TopSpin
Version: 3.1.0
Software Manual

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1 Introduction

1.1 About this manual

This manual is the TopSpin Installation Guide for Microsoft Windows and Linux and describes the installation of TopSpin 3.1 under Microsoft Windows 7.0 Professional and Linux CentOS 5.5.

The shown figures are obtained under Microsoft Windows 7.0 operating system because the appearance of the setup routine is nearly the same for both operating systems, Windows 7.0 and CentOS 5.5. Only if there are major differences, figures and instructions will be mentioned for both systems.

This installation guide is available:

• as a hardcopy
• as pdf file on the toplevel of the TopSpin DVD
• as the up to date version on the bruker web-server:
  http://www.bruker-biospin.com/documentation_nmr.htm
• Note that this manual does not contain the TopSpin Release letter. This is a separate document delivered as pdf- or text-files on the TopSpin DVD and also on the Bruker web-server (you will find it at the same URL as the Installation Guide.

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

1.2 Conventions

**Bold Arial**: commands to type in command line

*Cursive Arial*: path names and directories
1.3 Hardware and software requirements for TopSpin 3.1

1.3.1 Operating system requirement

TopSpin 3.1 on spectrometer computers is supported for:

- Windows 7.0 Professional
- CentOS 5.5

All operating system updates (hot fixes and service packs) at the time TopSpin 3.1 was released have been tested and are supported.

on Datastations TopSpin 3.1 is supported for:

- Windows 7.0 Professional
- Windows Vista (Business Edition)
- Windows XP Professional
- CentOS 5.5
- Red Hat WS 4

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

- on other Linux systems
- on Windows XP Home Edition

Bruker BioSpin does not recommend these systems for the use of TopSpin. Please note, the usage of not supported operating system is at one’s own risk.
1.3.2 Special PC Hardware requirements

To run TopSpin 3.1 (for acquisition) we recommend the following computer hardware:

- Memory $\geq$ 4 GB
- Video (graphics)-card memory $\geq$ 512 MB
- Ethernet card (to control a spectrometer, it is essential to have a second ethernet card)
- Mouse with 3-button possibilities
- DVD device

1.3.3 Spectrometer requirements

TopSpin 3.1 supports acquisition for AVANCE II and AVANCE III spectrometers. TopSpin 2.1 is the final version for AVANCE I spectrometer control.

1.3.4 Software requirements

- on DVD: 'TopSpin 3.1'
  - TopSpin
  - Flexlm Licence Manager
- For control of AV II spectrometer the following software must be installed and configured:
  - Hummingbird NFS Server Version 14 available on Bruker TopSpin NT Tool-kit 2 CD (H9437W2)
- For TopSpin Help and NMR Guide
  - Adobe Acrobat Reader

1. It is recommended not to use shared memory graphics, because in some cases memory problems could be observed.
### 1.3.5 NFS Server

With TopSpin 3.1 NFS Server is only required to control AVANCE II spectrometer. If your PC is used as a datasation, no NFS is needed.

#### 1.3.5.1 TopSpin NT Toolkit 2 CD

The Bruker BioSpin TopSpin NT Toolkit 2 CD contains the Hummingbird NFS Server and the OpenText NFS Solo 14 package with its NFS Server in the NFS 14 directory. The OpenText NFS Solo 14 is supported for Windows XP, Windows Vista and Windows 7 (32- and 64-bit), but together with TopSpin 3.0 it is only supported for Windows 7.0. The Hummingbird NFS Server 7.1 is supported for Windows 2000, Windows XP and Windows Vista.

The TopSpin NT Toolkit 2 CD can be ordered from Bruker BioSpin (part number H9437W2).

- Note: NFS 14 has to be used if your Operating System is Windows 7.

#### 1.3.5.2 How to install TopSpin NT Toolkit 2

- Log in as a Local Administrator
- Insert the CDROM TopSpin NT Toolkit 2
- Click `Start` → `Computer` (for Windows XP: Double-click the icon My Computer)
- A window 'Computer' will appear (for Windows XP:'My Computer');
  
  Double-click the CDROM icon
- A window showing the contents of the CDROM will appear:
  
  Click the NFS 14 folder and start the installer by double-clicking Msetup.exe for Windows 7. Right click the icon and click „Run as administrator“ for Windows XP: Double-click the icon
- A window 'Open Text NFS Solo 14' will appear:
  
  - Click Install Open Text NFS Solo. This window will change to the subtitle
'Install Open Text NFS Solo'
Click **Personal Installation**

- A window 'Setup Language Selection' will appear:
  Choose **English** (this description is written for the English one)
  Click **OK**

- A window 'Open Text Setup Wizard' will appear and display several progress bars. Finally it shows:
  The Open Text Setup Wizard will install… Open Text NFS Solo 14 on your computer…
  Click **Next**

- A window 'License Agreement' will appear:
  Click **I accept ...** → Click **Next**

- A window 'Customer Information' will appear. Insert the appropriate information or leave the information unchanged (it is important that this application will be installed for anyone who uses this computer):
  Click **Next**

- A window 'Destination Folder' will appear:
  Click **Next**

- A window 'User Directory Location' will appear:
  Select **Per User Directory**
  Click **Next**

- A window 'Setup Type' will appear:
  Click **Custom** → Click **Next**

- A window 'Custom Setup' will appear:
  Click **Connectivity Tools** and click X (meaning: This feature will not be available)
  Click **Accessories** and click X
  Click **Security** and click X
  Click the + button to open the **Open Text NFS** submenu
  Click **Name Mapping** and click the second button to install this feature and
all subfeatures
Click **NFS Administration** and click **X**
Click **NFS Client** and click **X**
Click **NFS Server** and click the second button to install this feature and all subfeatures
Click **Next**
- A window 'Additional Install Options for the Product' will appear:
  Click **Next**
- A window 'Ready to Install the Product' will appear:
  Click **Install**
- A window 'Installing Open Text product' will appear showing a progress bar
- A window 'Open Text Setup Wizard Completed' will appear:
  Click **Finish**
- A window 'Open Text NFS Solo 14 Installer Information' will appear:
  You must restart your system for the configuration changes made to **Open Text NFS Server 14** to take effect. Click **Yes** to restart now or **No** if you plan to restart later.
  Click **No**
- Back in the window 'Install Open Text NFS Solo':
  Click **Back**
  Click **Exit**
- Remove the CDROM and reboot the Windows PC.

### 1.3.5.3 Configuring the NFS Server for spectrometer control

Before you can configure the NFS Server you must first install packages on the TopSpin DVD, particularly the DISKLESS package.
1.3.5.4 Firewall configuration for the NFS Server

If you have enabled the firewall, you have to configure the firewall for the NFS Server. This can be done automatically during the TopSpin installation or later while executing the setfirewall.cmd\(^1\).

- Note: If you have installed the NFS Server after the TopSpin installation, you have to configure the firewall again!

1.3.5.5 Configuring NFS Solo 14

If your PC is controlling an AV II spectrometer, you must configure NFS after the installation of the DISKLESS package (part of TopSpin). This configuration requires that Open Text NFS Solo 14 Server is installed.

- Note: The NFS Server is only required for Bruker AVANCE II spectrometers. Bruker AVANCE III spectrometers do not need the NFS Server.

If you have NFS Solo 14 installed, proceed as follows:

[1] Create the user and groups

You can continue with step [2] if the users are already created (TopSpin DISKLESS installation creates them automatically).

Otherwise please create the following user and groups.

- 'diskless_user_sys' (with 'account is disabled')\(^2\) and the groups (with no members)
  - 'diskless_group_root'
  - 'diskless_group_other'
  - 'diskless_group_sys'

[2] Click Start → (All) Programs → Open Text NFS Solo 14 → Open Text NFS Server Configuration

---

1. <topspinhome>\prog\bin\Utilities\Miscellaneous\setfirewall.cmd

2. Creation and configuration of the necessary user and groups are most convenient if it is done in the user management tool of the management console and not in the user management of the control panel. For starting the management console click right on 'My computer' and choose 'manage'. A new window appears where you can choose 'local users and groups'.

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• A window ‘Open Text NFS Server Configuration’ will appear:
  Click the Security tab
  Unselect Allow Unmapped Access
  Unselect Allow Access for Root User from All Hosts
  Click the Shared File Systems tab
  Click Add
• A window ‘Browse for Folder’ will appear:
  In the field Folder browse for the location of the DISKLESS package (e.g.: C:\Bruker\Diskless\clients\spect)
  Important: the Uppercase letters in this path are necessary!
  Click Ok
• A window ‘Shared NFS Directory Properties’ will appear:
  Click the Network Restrictions tab
  Select Limit access to the hosts and netgroups listed below and click Add
• A window ‘Restriction Properties’ will appear:
  Enter spect in the field Entry Identification
  Select Allow Access for Root user
  Click Ok
  The entry „spect Host rw,root” will appear in the list
  Click Ok
  An entry „C:\Bruker\...” will appear in the list ‘NFS Shared File Systems’
  Click Ok
  If a message about the owner and group permissions of spect appears,
  Click Ok
  Click Ok
[3] Click Start → (All) Programs → Open Text NFS Solo 14 → Open Text NFS Tools → Name Mapping Server Configuration
• A window ‘Open Text Name Mapping Server Configuration’ will appear:
  Click the General tab
Click the **Browse** button for the Password file in the section ‘NFS Name Space’ and browse for the location of the DISKLESS package Password file (e.g.: C:\Bruker\Diskless\clients\spect\root\etc\passwd)

**Important:** the Uppercase letters in this path are necessary!

Click the **Browse** button for the Group file in the section ‘NFS Name Space’ and browse for the location of the DISKLESS package Group file (e.g.: C:\Bruker\Diskless\clients\spec\root\etc\group)

Click the **Configure...** button in the section ‘Name Mapping’

- A window ‘Name Mapping’ will appear:
  - Click the **Users** tab
  - Click the **Add...** button in the section ‘Selective Mapping’

- A window ‘Selective Mapping’ will appear:
  - Click both **Load...** buttons
  - Adding a User mapping select only the respective Windows user and the corresponding NFS user and click **Create**
  - Map Windows user **Administrator** to NFS user **root**
  - Map Windows user **diskless_user_sys** to NFS user **sys**
  - Click **Close**
  - Click the **Groups** tab
  - Click the **Add...** button in the section ‘Selective Mapping’

- A window ‘Selective Mapping’ will appear:
  - Click both **Load...** buttons
  - Adding a Group mapping, select only the respective Windows group and the corresponding NFS group and click **Create**.
  - Map Windows group **diskless_group_root** to NFS group **root**
  - Map Windows group **diskless_group_other** to NFS group **other**
  - Map Windows group **diskless_group_sys** to NFS group **sys**
  - Click **Close**
  - Click **Ok**

- Click **Ok**
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2 Installing TopSpin

2.1 Preparing for the Topspin Installation

For displaying the TopSpin Online Help, for parts of the NMR-Guide and the Release Letter the PDF viewer Acrobat Reader is required. It is not installed automatically as a part of TopSpin. It is available from Adobe as a download:

http://www.adobe.com/products

In the DOWNLOAD section choose Adobe Reader and follow the instructions on the screen.

Before starting the installation make sure you are logged in as a local administrator.

2.2 Packages on the TopSpin DVD

1. TopSpin: Acquisition and processing software
   - TopSpin Plot Editor: Object oriented WYSIWYG plot editor
   - GNU TOOLS: System tools required by TopSpin

2. CMC-a: CMC-assist

3. IconNMR: Icon-driven interface for Routine Spectroscopy and Automation

4. NMR-SIM: Program for numerical simulation of NMR experiments

5. NMR-GLP: Program for ’Good Laboratory Practice’ tests (requires separate license)

6. NMR-GUIDE: Web-browser based teaching and training program

7. NMR-DATA: example data sets

8. DISKLESS: Spectrometer operating system

1. automatically installed as part of the TopSpin package
2. automatically installed as part of the TopSpin package
2.3 Installing TopSpin

This chapter describes the installation of TopSpin 3.1 as a local administrator.

The main decision you have to make during installation is the location (directory) of the TopSpin version. If a previous TopSpin installation exists on your PC you can either:

- install the new version in parallel to the previous one
  e.g. old in C:\Bruker\TopSpin3.0 and the new in C:\Bruker\TopSpin3.1 (Windows)
  e.g. old in /opt/topspin3.0 and the new in /opt/topspin3.1 (Linux)
- install the new version in the same directory as the previous one
  e.g. both C:\Bruker\TopSpin (Windows)
  e.g. both /opt/topspin (Linux)

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 you can just start and re-use it.
Installing TopSpin

The TopSpin installation on a Windows system and a Linux system are very similar. For this guide the windows appearing during this installation are taken from a PC with a Windows 7.0 system. Only different or additional windows when using a Linux system will be shown at the relevant places.

a) If you have disabled User Account Control (UAC) you have to log in with an account that has local administrator rights

b) Close all windows on the desktop

c) Insert the DVD TopSpin 3.1

d) Start the installation

• If the Windows 7.0 autorun feature is enabled the popup window shown in Figure 2.1 will appear automatically. Click ‘Run install.cmd’.

Figure 2.1 AutoPlay window of TopSpin3.1 DVD

If the autorun function is disabled, open the Windows Explorer, select your DVD drive and double-click install.cmd."
Installing TopSpin

- Using the CentOS 5.5 Linux system a 'cd-rom file browser' will open when you have inserted the CD. If it will not be opened automatically click the now visible 'CD' icon on the Desktop. On KDE with konquerer, click 'install'. On Gnome with Nautilus, double-click 'install' in the right part of the window and the 'Run in a Terminal' button in the newly opened window.

Using Windows 7.0 now a 'Command Prompt' window (C:\windows\system32\cmd.exe) which informs about current installation process and a 'User Account Control' window will be opened. In the 'User Account Control' window you will be asked for your administration password.

![Image of Command Prompt window](image.png)

Figure 2.2 Second 'Command Prompt' window with 'Starting Installation' popup window

In the upcoming 'Command Prompt' window a small popup window will show information about the start of the installation (see Fig. 2.2).

1. Please note, that there is also a file called 'install' on the DVD. This is the installation script for Linux, under Windows you have to click on the file 'install.cmd'
Installing TopSpin

Using CentOS 5.5 a `/mnt/cdrom/install` shell (window) will be opened. First you have to enter the administrator password here. Then the installation will start and a log file is displayed in the same shell mentioned above.

After a short time the installer opens two additional windows shown in Figure 2.3 and Figure 2.4.

The `overall progress information` window (Fig. 2.3) will be visible during the whole installation process and will inform you about the progress.

![Overall progress information window of TopSpin installer](image)

The `Welcome` window (Fig. 2.4) gives you some initial information of the setup tool.
Click 'Next' to continue with the TopSpin setup.

In the 'overall progress information' window the setup parameters now change to running. This is also displayed in the 'Status' line at the bottom of this window.

After clicking the 'Next' button the following window will appear and allow you to decide if you want to install GPL licensed Cygwin Software. It is recommended to install both components. Click the 'Next' button.

A new window (Fig. 2.6) containing the Release Letter as a pdf document will be displayed.
Installing TopSpin

Figure 2.6  TopSpin Release Letter as pdf document in separate window
Installing TopSpin

- Please read the Release Letter! You can find all informations about news and bug fixes of the current version.

When you have finished reading the Release Letter, close the window by clicking the X button in the upper right corner.

After closing the Release Letter a new window for definition of the installation directory is displayed (Fig. 2.7)

![Figure 2.7](image)

Figure 2.7 Pop up window for defining an installation directory

The installation setup suggests the default Bruker directory for TopSpin. Figure 2.7 shows the one when using Windows 7.0. On the Linux system it is /opt/topspin3.1. By clicking the ‘Browse’ button you may define your own directory destination. In case of a non existing path you will be asked to confirm path creation for both Windows 7 and CentOS.

Click the ‘Next’ button and you will be led again to a new popup window for selecting the setup type (Fig. 2.8)
Installing TopSpin

Select one of the offered setup types:

- Select Data processing if you want to use TopSpin for data processing only.\(^1\)
- Select Data processing, acquisition and automation if you want to use TopSpin for spectrometer control. This will automatically install Diskless.\(^2\)
- Selecting Customized allows you to install selected programs only. If you have chosen this selection and click 'Next', a window with all available programs for the TopSpin installation (Fig. 2.9) will be displayed.

Select the packages you want to install.

Note that Diskless is only required if your PC controls a spectrometer.

The packages Perch, Aurelia Amix, SBASE and CMCQ Viewer, Protein Dynamic Center, Assure-RMS, Assure-RMSSBASE and GLP require a separate licence.

The selection shown in Figure 2.9 corresponds to Data processing, acquisition and

\(^1\) The packages TopSpin, NMR-Sim, NMR-Data, Magnet Information & Control System, CMC-assist and FLEXlm will be installed

\(^2\) The packages mentioned above and IconNMR, GLP, NMR-Guide and Diskless will be installed
Installing TopSpin

*automation* which is used in this guide.

![Program selection window for customized installation setup](image)

Figure 2.9  Program selection window for customized installation setup
If your setup selection is finished, click the ‘Next’ button.

Using a Linux system you will now be asked if the TopSpin installation directory should be set (or replaced if there was one before) in the ‘global PATH’ (Fig. 2.10)

![Linux window]

Do you want to replace the TopSpin installation directory in the global PATH?

If you do so, you will be able to start TopSpin by just typing ‘topspin’

Currently the global PATH contains the TopSpin installation directory

/opt/topspin3.0/prog/bin/scripts

- Yes, add the new TopSpin installation directory to the global PATH
- No, leave the global PATH unchanged

Figure 2.10  Global PATH question (Linux System)

Normally you will choose ‘yes’ and click ‘Next’. A new window (Fig. 2.11/ 2.12) prompts to select an NMR Super User now.
Installing TopSpin

Figure 2.11 Selection of NMR Super User (Linux System)

Figure 2.12 Selection of NMR-Super User (Windows System)
Click 'Next' and the next step requires entry of an Administrator Password (Fig. 2.13).

![Figure 2.13](Image)

Figure 2.13 Window for definition of NMR Administer Password

Enter your chosen password and re-enter it for confirmation in the second line. Then click the 'Next' button.

When using a windows system, you now will be prompted to select the installation directories for **Diskless** (Fig. 2.14). For Linux this will be created automatically.

![Figure 2.14](Image)

Figure 2.14 Window for defining the installation directory for Diskless
Installing TopSpin

Independent from the operating system you now have to define the mics (Fig. 2.15) and the NMR-Data (Fig. 2.16) directory.

![Figure 2.15 Window for defining the installation directory for MICS](image1)

You may accept the default directories for each installation directory or click the ‘browse’ button and select the desired one.

![Figure 2.16 Window to define the installation directory for NMR-Data](image2)

The directory for the license software flexlm will be created automatically for Windows 7. With Linux a selection window corresponding the ones in Fig. 2.15 or 2.16 will be displayed. Bruker recommends to use the given directory in this case to avoid problems with license management.
Installing TopSpin

The directories are:

- `C:\flexlm\Bruker` for Windows 7
- `usr/local/flexlm` for Linux

Always finish your selection by clicking the 'Next' button and the installer will lead you to the next one.

Anytime you might track the progress of the installation setup in the 'Overall progress information' window. Figure 2.17 shows it appearance during the directory definition step described above.

![Figure 2.17 'Overall progress information' window of TopSpin installer after directory selection](image-url)
Installing TopSpin

Clicking the 'Next' button after the final directory is defined will open a 'Question' window (Fig. 2.18) which asks regarding the Windows or Linux firewall handling. Bruker recommends to choose the automatic firewall configuration by selecting 'Yes'.

Figure 2.18 'Question' window about the Windows firewall

The installer recognizes if the firewall is installed and enabled on your PC. After clicking 'Yes', TopSpin installation will configure the firewall to enable spectrometer access. Clicking 'No' skips this step and an administrator must configure it later by running:

C:\Bruker\TopSpin3.1\prog\bin\Utilities\Miscellaneous\setfirewall.cmd (Windows 7)
/bin/sh/opt/Bruker/mics/setfirewall.sh.install (Linux)

Note: If your main directory (Windows 7) differs from C:\Bruker\Topspin3.1, you
have to use this one instead!

The installation setup is finished now. A summary of all target directories for the installation and the version number of each package is displayed in a new separate window (Fig. 2.19).

![Window with summary of all target directories for the installation](image)

**Figure 2.19** Window with summary of all target directories for the installation

If you want to change something, click the 'Back' button and the setup goes back to the selection of the setup type (Fig. 2.8).
Installing TopSpin

Clicking the 'Next' button immediately starts the installation of TopSpin, if your PC controls an AVANCE III spectrometer or if it should only be used for data processing (no spectrometer connected at all).

If your spectrometer belongs to the AVANCE II series and DISKLESS has been installed, for both operating system the TopSpin installation routine now wants you to shut the CCU of the spectrometer. The following window (Fig.2.20) is displayed now:

![Figure 2.20 Window for installing the CCU operation system](image)

Open a 'Command Prompt' window (click Start and type 'command prompt' in the search box, select 'Command Prompt' from the upcoming list) or a GNU shell (click Start → All Programs → Bruker → TOPSPIN → TOPSPIN 3.1 → GNU Shell) (Fig.2.21) and follow the instructions given in Figure 2.20. Check if your spectrometer is shut down, click 'Next'.
Now the installation starts.

![Figure 2.21 'Prompt' window for shutting down the spectrometer](image)

If you have other active TopSpin versions on your computer, they have to be closed. Otherwise the following error message (see Fig. 2.22) will appear and the installation (for every possible spectrometer type) will not start.

![Figure 2.22 Error message pointing out running programs](image)

The whole installation process takes up some time. You can see the progress in the 'Overall progress information' window e.g. as shown in Figure 2.23.
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Additionally you can see the progress of the installation in an upcoming window (Fig. 2.24). The steps consist of verification of already installed files in the selected target directories, extraction and check of extracted files per selected product.

For Windows the two initially opened 'command prompt' windows inform you about the source of installed programs and files ('command prompt' window:C:\windows\system32\cmd.exe) and the current log file ('command prompt' window shown in Fig. 2.2).

When the installation is finished a window (Fig. 2.25) is displayed when working with a Linux system. Read it carefully and click 'Seen' or 'Save as' if this information
Installing TopSpin might be relevant for your purpose.

Figure 2.24  Installation progress

Flexlm will use the TCP/IP port 1753. If you require a different port number for any reason, you will have to change the port number in the files

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

After changing the port number the license manager must be restarted.

Please see the release letter for further information.

Figure 2.25  Information at the end of TopSpin installation (Linux)
Installing TopSpin

Then the installation is finished and a summary of the installation result is given in a new popup window (Fig. 2.26).

Using a Windows operating system the same window (Fig.2.26) is displayed directly after all program files have been copied to your PC.

![Popup window which shows the status of the finished installation](image)

Figure 2.26  Popup window which shows the status of the finished installation

If one or more packages have not been installed successfully, check for possible reasons and run the installation again. The final window will display a 'Details' button. Click on it to get the details about the reason for problems or errors.
Additionally the 'cmd' window or shell respectively, will display all warnings and error messages issued by the installer. These warnings and error massages can be found in the installer log file.

If you contact the NMR support for installing problems, please make sure to attach the installation log file (see also Chapter 2.5).

After the final product confirmation dialog (Fig. 2.19) the log file is located in the TopSpin target directory and is named install.log. Before the final product confirmation dialog the log file can be found in

C:\Windows\Temp\install.log (for Windows operating system)
/tmp/install.log (for Linus operating system)

If all packages have been installed successfully click the 'Finish' button.

Clicking the 'Finish' button, the installation tool will check for extra tasks to be launched after the standard installation. These depend on your product selection and your operating system.

If you have selected Perch on Windows for installation, it will be launched now.

If you have selected the product Diskless on Linux, you will be prompted to restart the network service to enable the connection to the spectrometer CCU (Fig. 2.27), if your spectrometer belongs to the AVANCE II series. If you want to do this now click 'Yes'. If your PC is only a datastation you can click 'No'. For AVANCE III spectrometers this question will not appear.
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Figure 2.27  Question about network service restart (Linux)

In both cases this window will be closed, then the window shown in Fig.2.26 is displayed.

At least a window which informs you about the changes of the environment for the Magnet Information & Control System (MICS) program will be displayed (Fig.2.29). For more details about the program and setup please refer to:

Bruker\mics\docs\manual.pdf
When working under Windows, the installation is now finished and the two initially open 'Command Prompt' windows are closed automatically.

In the '/mnt/cdrom/install' window (Fig.2.29) you will be asked to hit enter to close this window.

TopSpin is now installed on your PC. You now have to store a valid license file and install this license (see chapter 3). Then your new software can be started (see also
2.4 Installation of TopSpin 3.1 on top or parallel to former versions

If on your PC a different TopSpin version to the TopSpin 3.1 or another TopSpin 3.1 is installed, you have to decide if the new installation should lead to a coexistent TopSpin version or should go on top the existing one (overwrite the existing one).

a) On the PC exists a different version of TopSpin (e.g. TopSpin 2.1)

Installation of TopSpin 3.1 parallel to an existing version means, you have two fully functional versions of TopSpin. Now you can carefully test the new Version 3.1 and later deinstall the older one.

Installation of TopSpin 3.1 on top of a former version means, you have only one version installed on your PC. This is convenient and does not lead to confusion. In this case the "Resolve conflicts" window (see Fig 2.29) will be displayed. It is recommended to confirm the suggested default with the NEXT button.

b) On your PC exists the same version of TopSpin

Installation of TopSpin 3.1 parallel to the existing version means, you have
two fully functional versions of TopSpin 3.1 on your PC. Installation of TopSpin 3.1 on top of an existing version 3.1 means, you have only one version installed on your PC. A backup of all modified Bruker files will be created. A window (Fig. 2.30) will inform you about the destination of this backup.

![Figure 2.30 Example of a 'Verification result' window after overwriting a TopSpin3.0 version](image)

2.5 Installation results

The installation stores its results in a log file named install.log.
Installing TopSpin

After installation is complete, the log file is stored in the TopSpin folder specified at the start of the installation. An existing log file is not overwritten, instead the new results are appended.

Before the installation begins to extract files to the hard disk, the log file is in the temporary folder C:\Windows\Temp (under Windows) or /tmp (under Linux). The current location of the log file is shown in the shell window that is displayed during installation.

Whenever you contact the support due to installation problems, please attach this log file.

2.6 Automatic installation of TopSpin

It is possible to run an automatic installation of TopSpin (also known as unattended or silent installation). This requires the use of a shell (bash under Linux), or Command Prompt (under Windows). In any case you will have to use the option -a (or --auto). All other options allow you to change the default settings of the installation.

In case of an error or obstacle the automatic installation will stop and display the appropriate message in a dialog window (see Fig. 2.31). In case of an obstacle (such as a running TopSpin session), the installation can still be completed manually when the obstacle has been removed. The results of the installation are stored in the log file as mentioned in section 2.5.

![Figure 2.32 Dialog window with message about error or obstacle during automatic installation](image)
Open a Command Prompt (under Windows) or a shell (under Linux). Then type the full path of "install" together with the desired options. You may want to start install -h first to get a list of available options. All options have to be typed on a single line. The Command Prompt allows you to continue a line on the next one by typing a caret (^) (under Windows) or a backslash (\) (under Linux) as the last character of the line. Most options have a short form (for easy typing) and a long form (for easy remembering). The install command together with its options may be put into a batch file for easy distribution or later reinstallation.

- **Note:** If you use the options below without -a, the installation runs in interactive mode, but changes the defaults to the values specified on the command line. This allows for more easy clicking through the dialogues without the need to change the settings when you have to attend a couple of installations.

Examples:

1. Let the DVD be in drive E:

   To install TopSpin, NMR-Sim, IconNMR, Diskless and FlexLM with TopSpin-Home=c:\Programs\Bruker\Topspin\3.1, type:
   
   E:\install -a -s topspin -s nmrsim -s iconnmr -s diskless -s flexlm --xwin-nmhome "c:\Programs\Bruker\Topspin\3.1"

   To install the CMCQ Viewer into the folder c:\Programs\Bruker\Cmcq, type:
   
   E:\install -a -s cmcqmain -d cmcqmain=c:\Programs\Bruker\Cmcq

2. Let the DVD be mapped to \my-pc\my-share

   To install the standard processing programs and specify the md5sum of an NMR administration password, type:
   
   \my-pc\my-share\install -a --setup-type po --nmradminpwenc
   a13ee062eff9d7295bfc800a11f33704
Installing TopSpin

3. Let the DVD be mounted as /media/cdrecorder

To install the standard acquisition programs and specify the md5sum of a plain NMR
administration password, type:

```
/media/cdrecorder/install -a --setup-type pa --nmradminpw TEDDY
```

To install TopSpin without GCC and specify not to add the installation directory to
the global path, type:

```
/media/cdrecorder/install -a -s topspin --gcc-off --globalpath 0
```

To get a list of the valid program shortnames, type:

```
E:\install -s help or
/media/cdrecorder/install -s help
```
3 TopSpin License

3.1 Questions and answers about the TopSpin license

1. Which program need a license?

TopSpin, TopSpin Plot Editor, NMR-Sim and NMR-Guide need a license. However, if you order a full license for TopSpin, you automatically get a license for all four programs.

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 and Plot Editor will offer only limited functionality.

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

GLP, AMIX, AURELIA, MAXENT, PARAVISION and Perch (only executable for Windows) do need a license which must be ordered for each program separately.

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

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

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

or contact your local Bruker-BioSpin representative.
## TopSpin License

<table>
<thead>
<tr>
<th>License Type</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acquisition, Processing, Automation (<em>IconNMR</em>), Plotting, Experiment Simulation and <em>NMR-Guide</em></td>
<td>Full licence period: 15 years, no restrictions</td>
</tr>
<tr>
<td></td>
<td>Demo licence period: 3 month, Node locked, uncounted, free of charge</td>
</tr>
<tr>
<td>Processing only</td>
<td>Processing and Plotting licence period: 15 years, full processing functionality, no <em>NMR-SIM</em>, no <em>NMR-GUIDE</em></td>
</tr>
<tr>
<td>Presenter</td>
<td>Viewing and Plotting licence period: 15 years, viewing and plotting, no <em>NMR-SIM</em>, no <em>NMR-GUIDE</em></td>
</tr>
</tbody>
</table>

Table 3.1: License types and their contents
TopSpin License

### 3. What kind of license do I need?

If you want to use **TopSpin 3.x** you need a FEATURE line 'TOPSPIN3' in your license.dat file. If you have 'TOPSPIN1' or 'TOPSPIN2' you can only start **TopSpin 1.x** or **TopSpin 2.x**.

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

If more than one license for TopSpin 3.1 are available, you only need one Feature

---

<table>
<thead>
<tr>
<th>License Type</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processing of 1D and higher dimensional data sets, Plotting, Spectrum and FID Simulation, quantification and <strong>NMR-Guide</strong></td>
<td></td>
</tr>
<tr>
<td>Student</td>
<td>license period: 3 years</td>
</tr>
<tr>
<td>full processing functionality, <strong>NMR-Sim, NMR-Guide</strong>, valid student certificate only online purchase, one per student, no upgrades</td>
<td></td>
</tr>
<tr>
<td>Processing license package for education in academia</td>
<td>license period: 3 years</td>
</tr>
<tr>
<td>features like Student license, floating license available in packs of 20, 50 or 100</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.1: License types and their contents
TopSpin License

TOPSPIN3. If more FEATURE lines TOPSPIN3 are available, only one would be read and accepted. To allow the parallel starting of TopSpin 3.0 more places are offered in the Feature.

In the following example the red number after the date defines the valid number of licenses for TopSpin 3.1.

```plaintext
FEATURE TOPSPIN3 bruker_is 0.0 18.-oct-2035 3 2B9E60C19A3C2D4F0DFC \vendor_info=" for hostid(s) : 001125323f2b" ISSUER=...
```

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

The Flexlm license manager is used and is delivered with the TopSpin DVD. The Flexlm package occupies about 3 MByte of disk space. It contains the 'lmgr' license manager, the 'lmutil' program, Help files and an example license.dat file.

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

   • your PC must have an Ethernet card
   • the network (TCP/IP) must be installed
   • the network service 'NetBIOS Interface' must be installed

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“.

   **Note: We use the term „server“, but the PC does not need to be a Server. An operating system supported by Bruker for TopSpin Datastations is sufficient.**

All computers that can communicate with the „license server“ computer can use the licences 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 licence 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 parallel from any 5 computers in the network.

The number of licenses is stated in the FEATURE for the respective program, it is the number behind the date.

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 server 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 licence servers can be inactive and the license management is then done by the remaining server(s).
- One requirement for 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 (Windows, Linux), but must be the supported systems
- The supported operating systems are the same as for TopSpin on Datastations (e.g. for TopSpin 3.0 they are Windows 7.0 Professional, Windows Vista Business Edition, Windows XP Professional, CentOS 5.5, Red Hat WS 4)

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 Student licenses. No other computer can use the license in the way described above for floating licences.
**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.

- **on a Windows PC:**
  
  `c:\flexlm\Bruker\licenses\license.dat`

- **on a Linux PC:**

  `/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 TOPSPIN3 bruker_l_ls 0.0 18.-oct-2035 2B9E60C19A3C2D4F0DFC
\HOSTID=001125323f2b vendor_info=" for hostid(s) : 001125323f2b" ISSUER=...
```

→ Node locked license for one **TopSpin** session that can be started.

```
FEATURE TOPSPIN3 bruker_l_ls 0.0 18.-oct-2035 2B9E60C19A3C2D4F0DFC
\vendor_info=" for hostid(s) : 001125323f2b" ISSUER=...
```

→ Floating locked license for session of **TopSpin** that can be started on every PC in the local network.

**10. How can I determine the Host-ID of my PC?**

See chapter 3.2.1

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

See chapter 3.2

**12. 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 licence. Must the license.dat file be identical on all hosts, servers and clients?

No, you can install license.dat on the server and all license clients are configured to contact the server and ask if the license is available in the up to date license file.

On the license server the the file license.dat must contain a SERVER line, a DAEMON line and a FEATURE line:

```plaintext
SERVER <Server_Name> <Server_HostID> <Port>
DAEMON bruker_ls <Daemon_Path>
FEATURE TOPSPIN3 ...
```

The license.dat file on the clients only contains the following entry:

```plaintext
SERVER <Server_Name> <Server_HostID> <Port>
USE_SERVER
```

So there is no need to ever change the license file on the client PCs.

14. 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.

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

No, it only needs to run the server for the counted licenses.

16. 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.
17. **What can I do if TopSpin cannot find the license.dat file?**

a) Open the Windows Explorer and go to `<Flexlm_Home>`\Bruker\ and double-click `lmtools.exe`

A window ‘LMTOOLS’ appears

![Image of LMTOOLS window](image)

b) Click on the ‘Bruker FLEXlm License Server’ entry and it will be underlayed in blue colour, then click the Start/Stop/Reread tab
c) Click **Stop Server** → wait 10s → Click **Start Server** → wait 10s → Click **ReRead License file** → wait 1-2 minutes → Click **OK**

d) Close the window 'LMTOOLS' by clicking on the X-button.

Using a Linux system open a Linux shell and re-read the license file. Therefore logon as root type:

```
/usr/local/flexlm/Brucker/Imrread -c /usr/local/flexlm/Brucker/licenses/licence.dat
```

**18. What can I do if TopSpin cannot find the license server?**

a) Check if you have a valid license file on you PC. If not, copy one to your system.

b) Install FLEXlm (from the TopSpin DVD). Do it with a customized setup (see Fig. 2.7) and select FLEXlm only (see Fig. 2.8)
3.2 Ordering and installing the TopSpin license

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

- the Host-ID of your PC (see chapter 3.2.1)
- the program for which you want to get a license, e.g. TopSpin
- the type of license (full, demo, processing-only, presentation and teaching, student)
- the number of licenses and your order number (not necessary for demo license)

Licenses can be ordered from the Bruker BioSpin web pages:

http:\www.bruker-biospin.com\nmr_license_requests.html

3.2.1 Determination of the correct Host-ID

The Host-ID is a 12-digit hexadecimal number. It is a 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 Host-ID for a Windows operation system in the following ways.

- Start TopSpin; a command prompt will pop up, which will list the Host-ID, if a correct license is not yet installed and if there is no license.dat file present in C:\flexlm\Bruker\license
- Click the Bruker Utilities icon on the desktop, then click Miscellaneous → get_hostid
- Open a Command Prompt and type in: ipconfig /all
  A configuration list will appear. The „Physical Address“ listed below „Ethernet adapter Local Area Connection“ represents the Host-ID.

Some Host-ID values may indicate problems:

a) If Host-ID ‚2‘ occurs, you may run Windows XP or higher and your network-adapter is disabled.
Click **Start** → **Control Panel** → **Network Connection**
Right-click all **Local Area Connection** xxx -items there click **Enable** (if it is visible)

b) If Host-ID '0' or 'ffffffff' occurs, you may run Windows XP or higher and your network adapter has no link to the network.
Establish a link to the network or install the **NWlink IXP/SPX/NetBIOS Compatible Transport Protocol**:
Click **Start** → **Control Panel** → **Network and Internet** → **Network and Sharing Center** → **Change Adapter settings**
Right-click **Local Area Connections** xxx
Click **Properties** → **Install...** → **Protocol** → **Add**
The 'Select Network Protocol' menu will appear after some seconds.
Click **NWlink** ... → **OK**
After some seconds the 'Properties' menu will reappear.
Click **Close**

See also c:\flexlm\Bruker\help\index.htm for FLEXlm related problems

The determination of the Host-ID for a Linux operation system can be done in the following way:

• Start TopSpin; a command prompt will pop up, which will list the Host-ID, if a correct license is not yet installed.
Open a Linux shell, enter `/sbin/ifconfig eth0` and take the number of HWaddr.

### 3.2.2 Installing a Demo license

A Demo license under Windows can be installed as follows:

[1] Log in as administrator
[2] Open the license.dat file with 'notepad':
   enter the FEATURE lines
set the filename in the ‘Save-as’ dialog into quotes ("license.dat" not only license.dat) otherwise Notepad will create a license.dat.txt file which will not work.

save and exit the file

A Demo license under Linux can be installed like this:

[1] Log in as administrator
[2] Open a Linux shell, type \texttt{nedit/usr/local/flexlm/Bruker/licenses/license.dat}, enter FEATURE lines, save and exit.

3.2.3 Installing a Student license

A TopSpin Student License contains the following features:

\texttt{TOPSPIN3\_STUDENT / TOPSPIN\_1D / TOPSPIN\_2D / XWINPLOT / NMRSIM / NMR\_GUIDE / AUTOLINK}\textsuperscript{1}

All FEATURE lines of the new license should be entered manually into the file:

\texttt{/usr/local/flexlm/Bruker/licenses/license.dat} (Linux)

or

\texttt{C:\flexlm\Bruker\licenses\license.dat} (Windows)

If the file ‘license.dat’ exists and the first two lines already start with ‘SERVER’ and ‘DAEMON’, you can simply add the new FEATURE lines of the TopSpin Student license. Include them right below the ‘DAEMON’ line.

If the file ‘license.dat’ exists but there are no lines starting with ‘SERVER’ and ‘DAEMON’, simply add the FEATURE lines into the file ‘license.dat’ and save the file to disk. A Student license does not need the ‘SERVER’ and ‘DAEMON’ lines.

If the respective path and/or the file ‘license.dat’ does not exist, create the respective directory path and paste the new FEATURE lines into a text file which has to be saved as ‘license.dat’.

\textsuperscript{1} The AUTOLINK license comes as a demo license which is valid for three months
TopSpin License

• Do NOT use advanced text editors like MS Word or Open Office Writer to create or edit this file. Use simple text editor programs like ‘nedit’ (Linux) or ‘notepad’ (Windows).

• When using ‘notepad’ please set the filename in the ‘Save-as’ dialog into quotes (“license.dat” not only license.dat) otherwise Notepad will create a license.dat.txt file which will not work.

If you get license FEATURES which already exist in your ‘license.dat’ file, create a backup of your original license.dat file then delete the older FEATURE lines.

• For example if you get a ‘FEATURE TOPSPIN3 ...’ and you already have a ‘FEATURE TOPSPIN2 ...’ just add the new one.

• But if you already have a ‘FEATURE TOPSPIN3 ...’ (for instance, because you have been using a demo license in the past) then you have to delete the old TOPSPIN3 FEATURE lines. New FEATURES can always simply be added.

Please be sure to enter the FEATURE lines exactly as stated, DO NOT INSERT any other symbols, spaces, or returns and DO NOT APPEND anything at the end of the lines.

Once the license file has been created like described above, save it to your disk and start TopSpin. The program is now ready to use.

3.2.4 Installing a full license on a license server

The Flexlm license is delivered on the TopSpin DVD and can be installed as described in chapter 2. The Flexlm is automatically installed as a Windows, respective Linux, service which is then automatically started.

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

SERVER petzi 001125323f2b 1700
DAEMON bruker_ls c: \flexlm\Bruker\bruker_ls.exe (→ Windows system)
DAEMON bruker_ls /usr/local/flexlm/Bruker/bruker_ls (→ Linux system)

FEATURE TOPSPIN3 bruker_ls 0.018-oct-2020 3 2B9E60C19A3C2D4F0DFC \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
**TopSpin License**

FEATURE TOPSPIN_1D bruker_ls 0.018-oct-2020 3 2B5E00712DB1321F2DDE \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE TOPSPIN_2D bruker_ls 0.018-oct-2020 3 6B7E009107D129E4DA95 \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE XWINPLOT bruker_ls 0.018-oct-2020 3 9B5E909100892E5F8A76 \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE TOPSPIN_ACQU bruker_ls 0.018-oct-2020 3 EBFE503139CA9BE6A280 \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE NMRSIM bruker_ls 0.018-oct-2020 3 ABFEA0F14EAF5A66EC \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE NMRGUIDE bruker_ls 0.018-oct-2020 3 7B7E30D13BDB911F3533 \ vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed

where ‘petzi’ is a hostname example and 001125323f2b a Host-ID example of one 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 TOPSPIN3 bruker_ls 0.018-oct-2020 3 2B9E60C19A3C2D4F0DFC \n
To inform Flexlm about a new license proceed as follows under a Windows operation system:

1. Open the Windows Explorer and go to `<Flexlm_Home>/Bruker` and double-click lmtools.exe.
2. A window ‘LMTOOLS’ appears. Click on ‘Bruker FLEXlm License Server’ (will be underlayed in blue colour). Click Start/Stop/Reread tab → Click Stop Server → Click Start Server → Click ReRead License file → Click OK
3. Close the window ‘LMTOOLS’ by clicking the X button.

To inform Flexlm about a new license under a Linux operation system, enter in a Linux shell:

```
/usr/local/flexlm/Bruker/lmreread -c /usr/local/flexlm/Bruker/licenses/license.dat
```
3.2.5 Installing a full license on a licence client

On a licence client, licenses can be installed as described for a Demo license in chapter 3.2.2. Set up the license.dat file only with following two entry:

SERVER <Server_Name> <Server_HostID> <Port>
USE_SERVER

So there is no need to ever change the license file on the client PCs.

You can also just copy the license.dat file from the license server as before to every client PC. In this case every change of the license.dat file has to be done on the server and on all clients.

3.2.6 Activiting the license file

If you have modified the license.dat file Flexlm must be informed about this new license file.

With a Windows system go on as described below:

1. Open the Windows Explorer and go to <Flexlm_Home>\Bruker\ and double-click lmtools.exe.
2. A window 'LMTOOLS' appears. Click on 'Bruker FLEXlm License Server' (will be underlayered in blue colour). Click Start/Stop/Reread tab → Click Stop Server → Click Start Server → Click ReRead License file → Click OK
3. Close the window 'LMTOOLS' by clicking the X button.

To inform Flexlm about a new license under a Linux operation system logon as root and enter in a Linux shell:

/usr/local/flexlm/Bruker/lmreread -c /usr/local/flexlm/Bruker/licenses/license.dat
3.2.7 Further information

For more information on the Flexlm license manager:

Click Start → run enter c:\flexlm\Bruker\help\index.htm, click OK when working with Windows.

Double-click Computer icon→ Files and select the following directories: usr → local → flexlm → Bruker → help and you will find an enduser.pdf (which is a Flexlm Enduser Guide) when working with Linux.
4 Basic Configuration of TopSpin

This chapter gives you some guidelines to full spectrometer or only processing configuration. Commands will not be discussed in detail here. For a full description please refer to the Acquisition Commands and Parameters (Chapter 3).

4.1 Starting and configuring TopSpin

There are two ways to start TopSpin on a windows system:

1. Double-click the icon TopSpin on the desktop
2. Click Start -> All Programs -> Bruker TOPSPIN -> TOPSPIN<vers.>

First of all a TopSpin 3.1 start window will open. It is shown in Figure 3.1. You will be informed about the Program Version, the installation directory and the valid license(s).

If there are any problems with the licences or the license management you will be informed here. TopSpin will not start then.

If everything is ok, the TopSpin main window will be displayed and the window shown in Figure 4.1 disappears into the background but remains open.

This procedure will be same with every start of TopSpin.
Basic Configuration of TopSpin

After the first startup of TopSpin a „LICENSE“ window will be displayed once. Please read the license agreement for Bruker TopSpin. If you agree, please click „I Accept“.

When starting TopSpin 3.1 for the first time, after opening of the „TopSpin main“ window and accepting the license agreement a popup window will be displayed (Fig. 4.2). Here you may choose between the new Flow User Interface or the traditional menu bar.

Follow the instructions in this window. If you do not want to get this window every time you start TopSpin, then mark the box on the left bottom (Don’t show this info again).
Basic Configuration of TopSpin

Figure 4.2  Popup window for defining the User interface

If necessary you can change the user interface (UI) anytime using the command `set`. This will open the 'User Preferences' window (Fig. 4.3) where the UI can be changed under *window settings*.

To enable or disable the **TopSpin 3.1** Flow User Interface, press the 'Apply' button and close this window. After restarting TopSpin the UI will have changed.
Basic Configuration of TopSpin

Figure 4.3 'User preferences' window

This window is also available by clicking the 'Manage' tab and then the 'Preferences' button when using the Flow User Interface or clicking the 'Options' button and then 'Preferences' when using the traditional menu bar.

For this manual the Flow User Interface will be used.

After the UI selection is finished, a 'Configuration Check' window (Fig. 4.4) will be displayed.
Now you can configure your system. This depends on the hardware of your spectrometer. If you do this, you are mainly in one of the following situations:

- You want to configure an only-processing-PC like your spectrometer-PC.
- You have to configure the software on a new hard disk without a backup of your spectrometer configuration, so you don’t have configuration files anymore.
- You have just installed the software in a new directory and the old spectrometer configuration is still known to the new software version.
4.1.1 Configuring a PC to control a spectrometer

If the PC does control a spectrometer be sure that your spectrometer is booted.

Press the ‘cf’ button of the ‘configuration check’ window or type cf in the command line of the TopSpin main window, if you have closed this window without any configuration or doing another one before.

Immediately the popup window shown in Figure 4.5 is displayed and you will be asked for your administrator password. Type in your password and press ‘Ok’.

Every time you want to access the configuration modus this password request will appear.

Figure 4.5  ‘Password request’ window

The first ‘cf’ window will appear. (Fig. 4.6).

Most likely you will select an existing configuration and click ‘Edit’ to confirm this configuration or modify it to your requirements. But you can also start from scratch by clicking ‘New’.

In this example the configuration ‘spect’ is an existing spectrometer configuration for an Avance III 300 spectrometer. We choose this one to explain the following steps.
Basic Configuration of TopSpin

Figure 4.6  First `cf window` with spectrometer connected to PC

After selecting the configuration and clicking `Edit` the window shown in Figure 4.7 is displayed.
Basic Configuration of TopSpin

Select Spectrometer and check the 1H frequency of the magnet. The debug module is used for troubleshooting only.
Figure 4.8  Third 'cf window' with spectrometer connected to PC
Basic Configuration of TopSpin

Then click 'Next' and the window shown in Figure 4.8 will appear.
Check all connections and modify them if necessary. Please keep in mind, that this is an example. Your specific entries will be different.
When finished click 'Next'.

A window for additional configuration (Fig. 4.9) will be displayed.

Figure 4.9 'cf window' for additional configuration

- Select 'Enable peak power check (POWCHK)'. Check the TopSpin manual regarding this important security feature and its requirements.
The 'Sample changer configuration' shown in the lower part of this window will only be displayed when using the older version of sample changer, BACS. Configure it as follows.

- Select 'Should the sample changer control the lift' if you have a sample changer. But it depends on how the air flow is connected. Normally you will tag this option.
- For 'Delay between SX and next command [s]' type in the length of this delay, e.g. 10
- BACS,SampleRall or SampleJet options: only fill in on request

With a newer version of sample changer, the Sample Xpress, the lower part of the window won't be displayed, because these options are not necessary for it.

Click 'Next' after you have finished all entries.
Basic Configuration of TopSpin

The nuclei table will be displayed (Fig. 4.10)

![Nuclei Table](image)

Figure 4.10 ‘cf window’ with nuclei table

Enter nuclei and frequencies in this table or check if the frequencies in the nuclei table are set correctly when using an existing configuration. Then click ‘Save’. If you are in doubt first ‘Restore’ and then ‘Save’.

Now the channel routing (Fig. 4.11) will be displayed. Check here if the preamplifier...
connections are set correctly and click ‘Save’.

![Image of channel routing window](image)

Figure 4.11 Channel routing during configuration

The result of ‘cf’ is now presented in a text window (Fig. 4.12). Check this list carefully and compare the result with a list of earlier configurations (if available). Then click ‘Print’ and store the output with your other spectrometer documentation. Now click ‘Next’ to close this window.
Basic Configuration of TopSpin

Figure 4.12 Configuration summary

Now the window ‘Additional configuration programs’ as shown in Figure 4.13 is displayed.
We will discuss the additional configuration programs **Expinstall**, **Edsolv** and **Edscon** in the following chapter (Chap. 4.1.2) where you first will learn how to configure **Topspin** without controlling a spectrometer. Most of the additional programs are needed there too.

**Edhead** and **Edprosol** require a spectrometer configuration and will be shown here.

After clicking **Edhead** a window like shown in Fig. 4.14 will be displayed.
Basic Configuration of TopSpin

Figure 4.14 Example of an ‘edhead’ window

In this window you have to define the current probe, edit the probe parameters and check the connections. Click the ‘Exit’ button to leave the window.

Now click the ‘Edprosol’ button to enter the solvent dependent parameter setup. It is necessary to execute ‘Edhead’ first because the probe parameters will be needed.

A window shown in Fig. 4.15 will be displayed.

Figure 4.15 ‘edprosol’ window
Basic Configuration of TopSpin

For detailed information about the parameters and how to define them please refer to the Bruker Edprosol manual.

4.1.2 Configuring a Processing-Only 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 or plotting you should configure it as that spectrometer.

To transfer the configuration of the spectrometer to the Processing-only PC execute the following steps:

[1] Save the desired configuration on your spectrometer PC with nmr_save (see chapter 4.2)

[2] Copy this archive file to the Processing-only PC.

[3] Restore the configuration with the nmr_restore command to the Processing-only PC (see chapter 4.2)


Press the „cf“ button of the „configuration check“ window or type cf in the command line of the TopSpin main window, if you have closed this window without any configuration or to repeat a previous one.

Immediately a popup window (Fig. 4.5) is displayed and you will be asked for your administrator password.

Type in your password and press „Ok“.

The first „cf“ window as shown in figure 4.14 will be displayed.

You will find the default configurations delivered with the TopSpin DVD (and all available spectrometer/datastation configurations you have saved before).

As an example, in this guide we will use the Bruker_default_av500 configuration which is delivered with the DVD. After selecting this configuration by clicking it, there are several options how to deal with it. They are shortly explained in the lower part
of this window.

First of all you can click the show button. A window as shown in Figure 4.16 gives information about the chosen configuration. Clicking the X at the top right side will close this window.

Figure 4.16  .cf' window to configure your system
Basic Configuration of TopSpin

The second button at the bottom of the .cf window allows you to delete one or more chosen configurations.

The 'New' button enable you to setup a new configuration from scratch.

The 'Edit' button allows you to edit and modify an existing configuration and clicking the 'Close' button you will leave the configuration modus.

To continue with our example, the Bruker_default_av500 configuration, we now click...
Basic Configuration of TopSpin

the ‘Edit’ button and examine the upcoming ‘Edit configuration’ window (Fig.4.17) and all following ones to get an idea of how to configure TopSpin for the several applications.

Figure 4.18 ‘Edit configuration’ window

First of all the Configuration name is accepted. Here you can set an own one if you start a new configuration. Then you decide, if you PC should control a spectrometer or should be a datastation only.
Basic Configuration of TopSpin

As the PC in our example shall not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing or plotting, we select 'Datastation' and set 500,13 MHz for the 1H frequency of the magnet (see Fig. 4.16, the chosen configuration represents a AV 500 spectrometer 500,13 MHz).

Now click the 'Next' button and the 'Edit nuclei table' window will be displayed. (Fig. 4.19)

![Figure 4.19 'Edit nuclei table' window](image)
Basic Configuration of TopSpin

You can delete or modify the values if necessary. For later modifications of the nuclei table you can always use the ednuc command to get this window.

Figure 4.20 'Channel Routing' window
Basic Configuration of TopSpin

After having finished this task click the ‘Next’ button and the ‘Channel Routing’ window (Fig. 4.20) is displayed.

Appropriate to your system the connections between amplifier, preamplifier etc. can be defined. For more information look up the **edasp** command in the TopSpin Acquisition Manual. The button bar at the bottom shows which actions are possible. For example clicking the ‘Info’ button displays the following popup window (Fig. 4.21)

![Spectrometer Information](image)

**Figure 4.21 Spectrometer Information**
Basic Configuration of TopSpin

In our example we do not change parameters of the default setting and leave the windows 'Spectrometer Information' and 'Channel Routing' by clicking the 'Close' button.

Immediately a Configuration summary will popup.

![Configuration summary](image)

Figure 4.22 Configuration summary
After examining the configuration summary and leaving it by clicking ‘Next’ a new window with additional configuration programs will be displayed (Fig. 4.23).

It is the same window as mentioned in chapter 4.1.1 where the PC was configured for controlling a spectrometer. The now described steps have to be done for both configuration examples.

![Additional configuration programs window](image)

Figure 4.23 ‘Additional configuration programs’ window
Basic Configuration of TopSpin

For our example(s) we will accept the default selections for all additional programs. All these additional configuration programs can also be added or changed at a later time by typing the annotation of the buttons in the command line of the TopSpin main window (e.g. edhead, expinstall, edprosol, edsolv, edscon).

You will be asked for the administrator password a couple of times.

[5] Edhead
This probe setup needs a configuration with a spectrometer. We will skip it here (see Chap. 4.1.1).

[6] Expinstall
Start with Expinstall by pressing this button a 'Password request' window as shown in Figure 4.5 will be displayed. Type in the administrator password and you will be led to the first 'Expinstall' window (Figure 4.24).

Click 'Next' if you either have no modified Bruker-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 with different names to the original Bruker files will not be affected during the installation

Now an 'Expinstall window' for selecting the type of installation will be displayed (Fig. 4.25)
Basic Configuration of TopSpin

Figure 4.24  First 'Expinstall' window

Expinstall installs pulse programs, AU programs, parameter sets and various other resources for spectrometer or datastation usage. It must be performed once after the installation of TOPSPIN. For spectrometer control do cf first. For a customized datastation configuration copy your spectrometer configuration directory (typically called "spect") to <TopSpin installation dir>/conf/instr.

WARNING:
Please archive all your MODIFIED Bruker PARAMETER-files, AU-programs and PULSE-programs before running "expinstall".
Here you have to select the type of installation. In our example we will use the customize one for Datastation as shown in Figure 4.25. (in chapter 4.1.1 it would be Spectrometer). Then click the 'Next' button.

In the now appearing window (Fig 4.26) you have to determine the type of acquisition. In this example it is a High Resolution System.
Click 'Next' and a new window (Fig. 4.27) will appear. Here you have to select the spectrometer or datastation configuration for which expinstall should be done. In our example select 'Bruker_default_av500' (in chapter 4.1.1 it would be the configuration 'spect') and click the 'Next' button.
Basic Configuration of TopSpin

Figure 4.27 'Fourth Expinstall' window for selection of configuration

In the now displayed window (Fig.4.28) you have to determine all items you want to use for your datastation (or spectrometer) configuration. Accepting the default settings is a good choice. Then click the 'Next' button.
Figure 4.28 ‘Expinstall’ window for selection of items to install to the configuration

The now displayed window (Fig. 4.29) allows you to define the printer and plotter you want to work with. The choice of the paper format is important because the chosen one will be copied to your working directory. Click ‘Next’ when finished.
In the now following window (Fig. 4.30) you determine the basic frequency of the spectrometer, the type of digitizer, acquisition mode and the pre-scan-delay. All settings should be correct. Nevertheless in case of a configuration to control a spectrometer they should be checked, then click ‘Next’.
Basic Configuration of TopSpin

Figure 4.30 'Expinstall' window to determine the basic frequency of the spectrometer, the type of digitizer, acquisition mode and the pre-scan-delay

After clicking 'Next' a summary of all you defined for the execution of expinstall is displayed (Fig. 4.31). Check this list regarding desired options and settings.

If you want to change something, click 'Back' until you reach the window(s) where corrections have to be done. Then click 'Finish'.
Basic Configuration of TopSpin

Figure 4.31 ‘Expinstall’ window with summary of all definitions for execution of Expinstall

The installation of the selected items will start now. Wait until this process has fin-
ished. In the status line at the bottom of the ‘Additional configuration programs’ win-
dow you can monitor the progress of the installation.

After finishing the configuration a ‘Cron check’ window (Fig.4.32) is displayed.

![Figure 4.32 ‘Cron check’ window](image)

Click ‘Automatic Backup’ and the ‘NMR Save’ window (Fig.4.33) will be opened. Here you can define the locations for saving and restoring the installation and user files in 4 separate tables.

At the bottom of the first table (Save installation files) you will find the ‘Automatic Backup’ button for setting a periodically saving of configuration specific files.

It might be useful to save the periodical backups on a network drive. You can do this by entering the network drive as location of backup file in the window shown in Figure 4.31. After clicking the ‘Automatic Backup’ button the chosen drive is set and cannot be edited anymore. (For more information see chapter 4.2.)
Basic Configuration of TopSpin

Figure 4.33 ‘NMR Save’ window

Pressing this ‘Automatic Backup’ button opens the ‘New periodical’ window where you can set job, options and rules for an periodical backup.

**Note:** The command box cannot be edited!
Press ‘OK for this window (you will be asked for the administrator password) and ‘Save’ in the ‘NMR Save’ window. The compilation of ‘xauw’ will start. When this process is finished the ‘Additional configuration programs’ window appears.
Basic Configuration of TopSpin

[7] Edprosol

This solvent dependent parameter setup can only be executed with a spectrometer configuration. Before executing this, Edhead must have been done. We will skip this here (see Chap. 4.1.1).


![Figure 4.35 Solvent table](image)

Check the solvent table (Fig. 4.35) and double-click on an entry if you want to change something. You will be asked for the administration password, then a window for the chosen solvent is displayed where changes can be done. Clicking the ‘Lock’ tab, the ’Spectrum Reference’ tab and the ’Properties’ tab the corresponding tables will be displayed instead of the solvent
table. You can handle them in the same way.

[9] Finish the additional configuration programs with 'Edscon' to set spectrometer parameters.

Check the spectrometer constants in the 'edscon' window (Fig. 4.36). Normally it is not necessary to change them. Click 'Save' and Close'

![Figure 4.36 'Edscon' window](image)

### 4.2 Backup and restore of important files with nmr_save

It is strictly recommended to create a frequently backup of the important files of your configuration of TopSpin.
There are a lot of reasons (e.g. head crash or theft of hard disk) for making weekly or monthly backup of important data. So you will be able to restore your spectrometer configuration in a short time.

TopSpin offers the command nmr_save for saving those important files. With nmr_save all installation specific files, like spectrometer information, licenses etc. are saved. Even the default directories listed in the 'Source Directories', like e.g. .pp are saved. All these files will be put together into one archive file.

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

The same function as nmr_save are 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 command nmr_restore and user_restore respectively restore installation and user-specific files to the same or a different installation.

**4.2.1 How to save information with nmr_save**

nmr_save can be started as followed:

- Start TopSpin and type in the command:
  nmr_save
- Start TopSpin and click
  Manage Configuration → Spectrometer → Safe|Restore installation → Save installation specific files

A window 'NMR_Save' (Fig. 4.37) will be displayed.
Basic Configuration of TopSpin

1. Accept or modify the 'Location of Backup file'
2. Enter the location of the 'Installation to be saved'
3. nmr_save will then offer a list of all available spectrometer configurations which are located in this installation. Select the correct in the field 'Spectrometer name'. In a typical setup your spectrometer configuration is called 'spect'. In a typical installation your configuration names will be listed here, your current instrument name and the three Bruker default configurations Bruker_default_av500, Bruker_default_avII700 and Bruker_default_avIII600.

Figure 4.37 NMR-Save window
Basic Configuration of TopSpin

[4] If you want to execute ‘Save installation specific files’ periodically click the button ‘Automatic Backup’. This will open a window for a command scheduling. Clicking ‘OK’ will accept the default values to execute \texttt{nmr\_save} one in a month.

[5] Now click ‘Save’

This will create an archive file of all necessary information from the selected installation/spectrometer configuration. It is called:

\texttt{nmr\_backup\_<date>-<time>.tar}

and is stored in the directory you selected above, typically:

\texttt{<TOPSPINHOME>/nmr\_backup}

The command \texttt{cron} performs command scheduling. It allows to execute commands periodically at predefined date/time in planned intervals. These intervals can be defined user-specific 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] \textit{Command}: The command to be executed

[2] \textit{Description}: A description of the command

[3] \textit{Execution scope}: The scope of the command execution, User of TopSpin

For scope ‘User’, the scheduled command will only be executed if \texttt{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 Administrator password.

[4] \textit{Off-schedule execution}: this flag allows you to execute commands that were scheduled to run at the time when \texttt{TopSpin} was off. These commands are executed after the next \texttt{TopSpin} startup.

\textbf{Note}: 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: between 00 and 59
Basic Configuration of TopSpin

- Hours 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 in the ‘from’ field. An asterix (*) in the ‘from’ field indicates all possible times. Clicking the ‘+’ button to the right of the field, adds an extra field of the same type, allowing multiple interval definition. Clicking ‘-’ removes the extra field.

4.2.2 Which information is stored with nmr_save

You can save (or restore all) Topspin user defined files. This includes:
- Spectrometer configuration files (cf)
- Parameter sets (rpar, wpar)
- Pulse program (edpul, edcpul)
- AU programs (edau)
- Plot editor layouts (plot, autoplot)
- Shim files (rsh, wsh)
- Gradient shimming field maps (gradshim)
- Icon-nmr user information (iconnmr)
- Program Licenses (Topspin, Nmr-sim, NMR Guide)
- Various lists like scl, f1, ds (edlist, zg, gs)
- Topspin macros (edmac)
- Probehead and solvent dependant parameters (edprosol)
- Lock parameters (edlock)
- Probehead information (edhead)
Basic Configuration of TopSpin

- Nucleus information (ednuc)
- RF Shapes and gradients
- etc.

Furthermore the files:
- prog/logfiles/heliumlog
- prog/logfiles/heliumlog.err
- Bruker/licenses/license.dat

will be saved with the ending .backup. Please note that these files will be stored in the folder conf/instr/, no longer in the original folder.

Furthermore the whole directory
- <diskless>/crco_data/cryotool_log/

will be saved.

4.2.3 How to restore information with nmr_restore

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.

nmr_restore can be started as followed:
- Start TopSpin and type in the command:
  nmr_restore
- Start TopSpin and click
  Manage Configuration → Spectrometer → SafeʃRestore installation → Restore installation specific files

A window 'NMR_Save' (Fig. 4.38) will be displayed.

[1] Enter the path where your archive file is stored in the field 'Location of backup file'. The default path is <TOPSPINHOME>\nmr_backup. A backup file created
by nmr_save will be shown in the field 'Name of backup file' if available. They always look like:

nmr_backup_20120206-1428.zip

where the first number represents the date and the second the time.

![Figure 4.38 NMR_save window with 'Restore installation files' tab selected](image)

[2] Enter the location of the 'Restore destination' (default is: <TOPSPINHOME>)

[3] Click the 'Restore' button and type the NMR administrator password in the upcoming Password request window.
Basic Configuration of TopSpin

[4] Execute the command cf
5 Deinstallation of TopSpin

5.1 Deinstallation under Windows 7.0

During the installation of TopSpin also a deinstallation routine (deinst.exe) is copied to your system.

If it should be desired or necessary to uninstall TopSpin stick to the following instructions:

[1] Click the start button of windows
[2] Open the 'Control Panel'
[3] Select uninstall a program and follow the instructions of this window
[4] Select the TopSpin Version you want to uninstall and click ,uninstall/change
[5] The following window will be displayed:

```
C:\ Bruker\TopSpin3.0\uninstall\deinst.exe

Uninstalling TopSpin 3.0

Installed in C:\ Bruker\TopSpin3.0

Installed at: 2010-12-16 13:36:13 * 8100

Do you want to uninstall this program? (yes/no) -
```

Type 'yes' or 'y' to uninstall this program.

[6] You will be prompted to type the Administrator Password

The deinstallation starts and might take a few minutes. When the deinstallation is finished ,all programs and icons of TopSpin x.y are removed from your PC.
5.2 Deinstallation under Linux?

During the installation of TopSpin also a deinstallation routine is copied to your system (into the sub folder uninstall).

If it should be desired or necessary to uninstall TopSpin stick to the following instructions:

[1] To deinstall a program under Linux, open a file browser like konqueror or a shell window.


[3] Then go to the sub folder “uninstall” and start uninstall-<program>.sh.

This will cleanly shut down running services, delete files in other directories and remove the entries in the GNOME or KDE menu. On the other hand, configuration files and acquired data will be left on the disk.

Examples:

To deinstall TopSpin and all dependent programs, run /opt/topspin3.0/uninstall/uninstall-topspin.sh

To deinstall NMR-Guide only, run /opt/topspin3.0/uninstall/uninstall-nmrguide.sh

To deinstall Diskless, run /usr/diskless/uninstall/uninstall-diskless.sh

To deinstall FlexLM, run /usr/local/flexlm/uninstall/uninstall-flexlm.sh
6 Contact

Manufacturer:

Address: Bruker BioSpin GmbH
Service & Support Department
Silberstreifen
D-76287 Rheinstetten
Germany

E-mail: nmr-software-support@bruker.de
WWW: http://www.bruker-biospin.com
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