yes but the partitioning was not done so far? Go to step 7
   - No? Go to step 7
7. To partition the new disk, type in the command **`fdisk /dev/sdb`**

In case you need help just type m and choose the possibility you want

8. After partitioning is done you have to create the filesystem on the new partitions. This can be done with the command

   `mkfs /dev/sdbx`

   where *x* is the partition you want to configure

9. Now you can add the new harddisk to the file `/etc/fstab`, open this file with a text editor and add a line like this

   `/dev/sdb1  /X  ext2  defaults  1 2`

   where */X* is an example for the mount point of the new harddisk. Be sure that the mount point you have choosen exists. If you want to use one that does not exists so far, you have to create this directory with the command

   `mkdir X`

   in case you want to use /X.

10. After reboot of the PC you can mount the new disk with the graphical tool

    <red hat> → System → Disk Management

Chapter 16

Appendix

16.1 Some notes for the helium handling

In the ***TopSpin*** home directory (default is `/opt/topspin`) in the directory `prog/logfiles` are two files named `heliumlog` and `heliumlog.err`. The `heliumlog` saves the current helium level in a new line every night at 3.00 am. The `heliumlog.err` documents possible errors during detection of the helium level.

16.1.1 Automatic notification for helium refill

TopSpin is able to send an email notification to a list of defined users if the helium level is equal or less than a predefined limit.

16.1.1.1 Set minimum limit of helium level

You can define the value of the helium level which should trigger the automatic notification (see next chapter)

1. Click **<red hat> → Editors → Text Editor**
2. A window *New Document - Text Editor* will appear
3. type in the percentage (without '%') of the helium level, that should activate the notification, e.g. **`25`**

4. Click **File → Save as**
5. Save the file as `heliumlimit` in the installation directory of ***TopSpin*** (default is `/opt/topspin`) in the subdirectory `conf/instr/<SPECT>`

16.1.1.2 Create shell script 'heliumwarn' for email notification

In this chapter you find an example for the shell script that will be execute the email notification in case the helium level is less than the entry (in %) in the file `heliumlimit`

1. Click **<red hat> → Editors → Text Editor**
2. A window *New Document - Text Editor* will appear
3. Copy the following example in the file

```
#!/bin/sh
# send an email when the helium level is too low
######################################################################
#-----------------------
# user defined variables:
#-----------------------
ADDRESSES="person1@domain person2@domain person3@domain"
INSTRUMENT="spectrometer identification"
MAIL="/usr/bin/mutt"
######################################################################
# no more changes are needed below this point. You may tailor #
# the variable MSG for specific needs though. Be careful!     #
######################################################################
#-----------------------------
# catch command line arguments:
#-----------------------------
MYSELF=$0
LEVEL=$1
LIMIT=$2
#--------------------------------------
# get the name of the spectrometer host:
#--------------------------------------
HOST=`hostname -f`
```

```
user=`whoami`
#---------------------------
# prepare the email message:
#---------------------------
MSG="\n\
Caution:\n\
The magnet of the spectrometer $INSTRUMENT \n\
has an helium level of $LEVEL % \n\
which is less than the limit of $LIMIT %: \n\
Please order liquid helium and refill this magnet.\n\
\n\
This email is automatically send from $MYSELF (user $USER) \n\
on $HOST to:\n\
- $ADDRESSES\n\
"
#-----------------
# mail the message:
#-----------------
echo -e $MSG|$MAIL -s "$INSTRUMENT : Helium refill" $ADDRESSES
exit 0
```

4. Modify the settings of "ADDRESSES" and "INSTRUMENT" and the text in the example as you like
5. Click **File → Save as**
6. Go in the installation directory of ***TopSpin*** (default is `/opt/topspin`) into the subdirectory `prog/bin` and save the file as `heliumwarn`

   Now the defined email addresses will get a notification if the actual helium level is the same or below the entry (in %) in the file

   `<TOPSPIN_HOME>/conf/instr/<spect>/heliumlimit`

   The notifications are sent only once but the procedure will be activated again if the helium level is again higher than the limit.

   Note that this script is only an example, if you would like to add more recipients to the notification list you had to add the respective addresses, if you like to have less addresses you have to delete the respective entries.

16.2 Script for saving important files

TOPSPIN offers a script (*xwinnmr.save*) for saving important files that are not delivered by Bruker BioSpin. This script can save and extract user specific data from the TOPSPIN_HOME directory and puts them into a tar-file. Files that start with an "." are ignored. The script can be started as follows:

- Open a Linux shell and enter

  <TOPSPIN_HOME>/prog/bin/scripts/ xwinnmr.save

Files and directories will be saved into the special tar-file `xwin_backup.tar` which is, by default, in the directory `<TOPSPIN_HOME>/xwin_backup`.

The ***xwinnmr.save*** script saves the same files and directories as the command *nmr_save* (see chapter 6.16.5). Nevertheless there are differences between xwinnmr.save and nmr_save. This is because of compatibility reasons with previous XWIN-NMR installations and corresponding individual scripts that calling the xwinnmr.save script. The differences between these two ways to create a backup are opposed in the following:

Script name	**default directory**	**name of tar-file**
xwinnmr.save	xwin_backup	xwin_backup.tar
nmr_save	nmr_backup	nmr_backup.tar

The options for ***xwinnmr.save*** starting from a command prompt are:
xwinnmr.save [-options]

- ***-help*** additional information
- ***-path <x>*** absolute path where backup tar-file `xwin_backup.tar` will be created
- ***-restore <x> <y>*** absolute path where backup tar-file `xwin_backup.tar` can be found (<x>) and absolute path where the restoring should take place (<y>) (installation directory of TOPSPIN)
- ***-replace*** overwrite the old backup.tar file
- ***-silent*** do not display any messages
- ***-source*** absolute path of ***TOPSPIN***/XWIN-NMR installation that should be saved

- ***-spect <x>*** spectrometer name (e.g. spect; default is the current name)
- ***-verbose*** print more information while backing up

For safety reasons the tar-file will not be replaced by executing the ***xwin-nmr.save*** script once again. So if you like to use the script several times, you have to move the `xwin_backup.tar` file from the directory `<TOPSPIN_HOME>/xwin_backup` on a backup medium (floppy, CD, DVD ...) and then start the script once again or you have to use the 'replace' option.

16.3 Where Do I Find What?

If you cannot find the required information in this manual, please check the manuals listed below.

Further useful information you can also find in the Release Letter for the respective TOPSPIN version.

- *TOPSPIN Users Guide*
  Window handling, displaying data, interactive data manipulation, user interface related items
- *Acquisition Reference*
  Description of all acquisition commands, parameters and files.
- *Processing Reference*
  Description of all processing commands, parameters and files.
- *AU Reference*
  How to write AU programs. Description of all AU macros, functions and variables. List of Bruker BioSpin AU programs.

For further manuals please refer to:

- TOPSPIN → **Help**
- *http://www.bruker-biospin.de/NMR/nmrsoftw/passwd/docu*
- NMR-GUIDE

Chapter 17

Bruker BioSpin addresses

Germany

Bruker BioSpin GmbH
Silberstreifen
D-76287 Rheinstetten
Tel: (++49) (721) 51 61 0
Fax: (++49) (721) 51 71 01

Bruker BioSpin Software Department
Silberstreifen
D-76287 Rheinstetten
Tel: (++49) (721) 5161 455
Fax: (++49) (721) 5161 943

http://www.bruker-biospin.de

ftp server: ftp.bruker.de

Email: nmr@bruker-biospin.de (sales)
mbu@bruker.de (service)
applik@bruker.de (application)
nmr-software-support@bruker.de (software)
license@bruker.de (licenses)

USA

Bruker BioSpin Corporation
15 Fortune Drive
Manning Road
Billerica, MA. 01821-3991

Tel: (++1)(978) 667 9580 5195 (center)
(++1)(978) 667 9580 5444 (application)
Fax: (++1)(978) 667 6168 (center)
(++1)(978) 667 2955 (application)

http://www.bruker-biospin.com
ftp server: ftp.bruker.com

Email: applab@bruker.com
center@bruker.com
software@bruker.com

Switzerland

Bruker BioSpin AG
Industriestraße 26
CH-8117 Fällanden

Tel: (++41)(1) 8 25 91 11
Fax: (++41)(1) 8 25 96 96

web server: www.bruker.ch
E-Mail: epweb@bruker.ch
all_ap@bruker.ch

France

Bruker BioSpin S.A.
34, rue de l'industrie
F-67166 Wissembourg/Cedex

Tel: (++33)(3) 88 73 68 00
Fax: (++33)(3) 88 73 68 79

web server: www.bruker.fr

E-Mail: support-rmn@bruker.fr (customer support)

England

Bruker BioSpin LTD.

Banner lane
Coventry CV4 9GH
Tel: (++44)(2476) 855200
Fax: (++44)(2476) 465317

web server: www.bruker.co.uk

Email:service@bruker.co.uk
apps@bruker.co.uk

Our webpage

http://www.bruker-biospin.de/NMR/about/offices

provides contact addresses of our facilities and offices worldwide

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