

TopSpin

Installation Guide
 User Manual
 Version 003

Innovation with Integrity

NMR

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1 Introduction

1.1 About this Manual

This manual is the TopSpin Installation Guide for Microsoft Windows, Linux and Mac OS. This installation guide is available:

- as PDF file on the toplevel of the TopSpin DVD
- as the up to date version on the Bruker web server: https://www.bruker.com/service/ information-communication/user-manuals/nmr.html

Note: This manual does not contain the TopSpin Release letter. This is a separate document delivered as PDF or HTML files on the TopSpin DVD and also on the Bruker web server.

Note: 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.

1.2 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All that you can enter"	Arial bold	Type or enter fromjdx zg
Button, Tab, Pane and Menu Names "All that you can click"	Arial bold, initial letters capitalized	Use the Export To File button. Click OK . Click Processing
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names Data Path Variables Table Column Names Field Names (within Dialog Windows)	Arial Italics	\$tshome/exp/stan/nmr/ lists expno, procno,
Parameters	Arial in Capital Letters	VCLIST
Program Code Pulse and AU Program Names Macros Functions Arguments Variables	Courier	go=2 au_zgte edmac CalcExpTime() XAU(prog, arg) disk2, user2
AU Macro	Courier in Capital Letters	REXPNO

Table 1.1: Font and Format Conventions

2 Installation

2.1 **Preparation**

The Linux distribution includes a built-in PDF viewer but it is preferred to have Acrobat Reader or Evince (on Linux) already installed. To display the TopSpin Online Help, for parts of the NMR-Guide and the Release Letter, a PDF viewer is required.

Acrobat Reader is not installed automatically as a part of TopSpin (on Linux, Mac OS and Windows). It is available from Adobe as download.

2.2 Packages on the TopSpin DVD

1 TopSpin		Acquisition and Processing Software		4. x
	TopSpin Plot Editor	Object oriented WYSIWYG plot editor. ³		Х
	Cygwin Tools Used for compilation of TopSpin AU programs. ³		Х	Х
	NMR-GUIDE	A web-based training and teaching tool providing a lot of theoretical and practical information on NMR spectroscopy and NMR methods for everybody interested in NMR. ²	Х	Х
	NMR-Sim	Program for numerical simulation of NMR experiments. ³	Х	Х
	CMC-q Viewer	Automation & Analysis ³	Х	Х
2	Central Audit File	Enables a Central Audit File for activity recording in TopSpin.	Х	Х
3	CMC-a	CMC-assist, a tool for structure verification based on NMR data.	Х	Х
4	IconNMR	Icon-driven interface for Routine Spectroscopy and Automation.	Х	Х
5	MICS	Magnet Information & Control System.	Х	Х
6	NMR-Data Example datasets		Х	Х
7	CodeMeter License manager required to start TopSpin programs. Runtime CodeMeter		Х	Х
8 AURELIA-AMIX-		Multiple object viewer ¹	Х	Х
	Viewer	During the installation the program is displayed as AMIX.		
9	SpectrOS	Spectrometer operating system for AVANCE NEO.		Х
		SpectrOS is needed for workstations controlling a spectrometer.		
10	Diskless	Spectrometer operating system for AVANCE III.	Х	
		Diskless is needed for workstations controlling a spectrometer.		
11	SBASE	Spectra base for AMIX ¹	Х	Х
12	Dynamics Center	Analysis of NMR data containing non-frequency dimensions (incl. Protein Dynamics) ¹	Х	Х
13	InsightMR	Reaction Monitoring	Х	Х

¹ Requires a separate license.

² Package is integrated in TopSpin4.x, package is selectable in TopSpin3.6.x

³ Installed by default together with the TopSpin package.

Packages available on a separate DVD:

	TopSpin	Acquisition and Processing Software	3.6. x	4.x
14	AssureNMR	The AssureNMR software provides automated multicomponent identity, quantification, classification, and detection of outliers with spectral databases and System Suitability Tests for GxP compliance. ¹	Х	X
15	AssureNMR- Methods	This directory includes Analysis Methods, for use with AssureNMR, that automate the analysis of poloxamers, molar substitution, tire rubber, heparin, Aloe vera and other common materials. Some of these methods may require separate software licenses for use (heparin and Aloe vera).	Х	Х

¹ Requires a separate license.

2.3 Windows and Linux Installation

This chapter describes the installation of TopSpin, which requires local administrator permissions. There are two possibilities:

- 1. User Account Control (UAC) is enabled. If you are logged in an as a normal user for the installation of TopSpin, you will be prompted during the installation for the name of a local administrator as well as his password. If you are logged in as a user with administrative rights, you will only be prompted to confirm that you want to continue the installation with these rights.
- User Account Control (UAC) is disabled. You must login as a user with administrator permissions and then install TopSpin. In that case, no question will be asked during the installation.

If a previous TopSpin installation exists on your Workstation 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\TopSpin4.0 (Windows)
 e.g. old in /opt/topspin3.0 and the new in /opt/topspin4.0 (Linux)

or

• 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)

Note: Bruker strongly recommends to always choose the parallel installation.

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation, start to work with the new version. If necessary, you can still go back to the previous TopSpin version.

Windows

- Close all windows on the desktop.
- Insert the TopSpin DVD and open the DVD drive with the Windows explorer.
- Double-click Install.cmd

Note: All current versions of Windows are initially installed with an option called Hide extensions for known file types enabled. In this case two files named *Install* are displayed. Click the one of type *Windows command script*.

A Command Prompt window displays the current installation process.

If you are logged in an as a normal user, a User Account Control window will be displayed. Enter the Administrator password.



Linux

- Insert the DVD to open a cd-rom file browser. If it will not be opened automatically click the now visible DVD 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 then click **Run in a Terminal** in the newly opened window.

On CentOS 7 a shell window will be opened.

 Enter the Administrator ("root") password here. The installation will start and and the location of the installation log file is displayed in the same shell described above on Windows.

Windows and Linux

After a short time the installer opens two additional windows shown in the following figures. The Overall Progress Information window will be visible during the whole installation .

BRUKER	Bruker NMR Software Installer including TopSpin and CMC-a
	Overall progress
Setup parameters	-
Check consistency	-
Select target direc	tories -
Prepare harddisk	-
Install files	-
Post processing	-
Status: Click 'Next' to	step through the setup process.

The second window displays a Welcome screen and lists the main programs that are part of the software distribution.

Welcome!
This setup tool will help you to install step by step Bruker NMR Software including - TopSpin with CMC-se - CMC-assist - Dynamics Center - Amix
Please terminate all running Bruker NMR Software before continuing with this setup
Note: To change the font size, type Ctrl - or Ctrl +
Back Encel Cancel

• Click **Next** to continue with the TopSpin installation.

The installer offers either to install only the Cygwin tools, to install the NMR programs without Cygwin, or to install the NMR programs including the Cygwin tools which is recommended. The Cygwin tools are used for the compilation of AU programs.

Selection of components to install			
 ✓ Install Bruker NMR Software ✓ Install GPL licensed Cygwin Software (recommended) 			
G Back	❷ <u>H</u> elp		

The release letter will be displayed in a PDF reader in the background, so you can proceed with the installation while reading the release letter.



• Click Next to continue with the TopSpin installation.

Please select an installation directory for TopSpin and CMC-assist				
C:\Bruker\TopSpin <version></version>				
G Back	Cancel	Disk usage		

- Click Browse to change the installation folder or enter the path in the text field.
- Click Next.

Note: This is also the directory where the installation log file will be located after the file extraction to the local hard disk has started. Please include the installation log file (install.log) in any request email concerning installation issues.

If the installation directory does not exist, the program asks if it should be created. The directory will be created only when the file extraction actually starts.

Exception: The installer will not allow to accidentally overwrite an existing installation of TopSpin with another version. If desired, the program can uninstall a previous version:

** Note: Cannot overwrite Top	oSpin <xyz> **</xyz>		
You cannot use C:\Bruker\Tops because it already contains To	Spin <xyz> as targe opSpin <xyz> .</xyz></xyz>	t directory for TopSpin <abc< td=""><td>></td></abc<>	>
• Select another	target directory for	TopSpin <abc></abc>	
C Uninstall TopSp	oin <xyz> automati</xyz>	cally	
G Back	O Next	Cancel	

- · When this exception note is displayed either
 - Check Select another target directory for TopSpin<version abc> and click Next to change the installation directory and continue with the setup type selection or
 - Check Uninstall TopSpin<existing version xyz> and Click Next to first uninstall the existing version and continue with the setup type selection.

Please select the setup type
C Data processing only
Installs Data Processing, Plotting and Simulation Components
C Data processing, acquisition and automation
Installs Data Processing, Acquisition and Automation Components for Spectroscopy Customized
Customized setup (allows component selection)
G Back O Next Cancel

- · Select one of the offered setup types:
 - Select Data processing only if you want to use TopSpin for data processing only. The packages TopSpin, NMR-Sim, NMR-Data, CMC-assist and CodeMeter will be installed.
 - Select Data processing, acquisition and automation if you want to use TopSpin for spectrometer control. This setup type provides the following packages: TopSpin, NMR-Sim, NMR-Data, CMC-assist, CodeMeter, IconNMR, SpectrOS and MICS.
 - Select Customized for a manual selection.

The Customize Products window has initial settings equal to the option **Data processing**, acquisition and automation.

Additionally:

 The option SpectrOS will be checked for the setup types Data processing, acquisition and automation and Customized if the current SpectrOS version on your spectrometer is outdated or equal. 2. The option **Codemeter Runtime** will be checked if the actual **Codemeter Runtime** version on your workstation is outdated.

		Please select products to install		
Sel.	Product	Description	Version	Size/MB
\checkmark	TopSpin	Acquisition & Processing Software		
	Central Audit File	Enable Central Audit File in TopSpin		
\checkmark	CMC-a	CMC-assist		
\checkmark	IconNMR	Automation Module		
\checkmark	✓ Diskless	Spectrometer Operating System		
		Magnet Information & Control System		
\checkmark	R NMR-GUIDE	NMR Encyclopedia		
\checkmark	MMR-Data	NMR Example Data Sets		
	CodeMeter Runtime	License Manager		
	🗆 Amix	Amix		
	□ SBASE	Spectra Base, Requires AMIX License		
	Dynamics Center	Dynamics Data Analysis		
	InsightMR	Process Monitoring		
	Select all	Clear all 🛛 Orre in	nfo >	
	<u> </u>	ck <u>O</u> nce	H I	

- · Click More info to check the already installed product versions.
- Click Next.

If a package dependency is not resolved correctly or the installation directory contains a TopSpin version that would be corrupted, the installer shows a dialog about the conflicts.

Conflict: The installation of IconNMR requires TopSpin <xyz> which is not installed in C:\Bruker\TopSpin<abc></abc></xyz>				
 Install TopSpin Do not install IconNMR 				
G Back	📀 <u>N</u> ext	<u>C</u> ancel		

Linux:

Select whether the current TopSpin installation directory should be added to the global path. This allows to start TopSpin by typing **topspin** on the command line.

Do you want to add the TopSpin installat	ion directory to the global PATH?
If you do so, you will be able to start Top 'topspin'	Spin by just typing
Currently the global PATH does not cont	ain any TopSpin installation directory.
● <u>Y</u> es, add the new TopSpin install ○ No, leave the global PATH <u>u</u> ncha	ation directory to the global PATH anged
G Back Dext	Cancel 😢 <u>H</u> elp

Windows and Linux:

NMR products are configured with special access for the account selected as the so-called NMR Super User.

Linux:

Select a name for a user account. If the account does not exist, it will be created.

Windows:

Select an existing account. This can be a local or a network account.

Please select the N	MR Super User.	
This can be eithe member of a dom	r a local account, or - if aain - a domain account	the computer is
Valid syntax: - USER ACCOUN - THALIA\USER A - DOMAINNAME	T or ACCOUNT or E\USER ACCOUNT	
THALIA\Administra	torln	~
G Back	€ <u>N</u> ext	<u>C</u> ancel

Windows and Linux:

• Enter and re-enter the NMR administration password.

Note: The NMR administration password is not related to any system password. This password will be required later when configuration commands in TopSpin are run, such as **cf**.

Please ((reques	choose an NMR Ac ted for commands	Iministration Passw i like 'cf', 'expinstall'	ord etc.)
Enter password: Re-enter password:			
G Back	Next	<u>C</u> ancel	😢 <u>H</u> elp

• Click Next.

Installation Directories for MICS, NMR-Data and SpectrOS

		Provera
C. (DIUKEI (IIIICS	 	- Diomac

• Select the installation directory for MICS.

Please s	elect an installation d	irectory for NMR-	Data
C:\Program Files\Br	uker\Topspin\alpha\o	examdata	Browse
G Back	🜔 <u>N</u> ext	<u>C</u> ancel	<u>D</u> isk usage

• Select the installation directory for NMR-Data.

Note: The next four dialog windows are displayed only when SpectrOS is included.

Note: On Windows do not use a path that contains parentheses, e.g. *C*:*Program Files (x86)*. Otherwise the firewall setup program will fail.

Please	select an installation	directory for Spect	rOS
C:\Bruker\spectros			Browse
G Back	Next	<u>C</u> ancel	<u>D</u> isk usage

• Select the installation direcory for SpectrOS.

Note: The installer will warn when downgrading SpectrOS to an earlier program version.

You are about	t to install an older prog	ram version.
Program: version to in version on d	SpectrOS stall: <abc> isk: <xyz></xyz></abc>	

• Click **Next**, if this is intended.

Note: Though not recommended, the Spectrometer Operating System can be installed while no spectrometer is connected to the workstation. In this case the network settings of the workstation will be configured for spectrometer control and the Spectrometer Operating System is installed on the local hard disk. When a spectrometer will be connected later, the Spectrometer Operating System can be transferred to the spectrometer with the program *post/updatespectros.sh* in the SpectrOS installation directory.

If Windows displays the message **Don't know how to open this program, please choose a program ...** then select *GNU\bin\bash.exe* in the TopSpin installation folder.

Exception: If the installation program cannot detect a spectrometer, it displays the following dialog window:

Note: No spectrometer found	4.
Spectrometer Operating Syst disk.	em will be installed on the local
Network will be configured for	or spectrometer control.
🕒 Back	<u>N</u> ext <u>C</u> ancel

• Click Next.

If the workstation controls a spectrometer, it should have two ethernet interfaces.

The installation tries to detect if manual changes have been made to the network interface configuration and to leave the file intact in that case. It will also save a copy of the original network interface configuration file in the SpectrOS installation directory.

Please specify Operating Syst	a network interface name for the Spectrometer em.
This should be network.	the network interface used for the spectrometer
eth1	-
G Back	Next <u>C</u> ancel

• Enter or select the name of the one connected to the spectrometer network.

Note: Bruker recommends to let the installer configure automatically the firewall for TopSpin commands. The firewall dialog is only displayed if a program was selected that requires firewall configuration, such as TopSpin on Windows, SpectrOS on Linux, CodeMeter on Linux, or MICS.

1	✓ Yes, configure system firewall automatically
	Automatically creates all firewall rules necessary for the products selected for installation
	Show necessary firewall rules
	This is useful if you intend to change custom firewall rules manually. The firewall rules will be shown after the products have been installed onto the hard disk

The last confirmation dialog is displayed before verification and file extraction to the local hard disk starts.

	The installati and will start	on has been setup now with these programs:	
Product	Version	Size/MB Target directory	
TopSpin			
CMC-a			
IconNMR			
SpectrOS			
NMR-Sim			
CodeMeter Runti	me		
	Open Source (GNU Public Lic Back	Components provided under cense v. will be installed	

- Check the summary of the selected components and target directories, before the installation starts.
- Click Next to start the file extraction.

The installer performs some checks before file extraction starts. In case of an error or obstacle any of the following dialog windows may appear.

Note: When other TopSpin versions are running on the computer, they have to be closed. Otherwise the following error message will appear:

	Running programs
	Terminate all applications of the program(s) you want to install before you proceed.
	The processes below are still running and cannot be overwritten during installation.
PID	Process name
3852	C:\Program Files\Bruker\Topspin\alpha\GNU\bin\bash.exe
4192	C:\Program Files\Bruker\Topspin\alpha\GNU\bin\bash.exe
800	C:\Program Files\Bruker\Topspin\alpha\prog\mod\cpr.exe
9440	C:\Program Files\Bruker\Topspin\alpha\prog\mod\cprserver.exe
8784	C:\Program Files\Bruker\Topspin\alpha\prog\mod\cprclient.exe
8032	C:\Program Files\Bruker\Topspin\alpha\jre\bin\java.exe
6636	C:\Program Files\Bruker\Topspin\alpha\prog\mod\dataserver.exe
3452	C:\Program Files\Bruker\Topspin\alpha\prog\mod\restartserver.exe
6616	C:\Program Files\Bruker\Topspin\alpha\prog\mod\cfserver.exe
4200	C:\Program Files\Bruker\Topspin\alpha\prog\mod\hconfserver.exe

Note: If a path was selected with an already existing TopSpin installation, the verification checks if any of the previously installed files have been changed, e.g. as patch or workaround for a bug. If so, the affected files are saved into a backup directory and information is displayed as in the next figure. The backup directory contains the program *restorefiles.pl* that can be run to restore the backup files.

Verification results
You can safely continue with the installation.
The modified files will be automatically saved in the sub directory backup\2017-03-24T1439 of the respective target directory of the product.
Below are the detailed results of the verification.
== Verification in C:\Bruker\TopSpin <xyz> for NMR-Sim ====================================</xyz>
The following files have been modified: C:\Bruker\TopSpin <xyz>\prog\nmrsim\pp\user\zgpg</xyz>

The installer displays the file extraction progress for each package.

Extracting NMR-Data		
exam2d_HC/3/acqus		
	Cancel	

The final dialog will display success or problems (during post installation) or errors if there are any. In that case please include the install.log in the TopSpin installation directory to your support request.

Installation finishe with the following	ed J results:
TopSpin	successful
CMC-a	successful
IconNMR	successful
SpectrOS	successful
NMR-Sim	successful
CodeMeter Runtime	successful
🕒 Back	€ <u>F</u> inish

· Click Finish.

2.3.1 CodeMeter Installation on Linux and macOS

- The **Linux** version of the CodeMeter runtime delivered with TopSpin comes as an RPM package and thus can only be installed on RPM based distributions like Red Hat (CentOS, Fedora) or Suse. If you use a different, not directly supported, distribution (Debian, Ubuntu,...), please download the CodeMeter Runtime here: https://www.wibu.com/support/user/downloads-user-software.html and follow the given installation details.
- CM runtime for diverse macOS versions are available on the same site.

2.4 Mac OS Installation

Insert the DVD and use Finder to inspect its contents. TopSpin for Mac OS X comes as a DMG file that is located in the root folder of the DVD. Double click the file TopSpin-<version>.dmg to open it. When the DMG is opened for the very first time, Mac OS X will verify its checksum. Due to the rather large size (around 500 MB) this may take a while (usually 30s on an iMac, probably longer on MacBook or MacMini). But the verification will happen only once. It is recommended to wait and let the system finish the check. Mac OS X will then mount the disk image and automatically display a Finder window with the Release Letter and the installation package file.



• Doubleclick TopSpin<version>.pkg.

The Welcome screen is displayed.

• • •	😺 Install Bruker NMR Software
	Welcome to the Bruker NMR Software Installer
 Introduction License Destination Select Installation Type Installation Summary 	This will install Bruker TopSpin (including CMC-se) and CMC-assist on your computer. You will be guided through the steps necessary to install the software.
BRUKER	Go Back Continue

• Click Continue.

000	💝 Install Bruker NMR Software			
	To continue installing the software you must agree to the terms of the software license agreement.			rms of
IntiLic	Click Agree to continue or click Disagree to cancel the installation and quit the Installer.			on and
• De:				
 Ins 	Read License	9	Disagree	Agree
SUMMARY SOFTWARE LICENSE AGREEMENT THIS AGREEMENT (hereafter "AGREEMENT") BETWEEN THE CUSTOMER ENTERING INTO THIS AGREEMENT BELOW (you') AND BRUKER BIOSPIN CORPORATION (hereafter "BRUKER"). LICENSE AGREEMENT. Subject to the provisions contained herein, BRUKER hereby grants to you a worldwide, revocable, non- exclusive license to use the proprietary software (the 'SOFTWARE')			WEEN THE IOSPIN hereby grants to 'SOFTWARE')	
BR	UKER	and documentation ('DOCUMENTATION') provided to Print Save	o you by BRUKER in Go Ba	ack Continue

• Click Agree.

• • •	😺 Install Bruker NMR Software
	Standard Install on "Macintosh HD"
 Introduction License Destination Select Installation Type Installation Summary 	This will take XyGB of space on your computer. Click Install to perform a standard installation of this software for all users of this computer. All users of this computer will be able to use this software.
BRUKER	Customize Go Back Install

• Click **Customize** to change some default settings, otherwise continue with **Install**.

Note: CodeMeter is deselected if it is already installed.

• • •	😺 Install Bruker NMR Software	
	Custom Install on "Macintosh HD" Package Name	Action Size
 Introduction License Destination Select Installation Type Installation Summary 	TopSpin C compiler C CMC-assist CodeMeter Runtime	Upgrade Upgrade Upgrade Skip
	Space Required: 1,55 GB	Remaining: 179,25 GB
BRUKER	Standard Install	Go Back Install

\bigcirc	Installer is t	rying to	o install new	software.
53	Enter your pas	sword to	allow this.	
Construction of the second sec	User Name:			
	Password:			
			Cancel	Install Software

- Enter user name and password of a user with administration rights.
- Click Install Software.

0 😑 0	🥪 Install Bruker NMR Software
	Installing Bruker NMR Software
 Introduction License Destination Select Installation Type Installation Summary 	Writing files
BRUKER	Go Back Continue
Please en	ter the NMR administration password
This nas	sword will be requested by TopSpin to
inis pu	authorize administrative tasks.
Password:	
Verify:	
	ОК

The NMR administration password is not related to any system password. This password will be required later when configuration commands in TopSpin are run, such as **cf**.

• Enter the NMR administration password and click **OK**.

Exception: The next two dialog windows are displayed only, when CodeMeter was installed and therefore a restart is necessary.

0 0	😺 Install Bruker NMR Software				
	When this software finishes ins must restart your computer. An	stalling, you re you sure Size			
Introductic	you want to install the software	1,43 GB			
License	Cancel	e Installation			
Destinatio		46,2 MB			
Installation Type					
Installation					
 Summary 					
	Space Required: 46,2 MB	Remaining: 180,67 GB			
Space Required: 46,2 MB Remaining: 180,67 GB Install CodeMeter Runtime on your computer. Please note that the CodeMeter Runtime Installation requires a reboot to start a driver to support CodeMeter CmDongle.					
BRUKER	Standard Install	Go Back Install			

Click Continue Installation.



• Click **Restart** to finish the installation.



· Click Close.

2.4.1 Differences of the Mac Version Compared to Other Platforms

In accordance to the guidelines for Mac applications, no target directory can be chosen during the installation. Unlike on other platforms, a parallel installation of several TopSpin instances of the same version is not supported. Installation is possible only on the root volume.

TopSpin on Mac OS X is a processing-only installation. Support for NUS (non-uniform sampling) data is fully implemented and available. NMR-Sim and the full NMR-GUIDE are available as well.

There is no acquisition support, nor IconNMR present.

Example Data Sets

On Mac OS X, the TopSpin installer currently installs a subset of the full example data sets only. If required, you can find the full set on the TopSpin DVD in the following file:

noarch/pack/nmrdata.tar.xz

Use a Finder window to navigate to the sub folder *mac/bin* of the DVD and double-click nmrdata-extract. This opens a window and asks for a folder where to extract the data. The program *nmrdata-extract* can alternatively be run in a terminal.

2.4.2 TopSpin Utilities

Completing the installation, the *Applications* folder contains the TopSpin application as well as a separate folder *TopSpin Utilities*. You can find the following tools there:

- SaveLogs: Used to collect log files and more required information for support incidents.
- **Terminate TopSpin**: In case TopSpin does not start as expected, components of the application may not have been terminated correctly from the last session and may still be active in memory. Use this tool to stop all running components. TopSpin should start normally after that.
- Uninstall TopSpin: This tool will remove the TopSpin installation from the harddisk. Use this only if you want to delete TopSpin completely. Security questions will protect from an unintentional use.

2.4.3 Additional Notes

During the release testing it has been observed that the presence of at least one virus scanning tool for Mac OS X may delay the start of TopSpin significantly (up to a couple of minutes). If you notice similar behavior we recommend to temporarily disable the virus scanner. TopSpin should start very fast then.

When starting TopSpin for the first time, the firewall of Mac OS may ask whether you want to allow or deny **access to cprclient**. This request is displayed only once and we suggest to choose **Allow**. (The installation procedure cannot do that automatically for you.)

2.5 Installation Results

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

When the installation is complete, the log file is stored in the TopSpin folder specified at the start of the installation or in */opt/topspin<version>* on MacOS. Under Windows and Linux, an existing log file is not overwritten, instead the new results are appended. On MacOS a new file is created every time a new TopSpin version is installed.

Before the installation begins to extract files to the hard disk, the log file is in the temporary folder

on Windows: C:\Windows\Temp

on Linux: /tmp

The current location of the log file is displayed in the terminal that is shown during the installation.

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

2.6 General Comment Regarding the TopSpin Factory Default Configuration when Installed on a Bruker Standard Workstation

TopSpin on a Bruker delivered workstation is installed with two user groups called NmrSuperUser and NmrUser together with two users called nmrsu and nmr. The user nmrsu belongs to the group NmrSuperUser, the user nmr belongs to the group NmrUser. Any newly created user can be associated with either of these groups or any other group. The default TopSpin installation is owned by the user nmrsu (group NmrSuperUser). Hence, this user owns all the TopSpin files and any manipulations to the configuration of TopSpin can only be done as this user. It is in the responsibility of the system owner to decide whether the TopSpin installation should be assigned to a different NmrSuperUser than nmrsu. This could either be a different local user or even a domain user. A reassignment of TopSpin to a different user can be accomplished through the TopSpin installations.

1. Procedure to change the NmrSuperUser of TopSpin under Windows:

Login with an administrator (root) account and open a TopSpin command prompt by opening the "TopSpin Utilities" desktop icon and double-click the command prompt. In the command prompt, enter the command:

perl\bin\perl prog\bin\installnmr <nmrsu>

2. Procedure to change the NmrSuperUser of TopSpin under Linux:

Open a shell window and become superuser (user: root). Change to the installation directory of TopSpin. In this example, TopSpin is installed in */opt/topspin*:

Enter the command:

./prog/bin/installnmr <nmrsu>

In both cases <nmrsu> refers to the name of the newly defined NmrSuperuser.

Under Windows, the user name for the so called NmrSuperUser must be the name of an existing user. Under Linux it can also be a non-existing user, which is then automatically created by the installation program. After running **installnmr**, the newly defined NmrSuperUser is the owner of all TopSpin program files. Logging in as this user allows you to remove files, change file permissions etc. The name of the NmrSuperUser is stored internally in TopSpin. Only the NmrSuperUser and users who belong to the administrator group are allowed to re-run installnmr (if that should be required).

In addition to this user, TopSpin also requires an NMR Administration password, which will be used for TopSpin internal configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TopSpin commands like **cf, expinstall** etc.

Note that the NmrSuperUser login password and the NMR Administration password have different purposes and are totally independent. Changing one of them does not affect the other.

Also note that the above described command **installnmr** also allows to change the NMR administration password.

Users belonging to	Install new software	Configure TopSpin	Run experiments
Windows/Linux Administrator-IT	Yes	Yes (if user belongs to group NmrSuperUser)	Yes
NmrSuperUser (Topspin Superuser/ Administrator)	No	Yes (requires NMR Administration Password)	Yes
NmrUser	No	No	Yes

The following table summarizes the groups and users and their meaning and rights:

2.7 Automatic Installation of TopSpin

It is possible to run an automatic installation of TopSpin (also known as unattended or silent installation). For that purpose

- On Linux run the shell script install with the command line option -a.
- On Windows run the batch file **install.cmd** with the command line option **-a**.

Other options that change the defaults can be added.

While you can launch install or install.cmd with any program, the examples below use the Command Prompt on Windows and a shell terminal on Linux. In that case the command and its options have to be typed in a single line.

Long lines can be split into several physical lines:

- On Linux type a backslash \ in the shell terminal as last character.
- On Windows type a caret ^ in the Command Prompt as the last character.

Note: When the automatic installation encounters an error or a warning, an appropriate error or warning message is displayed. After confirmation, the installation can be continued in interactive mode. Examples are:

- The installation directory cannot be used because there is already another TopSpin version.
- The verification check has detected modified files.
- There are processes running in the installation directory.

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 dialog windows without the need to change the settings when you have to attend a couple of installations.

Examples:

1. Scenario: The DVD is inserted in drive E:

• To list the available options, type:

E:\install -h

• To install TopSpin and IconNMR into the directory *C:\Programs\Bruker\Topspin* *<version>* , type:

E:\install -a -s topspin -s iconnmr -x C:\Programs\Bruker\Topspin\<version>

- To install the Dynamics Center into the folder C:\Bruker\DC, type:
 E:\install -a -d dc=C:\Bruker\DC
- 2. Scenario: The DVD is mapped to \\my-PC\my-share
- To install the programs in the group Data processing only: \\my-PC\my-share\install -a --setup-type po
- To specify an empty NMR administration password via its md5sum: \\my-PC\my-share\install -a --nmradminpwenc d41d8cd98f00b204e9800998ecf8427e
- 3. Scenario: The DVD is mounted as /media/cdrecorder
- To install the programs in the group **Data processing, acquisition and automation**: /media/cdrecorder/install -a --setup-type pa
- To specify the plain NMR administration password, type: /media/cdrecorder/install -a --nmradminpw TEDDY
- To install TopSpin without GCC, type: /media/cdrecorder/install -a -s topspin --gcc-off
- To specify not to add the installation directory to the global path, type: /media/cdrecorder/install -a --globalpath 0
- To get a list of valid program shortnames that can be used in the command line, type: /media/cdrecorder/install -s help

3

TopSpin License Management and Product Order

TopSpin uses the new Code Meter license management. A license can be ordered from the Bruker website. Just go to *https://www.bruker.com/nmr_license_requests.html* and fill out the request form. The License department will process the order details and generate an **activation ticket** and provide it to the customer. A ticket consists of a 25 character code like e.g.:

PH3T4-9D9U9-FNSGP-J9FXP-TTNXC

This code works as an access key to the purchased license package. It authorizes the customer to assign the license package to a computer of personal choice.

Install the software product on the computer system. During installation you may also be requested to install the package **CodeMeter Runtime**. This is the component of the license management system. Most installation routines will perform this task automatically.

A Free TopSpin Evaluation license can be ordered on the following web page:

https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/topspin-demo-licences-generation.html

A Free TopSpin Processing license for Academia can be ordered on the following web page:

https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/nmr-topspin-license-for-academia.html

For further information please look up the Code Meter License Management User Manual H162728.

4 Basic Configuration of TopSpin

This chapter provides some guidelines to full spectrometer or processing-only configuration. Commands will not be discussed in detail here. For a full description please refer to the **Acquisition Commands and Parameters** Manual.

There are several ways to start TopSpin on Windows:

- · Double-click the TopSpin icon on the desktop or
- Click Start | All Programs | Bruker TOPSPIN | TOPSPIN

First of all a TopSpin start window will open with details about the program version, the installation directory and the valid license(s).



If there are any problems with the licenses 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 the figure below disappears into the background but remains open.

This procedure will be same with every start of TopSpin.

After the startup of TopSpin a LICENSE window will be displayed. Please read the license agreement for Bruker TopSpin.

🍐 UC	CENSE CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR CONTRA	X
	Accept, Do Not Show License Again Accept Cancel	
Pleas	se read and accept license.	
if you	I don't agree, press Cancel. The program will terminate in this case.	
1	BRUKER BIOSPIN CORPORATION	Â
2	15 Fortune Drive	
3	Billerica MA 01821	=
4	978 667 9580	
5		
6	Software Copyright/License Documents	
7		
8	SOFTWARE LICENSE AGREEMENT	
9	THIS AGREEMENT (hereafter "AGREEMENT") BETWEEN THE CUSTOMER ENTERING INTO	
10	THIS AGREEMENT BELOW ('you') AND BRUKER BIOSPIN CORPORATION (hereafter	
11	"BRUKER").	
12		
13	LICENSE AGREEMENT.	
14	Subject to the provisions contained herein, BRUKER hereby grants to you a worldwide, revocable, non-	
15	exclusive license to use the proprietary software (the 'SOFTWARE') and documentation	
16	('DOCUMENTATION') provided to you by BRUKER in accordance with the sales agreement. As	
17	described below, your use of the SOFTWARE, when enabled, is limited to a specified number of	
18	simultaneous users.	
19		
20	SOFTWARE AND DOCUMENTATION.	
21	BRUKER shall furnish the SUFTWARE to you on media in machine-readable object code form and may	
22	also provide the DOCUMENTATION containing instructions for operation and use of the SOFTMARE.	
23	All items will be delivered via electronic means such as internet download (e.g., via FTP). You may	
24	inspect the SUFTWARE prior to accepting delivery of the SOFTWARE.	
25		-
	1:1	

• Click I Accept.

If you do not wish to answer the License question again upon the next start of TopSpin, click I Accept, Do Not Show License Again.

The TopSpin GUI is displayed.

C TopSpin		⇔_□×
Ξ <u>Acquire</u> <u>P</u> rocess A <u>n</u> alyse <u>M</u> anage	© ?	BRUKER
送 Sample - ♯ Lock V Tune - U Spin - 帮 Shim - パ Prosol - 座 Gain - ト Go - More -	88 66 68	😋
*2 /2 \$ ↔ \$ ⇔ ± Q Q 勹豆圡 ⊼ 늪 ▶ ■ @ ₩ ଓ 讐骨 # ↓ ↓ ♥		
Search Clouder Copporer and ata		
No structure available.		

The user interface can be changed with the command **set** or with the toolbar button This will open the User Preferences window. In the group Window Settings the window can be customized.

🖕 Preferences		×
Administration Items Window Settings Processing Preferences Text Editors Regulated Environments Miscellaneous Mobile Connection Directories Acquisition More Preferences	Administration Items Auto-open last used dataset when restarting TopSpin Show TopSpin data examples directory in data browser Setup users for TopSpin-internal login/logoff and esign Automatic termination of TopSpin when idle time exceeded Automatic locking of TopSpin when idle time exceeded Enable automatic command spooling Window Settings Change fonts by points Open new internal windows "cascaded" rather than "maximizer Configure cascaded windows 'Arrange' internal windows is only applied to dataset windows Tabbed pane layout	Change Change Change d" Change
Searc	ch <u>Apply</u> <u>C</u> lose	<u>R</u> eset

With the first start of TopSpin a Configuration Check window will be displayed:

Configuration check	
Warning:	
"Expinstall" has not been executed for this installation yet! Some functions of the program will not work correctly until "expinstall" has been executed.	
For spectrometer control press "Cf" to execute "cf" first, for datastations press "Expinstall" to execute "expinstall" or press "Close" to ignore this message and execute "cf" or "expinstall" later.	
Do not show this message again	
Cf Expinstall Close	

Note: The TopSpin system configuration depends on the spectrometer hardware. Mainly three scenarios need to be considered:

- · Configuration of a Workstation to control a spectrometer
- Configuration of a processing-only Workstation using an existing spectrometer configuration.
- Configuration of a processing-only Workstation

4.1 Configuration of a Workstation to Control a Spectrometer

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

- Click **cf** in the Configuration check window or type **cf** in the command line of the TopSpin main window.
- Enter the NMR administration password in the next window and click Ok.

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

🝦 Password request	×
Please enter the NMR administration password:	
	Cancol
<u></u> K	Gancel

The first cf window is displayed.

🖕 Cf		×
	Select Spectrometer	
△ Spectrometer	Location/Configuration	Datastation
Avance 600MHz	configured in Bruker_default_TRX_600	Yes
CAB AV4 400 MHZ BASIC	at IP 149.236.99.9	No
	New Spectrometer Delete	Spectrometer
	<u>N</u> ext >	▶ <u>C</u> ancel

Most likely you will select an existing configuration and click **Next** to confirm this configuration. Click **New Spectrometer** to start a new configuration.

In this example the configuration CAB AV4 400 MHZ BASIC is an existing spectrometer configuration for an Avance Neo 400 MHz spectrometer.

If only the Bruker_default_TRX_600 configuration is shown (see below), then a previous configuration could either not be detected or does not exist.

🖕 Cf		×
	Select Spectrometer	
△ Spectrometer	Location/Configuration	Datastation
Avance 600MHz	configured in Bruker_default_TRX_600	Yes
	New Spectrometer Delete	Spectrometer
	Next :	> Cancel

If an older TopSpin version with an appropriate configuration exists, then you can load it by clicking on **New Spectrometer**. The following window will be displayed:

Create new Sp	pectrometer Configuration		×
 import 	as Datastation ~ from	C:\Users\nmrsu	Browse
⊖ AV	connected to workstation at local IP address	149.236.99.9	
		Cancel	ОК

Select one of the following three options:

- 1. Import a datastation from ... This will be explained in chapter *Configuration of a Processing-Only Workstation Using an Existing Spectrometer Configuration* [▶ 44] and *Configuration of a Processing-Only Workstation* [▶ 48] and only makes sense when you configure a processing-only workstation and not a spectrometer.
- 2. Import as spectrometer from... Browse to the TopSpin configuration directory where you want to import from.

Create new Sp	ectrometer Configuration		×
 import 	as Spectrometer v from	C:\Users\nmrsu	Browse
⊖ AV	connected to workstation at local IP address	149.236.99.9	
		Canc	el OK

3. Use the option AV connected to workstation at local IP address 149.236.99.9. This is the recommended option, if available.

Create new Sp	ectrometer Configuration		×
⊖ import	as Spectrometer v from	C:\Users\nmrsu	Browse
AV	connected to workstation at local IP address	149.236.99.9	
		Cance	el OK

Both options 2 and 3 will bring you back to the main cf window. It will now show the imported configuration.

🖕 Cf		×
	Select Spectrometer	
△ Spectrometer	Location/Configuration	Datastation
Avance 600MHz	configured in Bruker_default_TRX_600	Yes
CAB AV4 400 MHZ BASIC	configured in remote_spect	No
	New Spectrometer Delete	Spectrometer
	Next >	Cancel

• Click **Next** to continue the configuration. A window with the basic spectrometer frequency will be displayed.

🖕 Cf		×
	Edit Configuration Parameters	
Spectrometer Description Description	CAB AV4 400 MHZ BASIC	
Spectrometer Data 1H Spectrometer frequency	400.130 MHz	
Security Options Enable power check		
Magnet Data Magnet polarity	SN (Bruker) ~	
	< <u>P</u> revious <u>N</u> ext > <u>C</u> ar	ncel

• Check or enter the spectrometer description, the 1H frequency of the magnet and magnet polarity. Enable **power check** and click **Next**.

The progress of the configuration procedure is displayed.

🖕 Cf	×
wait for server to handle parameters	
read BIS from HPPR/2 module P4 done	^
check ethernet hardware	
there are 7 DHCP controlled devices and 12 devices with fixed IP to check	
try to connect 19 devices at the spectrometer subnet	
connected: BLA-W144063-000028 at IP 192.168.99.16	
connected: ELCB_Z100818_6612 at IP 192.168.99.10	
connected: BACS2_H15000-01_733 at IP 192.168.98.2	
read configuration data from BSMS/2	
edit parameters	
send user input to server	
wait for server to handle parameters	
edit parameters	
get permission to continue configuration	
continue configuration	
parse input from user	
check for questions from server	
send user input to server	
wait for server to handle parameters	
get permission to continue configuration	
continue configuration	
parse input from user	
check for questions from server	
configure AQ facks	
contact restartserver	
contact adrackserver	
read board configuration from adrackserver	
configure EPU	
configure 184 1200	
read sequencer types from its ison at 192.100.100.14	
read all ks values from ikk 1200 1 done	
Consigning the 1500	
read sequencer types from TAX 1200 at 152.100.100	
read all k5 values from FRA 1200 2 done	
contiguite Gio	
read sequence: types from 610 at 152.166.160.30	
configure DACK	
configure DSM_429V	
configure PSM-D	
configure FANTDAY	
configure DEE 1200	
configure HPDP/2 COVER2	
read HPP//2 controller configuration	
read nreamblifter module configuration	
read BIS from HPDR/2 module Cl done	
read BIS from HPPR/2 module Pl done	
read BIS from HPPR/2 module P2 done	
read BIS from HPPR/2 module P3 done	
read BIS from HPPR/2 module P4 done	
check ethernet hardware	
there are 7 DHCP controlled devices and 12 devices with fixed IP to check	
try to connect 19 devices at the spectrometer subnet	
connected: BLA-W144063-000028 at IP 192.168.99.16	
connected: ELCB Z100818 6612 at IP 192.168.99.10	
connected: BACS2 H15000-01 733 at IP 192.168.98.2	
read configuration data from BSMS/2	~
	-
	Cancel

Depending on the hardware configuration optional devices will be displayed. Please keep in mind that this is an example. Specific entries may be different.

🖕 Cf	×
Edit Co	onfiguration Parameters
Optional Amplifier Devices	
19F Lockswitch connected to Amplifier at Blanking Signal	0 ~
2H Lockswitch connected to Amplifier at Blanking Signal	0 ~
PC running LC-NMR Software HyStar connected to	no ~
	< <u>Previous</u> <u>Next</u> > <u>Cancel</u>

• When finished, click Next. A summary window will be displayed.

<pre>Troubartow Hardware for any formation of formation of perturbations info</pre>				
<pre>HTERAIDCONFINEMENT THE ADDRESS AD</pre>	Summary			
<pre>intervalues development is constructed by the set of the set</pre>				
<pre>h</pre>				
<pre>v</pre>	ath : /ont/tonenin/conf/instr/smact/unner info			
<pre>image is special 6.00.1.11 image is special 6.00.1.11 image is special for the special fo</pre>	ath : /opb/soppin/conf/instr/spect/user/info			
<pre>trailed a: //griverspin :: ::::::::::::::::::::::::::::::</pre>	- Tenshin (0.0 h) (0.0 h)			
<pre>t : flidefpui : Could line relation 7.1.1511 (Court) : Could line relation : Court of line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line relation : Court if line</pre>	installed in : /ort/topspin			
<pre>: Control Lines relates 7.1.101 (User) : Control Control Lines relates 7.1.101 (User) : control Control Control Control Control (Control Control Contro Control Control Contro Control Control Control</pre>	iost : BladeEpu			
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<pre>r</pre>	PU : Intel(R) Core(TM) i7-4700EQ CPU @ 2.40GHs (8 cores at 1703 MHs with Hyperthreading)			
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<pre>frequency: 400.13 MHz frequency: 400.13</pre>	ystem : Avance Neo 400 NMR spectrometer			
<pre>respice (DB JV4 400 BET ADJC frequent in: Electropy / yespin/comf/impr/impr/impr/impr/impr/impr/impr/impr</pre>	M-frequency : 400.13 MMs			
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Section: Ref. 1 10: 1 Ministim: at 10: 1 [10: 10: 10: 10: 10: 10: 10: 10: 10: 10:	TRX 1200: AV4 TRANSCEIVER 1200 2148291/00178 ECL 01.03			
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Price: III of at mid. DEX as (der/%o/det.S. DED at (der/%bd/edd.4 Toka: Toka: Toka: Toka: Decasion: Back 1 Elso : Decasion: Back 1 Elso : D	Connection: at IP 192.168.180.14 via PCIe #3			
<pre>FALMA TAUMINE TRADECITER 10:0 144884/0017 ECL 01.03 Minimis AS JF 352.161.00.16 vuk FCL 61 Finance Taumine Taumin</pre>	Devices: MTD at mtdl, DRX at /dev/bbu/drx3.5, RTD at /dev/bbu/rtd3.4			
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Mark AFA 40 CHARSE 214800/0057 ECL 00.01 Mark AFA 40 CHARSE 214800/0057 ECL 00.02 MARKAN, NFA 40 CHARSE 214800/0057 ECL 00.02 MARKAN, NFA 40 CHARSEN 214800/0058 ECL 00.02 DEWLS COURSE: MERU/2 Coverse 2114807/0068 ECL 00.02 Medua 1: NETA/2 DEWLS DEWLS DEWLS DEWLS 2114807 Medua 1: NETA/2 DEWLS DEWLS DEWLS 2114807 DEWLS DEWLS 2114807 DEWLS DEWLS 2114807 DEWLS DEWLS 2114807 DEWLS DEWLS 2114807 DEWLS 2114807 DEWLS DEWLS 2114807 DEWLS	PSM-A: AV4 PSM-A 2149510/00066 ECL 01.02			
Sme-MFY, NAF SDM-MFY 214985/011 ECL 00.00 NUTRAK: NAF SDM - MFY 214985/0108 ECL 00.01 NUTRAK: NAF AGT TAK 114950/0108 ECL 00.01 NUTRAK: NAF AGT TAK 114950/0108 ECL 00.01 STATULE - STATULE - ST	RACK: AV4 AQ8 CHASSIS 2149500/0057 ECL 00.01			
<pre>Steve: Ar Steve 2144520/0008 ECE 00.01 Steve: Ar Steve 2144520/0008 ECE 00.00 Steve: Course: MSFA/Course 2114547/0008 ECE 00.00 Steve: Course: MSFA/Course 2114547/0008 ECE 00.00 Steve: Course: MSFA/Course 2114547/0008 ECE 00.00 Type : MSFA/C Course: MSFA/Course/Linksong in ED Steve: Ar Ministry 200.00 in ED Steve: Ar Ministry 200.00 Module 1: ET BreiDott, MF0000 from 2016107 Module 1: If Module 1: If Module 1: If BreiDott, MF0000 from 2016107 Steve: Ar Ministry 2000 from 2016217 Steve: Ar Ministry 2000 from 2016217 Steve: Ar Ministry 2000 from 2016218 Steve: Ar Ministry 2000 from 2016218 Steve: Ar Ministry 2000 from 2016218 Steve: Ar Ministry 2016 from 2016218 Ste</pre>	PSM-48V: AV4 PSM-48V Z149850/0111 ECL 00.00			
ANTAR: NA AOF TAT TAT 114050/004 ECL 00.00 HT100: XM HTMLTC: 100014970/0046 ECL 00.00 HTMLTC: XM AOF TAT 114097/10046 ECL 00.00 HTMLTC: XM AOF TAT 114097/10046 ECL 00.00 HTMLTC: XM AOF TAT 114097/10046 ECL 00.00 TAT 11407/10040 ECL 00.00 HTMLTC: XM AOF TAT 11407/10046 ECL 00.	PSM-D: AV4 PSM-D 2149520/0059 ECL 00.01			
<pre>MF 1000.WAX MEREMENT 1000 114819/0004 EX 01.02 MF 1000.WAX MEREMENT 1000 114819/0004 EX 01.02 MF 1000.WAX MEREMENT 100 FORM 1 : EVEN 100 FORM 1 : EVEN</pre>	FANTRAY: AV4 AQS FAN TRAY 2149501/0056 ECL 00.00			
<pre>SPAC = COME: MFM2 = Cover 2 lister/1009 # C = 0.0. Two for the space of the s</pre>	REF 1200: AV4 REFERENCE 1200 2148270/00066 ECL 01.02			
<pre>trrd: prev) preampling connectes ViA Apack Type : DTP() risk100 Publication finances = c. Connective Publication finances = c. mo LEO depire for tuning and matching Module 1: HTEMINISHIG (virtual 50 dm orference: 100.04/0.1deg, reflection meter) BM=TLORED, BM=CODEF from 20161010 Module 1: DT BM=DCODEF, BM=CODEF from 20161017 Module 4: ATBNT THE FM=TLORED4, BM=CODEF from 20161017 Module 4: ATBNT THE FM=TLORED4, BM=CODEF from 2016116 PM=TLORED4, BM=CODEF from 2016116</pre>	HPPR/2 COVER: HPPR/2 Cover2 2124567/02088 ECL 00.03			
<pre>provide Crew(); with DED Application finances = c. no LED dapls (result); winning and matching Module 1: HEUMI HEUMI (virtual 50 Gm seference: 100.04/0.1deg, reflection meter)</pre>	nrrk: - nrrk/2 prempilter connected via Aquaca			
no LEO deplay for tuning and marching Mohle 1: HEMI (HIMI (HIMI) Of the reference: 10.0%/0.1deg, reflection meter) PEFILORIO, SHPOORE from 2016110 Mohle 2: IS PEFDOOREN, SHPOORE from 2016100 Mohle 3: ISF PEFDOOREN, SHPOORE from 2016107 Mohle 4: SHPOOREN SHPOORE from 2016110 PHFLOREN, SHPOORE from 2016110 PHFLOREN, SHPOOREN from 2016110	Type : hFFV_			
Module 1: HEIM 1914 (ritual 50 Cm erference: 100.04/0.1deg. reflection meter) PFECORD, SPECORT, SPECORT, SPECORF fram 2014[10] Module 2: 12 Module 4: 117 Module 4: 1217 PHETORESS, SPECORF fram 2014[21] PhetoRess, SPECORF, SPE	controlation cover, a provide and an and a section of the section			
PP=100203, BP=0048 from 2016118 PP=200473, BM=0006 from 2016100 PP=200473, BM=0016 from 2016100 PP=200483, SM=0019 from 2016107 Module 4: XBM=00197 from 2016116 PM=10684, SM=00197 from 2016116 Pfmft Newt> Came	Module 1 : MFINA 19FIN (virtual 50 Chm reference: 100.0%/0.1deg, reflection meter)			
Module 2 : 17 SHP0200471, SHP02006 from 20141026 Module 3 : 187 SHP0200471, SHP02006 from 20141017 Module 4 : FSSETTER SHP02077 from 20141017 Module 5 : SHP00077 from 20141016 SHP02077 from 20141016	PN=2103203, SN=00640 from 20161110			
PHEDOATD, BH=0000 from 20161006 Module 1: 10 F PHEDOATD, BH=0011 from 20161017 Module 4: XBH=00137 from 20161116 PH=1106964, BH=00137 from 20161116 PH=1106964, BH=00137 from 20161116	Module 2 : 2H			
Module 3 : 197 BUICODESS, SH=0013 from 20141017 Module 4 : XB107 HP BH=010694, BH=0027 from 20141016 PHINT Newt> Cance	PN=2002471, SN=00206 from 20161026			
PH=D00489, SH=0012 from 2016107 Module 4: XBH=00127 from 20161216 SH=2106964, SH=00127 from 20161216	Module 3 : 19F			
Module 4: XELIFIER BH=2106994, SH=00197 from 20161216 Print Newt> Cance	PN=2003493, 5N=00213 from 20161017			
speciologi, steoory free coldicid	Module 4 : XBB19F 2MP			
Print Next > Cance	DN=2106984, SN=00227 from 20161216			
Print Next > Cance				
Print Next > Cance				
		Print	Next >	Cance

🛊 u 🛛 🕹
Summary
^
Transmitters at the spectrometer submet:
BLA-W144062-000028 W144062/000028 ECL 00:
- Firmars - 19.106318
- Amplifier = AV4 BLABBH2H 500/100/150 200-600: #144062/000026 ECL 00 - Controller = BLA CONTROL BOARD 7: #123926/000945 ECL 20
ITEX 2109889/0210 ECL 04.01: - TCP/IP address = 102.180.98.10
- Amplifier = BSMS/2 LOCE TRANSCEIVER 400: 2109888/02120 ECL 04.01
83N5: 83N5/2 connected to ethernet
- LLUB furmare version = 20161026
- GAB current limits = 0.0/X, 0.0/Y, 10.0/Z (in A) - SCB channels = 40
- Shim System = B0383-3B
- Artive shims: Z 2 28 24 25 X XZ X22 (X2-Y1) XY Y YZ YZ2 (X2-Y1)Z2 X24 X28 26 (X2-Y1)Z YZ4 YZ8 XYZ2 XYZ X8Z X8 Y3Z Y3 Z7 28 X25 YZ6 (X2-Y1)Z
- Magnet polarity: SN (Bruker), uses standard NO polarity L-TRN: # BSNS/2_LOCK TRANSCIPUEN 400: 1109809/021D0 ECL 04.01
- Lock: on L-TEX board, supports 2H, 18F - VTI ASP = RNM/2 ASP ATMONG & PATTERNATION: 2118191/03730 ECL 05 02
- VTU_VFSB1 = AV4 VARIABLE FOWER SUFFLY BD DC: 2139805/00043 ECL 01.01
VTU: in BSN9/2 connected to ethernet
- TCW/IV address = 192.100.99.10
Sample Changers at the spectrometer subnet:
Sample Changer 1: BAC52 H15000-01_722 - TCP/IP address = 102_168.08.2
- Protocol types = BOAD
SGUI NORM output -> imput 2 of transmitter 1 (AV4 BLAEBHIH 500/100/150 200-600BSMS/2 LOCK TRANSCEIVER 400 W144062/000028 at TCP/IP 192.168.99. SGUI AUX output -> imput 1 of transmitter 2 (BSMS/2 LOCK TRANSCEIVER 400 2109888/02120 at TCP/IP 192.168.99.10)
SGU2 MORA output -> input 1 of transmitter 1 (AV4 ELABEM2H 500/100/150 200-600B5M5/2 LOCK TRANSCEIVER 400 W144063/000028 at TCP/IP 152.168.99. SGU2 ADX output -> open
Blanking cable connections (detected)
- amplifier B-500W uses blanking 2
- amplifier 1H-100W uses blanking 1 - amplifier 2H-150W meeds no blanking
transmitter 2 = 55M5/2 LOCK TRANSCEIVER 400 2109008/02120 at TCP/IP 192.160.99.10:
- amplifier 2N-5W uses blanking 9
Refeatives (setures as estimate) and (set
ovicchox (unanowi no suppus) rousing
<pre>transmitter 1 = AV4 BLABEMIN 500/100/150 200-600BEMS/2 LOCK TRANSCEIVER 400 W144063/000028 at TCP/IP 192.160.99.16: - amplifier 1H-100W at blanking 1 can be routed to switchbox output 3 (unknown)</pre>
- amplifier B-500W at blanking 2 can be routed to switchbox output 1 (unknown) and output 2 (unknown)
Breamliffer connections (detected)
Tune-SGU1 -> 2H -> REC1
Tune-36U1 -> 19F -> REC1 Tune-36U2 -> XBE19F 2HF -> REC2
× v
Print Next > Cancel

• Click **Next**. The channel routing window will be displayed. Check and correct it, if necessary.

Channel Routing			×
Amplifier		Preamplifier	Receiver
1H 100 W		HPLNA 19F1H	REC1
	MAIN	2H	
BB 500		19F	l .
		XBB19F 2HP	REC2
2H 5 W			
settings			
show cf wiring	show receiver wiring		
⊖ show probe wiring	Select HP Stage for default routing		
	Sa <u>v</u> e and Close Save	Clear cable connections	Param <u>C</u> lose

• Check and correct the connections, if necessary. Click **Save and Close** or **Close**. The Additional Setups window will be displayed:

💩 Cf		×
	Additional Setu	os
Important		
Edprobe	Probe setup	
Expinstall	Installation of standard experiments	
Paracon	Update installation of user experiments	
Edprosol	Solvent dependent parameter setup	
Optional		
Ed <u>c</u> stm	Edit customer/system information	
Ed <u>n</u> uc	Edit nuclei table	
Ed <u>s</u> olv	Solvent table setup	
Edscon	Spectrometer parameters setup	
<u>V</u> tudisp	Temperature control unit setup	
MICS update	Magnet Information & Control System	
		<u>Einish ></u>

• Note: The most important next configuration steps are Edprobe, Expinstall and Edprosol.

Edprobe

• Click **Edprobe**. The Edprobe window will be displayed.

🖕 Edprobe M <u>a</u> nage <u>H</u> elp				_		×
Current probe: Nickname: Probe ID: Description:	(Automatically Z820201_028 PA BBI 400S	detected) 0 LH-BB-D-05 Z				
△ Nickname	Probe ID		Description			
2	Z820201_0256	PA BBI 400S1 H	BB-D-05 Z			
Edit Pr	roperties Ed	it <u>R</u> F Connections	<u>S</u> et as current	De <u>l</u> ete	<u>C</u> I	ose

If the current probe is recognized through the PICS (Probe Identification Control System), then it will automatically be selected.

• Click **Edit Properties** to check or set the properties. Click **Close**. The probe RF connections will be displayed.

edprobe: Edit RF Connections			×
Amplifier	Preamplifier	Probe: Z820201_0280	
1H 100 W BB 500	HPLNA 19F1H 2H AUX 19F XBB19F 2HP	1H connector 1 on coil 1 2H connector 2 on coil 1 31P-109Ag connector 1 on coil 2	
	Sa <u>v</u> e and Clos	se Clear cable connections Info Param	<u>C</u> lose

• Check and correct them, if necessary. Click Save and Close or Close.

Expinstall

In the Additional Setups window, click Expinstall. A Password request window is displayed.



• Enter the NMR administration password to display the first Expinstall window.

Experiment installation and AU compilation
Expinstall
Expinstall installs pulse programs, AU programs,
parameter sets and various other resources for spectrometer
For spectrometer control do cf first.
For a customized datastation configuration copy your
spectrometer configuration directory (typically called "spect")
to <topspin dir.="" installation="">/conf/instr.</topspin>
WARNING:
Please archive all your MODIFIED Bruker PARAMETER-files, All-programs and PULISE-programs before running
"expinitali".
< Back Next > Einish Cancel

- Click Next. If there are no modified Bruker-Parameter files, AU-programs and Pulseprograms or files and programs are archived in a different directory. Individual Parameter files, AU-programs and Pulse-programs with different names to the original Bruker files will not be affected during the installation.
- In the next window select the type of acquisition. In the example a High Resolution System has been checked.

🖕 Expinstall for Spectrometer	x
Select the type of acquisition: I High Resolution Systems Solid State Systems	A III
Micro-Imaging and Diffusion Systems	
۳	
< <u>B</u> ack <u>N</u> ext > <u>Finish</u>	<u>C</u> ancel

• Click Next.

🖕 Expinstall for Spectrometer	×
Available encetremeter or detectation configurations:	^
Available spectrometer of datastation conligurations.	
Select the configuration you want to use:	
CAB AV4 400 MHZ BASIC V	
Bruker_default_TRX_600	
CAB AV4 400 MHZ BASIC	
\$	>
< <u>B</u> ack <u>N</u> ext > <u>F</u> inish <u>C</u> an	cel

- Select the spectrometer or data station configuration for expinstall. Here the CAB AV4 400 MHZ BASIC has been selected. If this window is not displayed, then TopSpin has found only one valid configuration, namely the one for the current spectrometer, and immediately continues with the next window. Click Next.
- In the next window select the items to use for the spectrometer or the processing-only Workstation configuration. Accepting the default settings is a good choice. Then click **Next**.

🖕 Expinstall for Spectrometer
Select the items you want to install:
✓ Install Pulse Programs
✓ Install Bruker AU Programs
Recompile All User AU Programs
☑ Install Library CPD Programs
Install Library Gradient Files
Install Library Shape Files
Convert Standard Parameter Sets
Install Standard Scaling Region Files
Install Bruker Python Programs
Select all Select none
< <u>Back</u> <u>Next</u> > <u>Finish</u> <u>Cancel</u>

• In the next window enter the basic frequency of the spectrometer and the pre-scan delay. All settings should be correct. Nevertheless in case of a configuration to control a spectrometer they should be checked. Click **Next**.

Basic Configuration of TopSpin

Expinstall for Spectrometer			X
Select the basic frequency of	your spectror	neter:	
Basic frequency (MHz):	400.13		
Select the pre-scan-delay DE:			
Default pre-scan-delay (µs):	6.5		
Select the plotter paper format	i:		
Paper format:	A4 / Letter	~	
< <u>B</u> ack	<u>N</u> ext >	<u>Finish</u>	Cancel

• Click **Next** to display a summary of options executed by **expinstall**.

Expinstall for Spec	trometer	×
Expinstall will be e	xecuted with following options:	
Installation for S	Spectrometer	
(High Resolutio	n)	
Configuration n	ame: CAB AV4 400 MHZ BASIC	
Install Pulse Pr	ograms	
Install Bruker A	U Programs	
Install Library C	PD Programs	
Install Library G	radient Files	
Install Library S	hape Files	
Convert Standa	ard Parameter Sets	
Install Standard	Scaling Region Files	
Install Bruker P	ython Programs	
Basic frequenc	y: 400.13 MHz	
Pre-scan-delay	6.5 µs	
Paperformat:	A4 / Letter	
	< Back Next > Finish	<u>C</u> ancel

· Check this list.

• To change an option, click **Back** to the window(s) where corrections have to be done. Then click **Finish**.

The installation of the selected items will start now. Wait until this process has finished. In the TopSpin status line the progress of the installation is monitored. At the end of expinstall a Cron check window is displayed.

Cron check	×
An automatic periodical backup of your TopSpin configura	tion
can be defined in TopSpin. Currently you do not use this to	ool.
Press "Automatic Backup" to open the configuration tool.	
Do not show this message again	
Help Automatic_Backup Cos	е

• Click Automatic Backup to open the NMR Save window.

ave installation files Restore installation files Save user files Save installation specific files. Installation specific files are collected and stored into a compressed file. This compressed file of to copy the files from a previous installation to a new installation or to create a backup of the installation specific files. Note: To save user specific files use the "Save user files" tab. Location of backup file: C:\Bruker\TopSpin <version>\nmr_backup Overwrite existing backup file: Browse Overwrite existing backup file: Bruker\TopSpin<version> Installation to be saved (TopSpin home) C:\Bruker\TopSpin<version> Spectrometer configuration (e.g. spect) Bruker_default_TRX_600 Display default information: O Execute "Save installation specific files" periodically Automatic Backup Log: Log:</version></version></version>		
Save installation specific files. Installation specific files are collected and stored into a compressed file. This compressed file of o copy the files from a previous installation to a new installation or to create a backup of the installation specific files. Note: To save user specific files use the "Save user files" tab. Location of backup file: Location of backup file: Location of backup file: C_\Bruker\TopSpin <version>\mmr_backup Browse Overwrite existing backup file: Display default information: Execute "Save installation specific files" periodically Log:</version>		
Istallation specific files are contected and stored into a compressed me. This compressed me to o copy the files from a previous installation to a new installation or to create a backup of the installation specific files. Note: To save user specific files use the "Save user files" tab. Location of backup file: Determine existing backup file: Installation to be saved (TopSpin home): C:\Bruker\TopSpin <version> Browse Spectrometer configuration (e.g. spect): Bruker_default_TRX_600 Display additional information: Display additional informat</version>	on he	
ote: o save user specific files use the "Save user files" tab. ocation of backup file: Derwrite existing backup file: Destallation to be saved (TopSpin home): C:Bruker:TopSpin <version> Browse pectrometer configuration (e.g. spect): Bruker_default_TRX_600 Display additional information: O xecute "Save installation specific files" periodically Automatic Backup og:</version>	an be	e usei
o save user specific files use the "Save user files" tab. ocation of backup file: Browse Dverwrite existing backup file: Browse installation to be saved (TopSpin home): C:\Bruker\TopSpin <version> Spectrometer configuration (e.g. spect): Bruker_default_TRX_600 Display default information: Image: Comparison of the same of the</version>		
ocation of backup file: C:\Bruker\TopSpin <version>\nmr_backup Browse Dvervrite existing backup file: Istallation to be saved (TopSpin home): C:\Bruker\TopSpin<version> Browse Spectrometer configuration (e.g. spect): Bruker_default_TRX_600 Sisplay default information: Secute "Save installation specific files" periodically Automatic Backup og:</version></version>		
.ocation of backup file: C:\Bruker\TopSpin <version>\nmr_backup Browse Dverwrite existing backup file: Installation to be saved (TopSpin home): C:\Bruker\TopSpin <version> Browse Spectrometer configuration (e.g. spect): Bruker_default_TRX_600 Display default information: O Execute "Save installation specific files" periodically Automatic Backup .og:</version></version>		
Diverwrite existing backup file:		
Installation to be saved (TopSpin home): C:\Bruker_TopSpin <version> Browse Spectrometer configuration (e.g. spect): Bruker_default_TRX_600 Splay additional information: Secute "Save installation specific files" periodically Automatic Backup .og:</version>		
ipectrometer configuration (e.g. spect): Bruker_default_TRX_600 ipsplay default information: ixecute "Save installation specific files" periodically Automatic Backup .og:		
Iisplay default information: iisplay additional information: xecute "Save installation specific files" periodically dutomatic Backup og:		
Display additional information: O Execute "Save installation specific files" periodically Automatic Backup og:		
Execute "Save installation specific files" periodically Automatic Backup		
		^
Sa	e	Close

- Define the locations for saving and restoring the installation and user files.
- Click Automatic Backup to periodically save the configuration specific files.

It might be useful to save the periodical backups on a network drive. Enter the network drive as location of backup file in the NMR_Save window. Click **Automatic Backup**, the chosen drive is set and cannot be edited anymore. For more information see *Backup and Restore of Important Files* [> 49].

• Set job, options and rules for an periodical backup.

Note: The command box cannot be edited!

ommand	nmrsave	-date -pat	h "C:\Bruk	ker\TopS	Spin <version>\nm</version>	r back	UD" -SO	urce "	C:\F
escription	Execute NMR_SAVE								
xecution scope	TopSpin (requires authentication)								
7 Direct execution	'n								
Direct execution	on	from	26	to:	Janore	~	+		^
Direct execution ules Minute of the ho Hour of the day	on our	from: from:	26	to:	Ignore	~ ~	+		^
Direct execution ules Minute of the ho Hour of the day Day of the mon	on our v th v	from: from: from:	26 × 16 × 28 ×	 to: to: to: 	Ignore Ignore Ignore	~	+ + +		
Direct execution Ules Minute of the ho Hour of the day Day of the mon Month of the ye	on our y th y	from: from: from: from:	26 × 16 × 28 ×	 to: to: to: 	Ignore Ignore to: Ignore	> > >	+ +		

- Click OK and enter the NMR administration password.
- In the NMR Save window, click **Save**. The compilation of **xauw** will start. When this process is finished the Additional configuration programs window is displayed.

Edprosol

• Click **Edprosol** to enter the probe and solvent dependent parameters. It is necessary to execute Edprobe first (see above) because the probe parameters are needed.

Basic Configuration of TopSpin

edprosol								_		×
<u>File Edit View F</u>	<u>-l</u> elp									
		Saved Ob	serve and Sav	ed De	ecouple Prosol Para	ameter Set for:				
Probe: Z820	0201_	_0280 PA BBI 4005	61 H-BB-D-05	Z	Select	Solvent: g	ener	ic		~
		Obs	serve		C	ecouple				
		1H	~	Nu	Icleus 1H	~				
		Obs	serve		D	ecouple)				
Observe Com	ment	: Default 1H obs 4	100		Decouple Comn	nent: Default	1H de	ec 400		
90 deg. Pulses	HR	Square Pulses HI	R Shape Pulse	es O	thers					
		Observe	;			Decouple				
Nucl	leus	Pulse Width[µs]	Power[W]	Set	Pulse Width[µs]	Power[W]	Set	Nucleus		
11	H	10.00	6.3096	\bigcirc	10.00	6.3096	\bigcirc	1H		^
2H@	@1	280.00	2.9992	\bigcirc	280.00	2.9992	\bigcirc	2H@1		
2H@	@2	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	2H@2		
61	Li	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	6Li		
71	Li	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	7Li		
9B	Be	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	9Be		
10	в	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	10B		
11	в	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	11B		
13	C	15.00	80.910	\bigcirc	15.00	80.910	\bigcirc	13C		
14	N	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	14N		
15	N	30.00	104.95	\bigcirc	30.00	104.95	\bigcirc	15N		
17	0	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	170		
211	Ne	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	21Ne		
231	Na	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	23Na		
251	Mg	0.00	0.0000	0	0.00	0.0000	0	25Mg		
27	AI	0.00	0.0000	0	0.00	0.0000	0	27AI		
29	Si	0.00	0.0000	0	0.00	0.0000	0	29Si		
31	Р	0.00	0.0000	0	0.00	0.0000	0	31P		
33	S	0.00	0.0000	\bigcirc	0.00	0.0000	\bigcirc	33S		
35	CI	0.00	0.0000	\bigcirc	0.00	0.0000	Ø	35CI		~
			<u>L</u> ast S	ave	Print Copy	r to Sol <u>v</u> ent	Cop	oy to Pro <u>b</u> e	5	ave

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

Optional commands

You may want to check the optional configuration commands as listed below in the last cf window.

🖕 Cf		
	Additional Setu	os
Important		
Edprobe	Probe setup	
E <u>x</u> pinstall	Installation of standard experiments	
Paracon	Update installation of user experiments	
Edprosol	Solvent dependent parameter setup	
Optional		
Ed <u>c</u> stm	Edit customer/system information	
Ed <u>n</u> uc	Edit nuclei table	
Ed <u>s</u> olv	Solvent table setup	
<u>E</u> dscon	Spectrometer parameters setup	
<u>V</u> tudisp	Temperature control unit setup	
MICS update	Magnet Information & Control System	
		<u>Einish</u> >

• When done, click **Finish**.

4.2 Configuration of a Processing-Only Workstation Using an Existing Spectrometer Configuration

If the Workstation 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 like that spectrometer.

To transfer the configuration of the spectrometer to the processing-only Workstation execute the following steps:

 Save the desired configuration on your spectrometer Workstation with nmr_save (see Backup and Restore of Important Files [> 49])

🖕 NMR_Save		×
Save installation files Restore installation	files Save user files Restore user files	
Save installation specific files. Installation specific files are collect to copy the files from a previous in of the installation specific files. Note: To save user specific files use the	eted and stored into a compressed file. This compress nstallation to a new installation or to create a backup e "Save user files" tab.	sed file can be used
Location of backup file:	C:\Bruker\TopSpin <version>\nmr_backup</version>	Browse
Overwrite existing backup file:		
Installation to be saved (TopSpin home):	C:\Bruker\TopSpin <version></version>	Browse
Spectrometer configuration (e.g. spect):	remote_spect ~	
Display default information: Display additional information:	•	
Execute "Save installation specific files" Log:	periodically Automatic Backup	
Backing up of NMR data was successful The backup file C:\Bruker\TopSpin <version>\nmr_backu</version>	! p/nmr_backup_20170705-1714.zip	
has been generated!	###	×
		Save Close

- Copy this archive file to the processing-only Workstation.
- Restore the configuration with the nmr_restore command to the processing-only Workstation (see Backup and Restore of Important Files [> 49])

Save installation files Restore installation specific files. Installation specific files are restored from a previously created backup file. This backup file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files. Note: You can only restore files that are named correctly (nmr_backup_"date"). To restore user specific files use the "Restore user files" tab. Browse Location of backup file: C.\Bruker\TopSpin <version>\nmr_backup Browse Name of backup file: C.\Bruker\TopSpin<version> Browse Display default information: Image: Clarkit information: Image: Clarkit information: Image: Clarkit information: Log: now converting gradshim files converting of gradshim files finished! Image: Clarkit information: Image: Clarkit information: Human Image: Clarkit information: Ima</version></version>	NMR_Save						X
Restore installation specific files. Installation specific files are restored from a previously created backup file. This backup file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files. Note: You can only restore files that are named correctly (nmr_backup_"date"). To restore user specific files use the "Restore user files" tab. Location of backup file: C:\Bruker\TopSpin <version>\nmr_backup Name of backup file nmr_backup_20170705-1714.zip Restore destination (TopSpin home): C:\Bruker\TopSpin<version> Display default information: Image: Converting of gradshim files converting of gradshim files finished! files finished!</version></version>	Save installation files Restore installati	ion files	Save user files	Restore user	files		
Installation specific files are restored from a previously created backup file. This backup file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files. Note: You can only restore files that are named correctly (nmr_backup_"date"). To restore user specific files use the "Restore user files" tab. Location of backup file: C:\Bruken\TopSpin <version>\nmr_backup Restore destination (TopSpin home): C:\Bruken\TopSpin<version> Browse Display default information: Display additional information: C:\Bruken\TopSpin</version></version>	Restore installation specific files.						
Note: You can only restore files that are named correctly (nmr_backup_"date"). To restore user specific files use the "Restore user files" tab. Location of backup file: Name of backup file: Nam	Installation specific files are restored f can be used to copy the files from a p restore a backup of the installation sp	from a prev previous inspecific files.	viously created stallation to a r	I backup file. Th new installation	nis backup or to	file	
Autor an only restore files that are named correctly (nmr_backup_"date"). To restore user specific files use the "Restore user files" tab. Location of backup file: C:\Bruker\TopSpin <version>\nmr_backup Name of backup file nmr_backup_20170705-1714 zip Restore destination (TopSpin home): C:\Bruker\TopSpin<version> Display default information: Image: Converting gradshim files Converting of gradshim files finished! ####################################</version></version>	Note:						
Location of backup file: C:\Bruker\TopSpin <version>\nmr_backup Browse Name of backup file nmr_backup_20170705-1714 zip Restore destination (TopSpin home): C:\Bruker\TopSpin <version> Browse Display default information: Display additional information: Converting gradshim files converting of gradshim files finished!</version></version>	You can only restore files that are nar To restore user specific files use the "	med correc 'Restore u	ctly (nmr_back ser files" tab.	up_"date").			
Name of backup file mmr_backup_20170705-1714.zip Restore destination (TopSpin home): C:\Bruker\TopSpin <version> Display default information: Image: Close in the second s</version>	Location of backup file:	C:\Bruke	r\TopSpin <ver< td=""><td>sion>\nmr_bac</td><td>kup</td><td>Browse</td><td>•</td></ver<>	sion>\nmr_bac	kup	Browse	•
Restore destination (TopSpin home): C:\Bruker\TopSpin <version> Display default information: Display additional information: C.\Bruker\TopSpin <version> Display additional information: Display additional information: C.\Bruker\TopSpin <version> Display additional information: Display additional in</version></version></version></version></version></version>	Name of backup file	nmr_bac	kup_2017070	5-1714.zip		•	
Display default information: Display additional information:	Restore destination (TopSpin home):	C:\Bruke	r\TopSpin <ver< td=""><td>sion></td><td></td><td>Browse</td><td>•</td></ver<>	sion>		Browse	•
Display additional information:	Display default information:	0					
Log: now converting gradshim files converting of gradshim files finished! ####################################	Display additional information:	O					
Log. now converting gradshim files converting of gradshim files finished! ####################################	1.02						
####################################	Log.						
All data have successfully been restored!	converting of gradshim files finished!						
All data have successfully been restored!							
All data have successfully been restored!							
All data have successfully been restored!							
All data have successfully been restored!							
All data have successfully been restored!							
All data have successfully been restored!	****						
Restore	All data have successfully been resto	ored!					
Restore Close	***************************************						
Restore	•	ш					•
						Restore	Close

- The spectrometer configuration is now available. It will appear in the expinstall window and can be used to configure the Processing-only system.
- Click cf in the Configuration check window or type cf in the command line of the TopSpin main window. Enter the NMR administration password when prompted for it. In the cf window, click New Spectrometer. Enter the pathname to the above imported spectrometer configuration or click Browse to select it.

C	ireate new Sp	ectrometer Configuration		×
	import	as Datastation - from	C:\Users\michael.engelhardt	Browse
	© AV	connected to workstation at local IP address	149.236.99.9	I
			Canc	el <u>O</u> K

Here the configuration stored as remote_spect has been selected:

🕌 Select				x
Look jn	instr 🔒	•	1 🕫 🖽	·
Zuletzt ve Desktop	autoshim Bruker_defau Probeheads remote_spect servtool topshim	lt_TRX_600 (Avance 600MHz) t (CAB AV4 400 MHZ BASIC)		
Eigene D				
Computer				
	Folder name:	C:\Bruker\TopSpin <version>\conf\instr\remote_spect</version>		Select
Netzwerk	Files of type:	All Files	•	Cancel

• Click **Select**, the name will be entered in the *from* field:

Create new Sp	ectrometer Configuratio	on			×
import	as	Datastation	• from	C:\Bruker\TopSpin <version>\conf\instr\remote_spect</version>	Browse
© AV	connected to works	tation at local IP	address	149.236.99.9	
					ancel <u>O</u> K

• Click **OK** and enter a suitable name for the spectrometer configuration to describe it in a meaningful way, e.g. av400_neo:

Save in:	🍌 instr	•	r
Luletzt ve Desktop	 autoshim Bruker_defau probeheads remote_spect servtool topshim 	ult_TRX_600 (Avance 600MHz) t (CAB AV4 400 MHZ BASIC)	
igene D			
Computer			
	Folder <u>n</u> ame:	C:\Bruker\TopSpin <version>\conf\instr\av400_neo</version>	Save

• Click Save.

Basic Configuration of TopSpin



The cf window will be displayed. Click Cancel and continue with edprobe and expinstall.



In the **expinstall** window, the available spectrometer list should show the av400_neo entry. Select it and continue as outlined in the previous chapter.

4.3 Configuration of a Processing-Only Workstation

If the Workstation does not control a spectrometer and is just used for processing only, then only expinstall needs to be executed. Proceed as outlined in the previous chapters and for instance select **Bruker_default_TRX_600** as an example configuration.

🖕 Expinstall for Spectrometer	:	×
Available spectrometer or datastation configurations:		^
Calact the configuration you want to you		
Select the conliguration you want to use.		
Bruker_default_TRX_600 ~		-
Bruker_default_TRX_600		
CAB AV4 400 MHZ BASIC		
1		~
	-	_
< <u>B</u> ack <u>N</u> ext > <u>F</u> inish	<u>C</u> ancel	

5 Backup and Restore of Important Files

It is strictly recommended to frequently create a backup of the important files of your configuration of TopSpin.

There are many good reasons for weekly or monthly backup of important data, e.g. head crash or theft of hard disk. It will allow to restore the 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 stored in one archive file.

Note: The commands nmr_save and nmrsave have identical functions.

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

The same function as nmr_save is 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 as defined in the user preferences, and the user specific directory *<USER_HOME>/.topspin-/ <Workstation_NAME>/prop* are saved. All these user specific files will be stored in one archive file.

The command **nmr_restore** and **user_restore** respectively restore installation and userspecific files to the same or a different installation.

5.1 How to Save Information with nmr_save

Start TopSpin and enter nmr_save or nmrsave

or

Start TopSpin and click

Manage | Safe/Restore installation | Save installation specific files

🛃 To	opSpin		↔	×
	<u>P</u> rocess A <u>n</u> alyse <u>I</u>	Manage	ې نې، ؟ ۵) E R
Ŀ	Spectrometer 🗸 🖉 Security 🗸	Commands - En Remote		4
*2	Spectrometer power on/off (pdudisp)	Save Installation Specific Files (nmr_save)		
	Hardware Detection	Saves spectrometer installation specific files		-
Searc	Experiments/Parameters	in a backup TAR-file. The saved files can be restored to the same or a different TopSpin		
E-C:\	Manage temporary acquisition data	installation using the command nmr_restore.		
	BSMS Control			
	CryoProbe Control			
	ProdigyDisplay			
	Save/Restore Installation			
Struc	Spectrometer Usage (account)			
	No structure available.			

The NMR_Save window will be displayed.

	Restore installation t	iles Save user files Restore user files	
save installation specific fil o copy the files from f the installation spe lote: o save user specific	cific files. es are collected and a previous installatio crific files.	stored into a compressed file. This compressed file in to a new installation or to create a backup user files" tab.	e can be used
Location of backup 1 Dverwrite existing be nstallation to be sav Spectrometer config Display default infor Display additional in Execute "Save instal	file: ackup file: ved (TopSpin home): uration (e.g. spect): mation: formation: lation specific files" p	C:\Bruker\TopSpin <version>\nmr_backup C:\Bruker\TopSpin<version> C:\Bruker\TopSpin<version> eriodically Automatic Backup</version></version></version>	Browse

- Accept or modify the location of the backup file.
- Enter the location of the installation to be saved.
- nmr_save will then offer a list of all available spectrometer configurations which are located in this installation. Select the correct spectrometer name, e.g. BRUKER_default_TRX_600.
- For a periodical backup click **Automatic Backup**. This will open a window for a command scheduling. Click **OK** to accept the default values to execute **nmr_save** once a month.
- · Click Save.

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

nmr_backup_<date>-<time>.tar

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

<TOPSPINHOME>\nmr_backup

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-specific or by default. It offers full flexibility in time definition, off-schedule execution and user control. When called from **nmr_save**, the fields contain default values as in the next figure.

CONTRACTOR INCOMENDATION	nmrsave -	date -nath	"C:\Bruker\	TonSnin	v>\nmr hackur	" -sour	re "C·V	Bruker\
Johnmand	.mm save -	date -patri	C. Drukery	ropopiir		-30ui		Diakers
Description	Execute NMR_SAVE							
Execution scope	TopSpin (requires authentication)							
tules	iour 🗸	from:	53 ~	to:	Ignore	~	+	-
Minute of the h	our							
Minute of the h	/ ~	from:	15 ~	to:	Ignore	~	+	-
Minute of the h Hour of the day Day of the mor	y v	from:	15 ~ 1 ~	to:	Ignore Ignore	~	+	-
Minute of the h Hour of the day Day of the mor Month of the ye	y v ith v ear v	from: from: from: *	15 × 1 ×	to: to: v to:	Ignore Ignore Ignore	>	++++++	-

The following fields are available:

- Command: The command to be executed
- · Description: A description of the command
- **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 NMR administration password.
- 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.

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
- 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 an extra field of the same type, allowing multiple interval definition. Clicking **-** removes the extra field.

5.2 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)
- IconNMR 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 (edprobe)
- Nucleus information (ednuc)
- RF Shapes and gradients
- etc.

Furthermore the files:

prog/logfiles/heliumlog

prog/logfiles/heliumloig.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.

5.3 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.

• Start TopSpin and enter **nmr_restore**

or

Start TopSpin and click Manage Configuration | Spectrometer | Safe\Restore installation | Restore installation specific files

The NMR_Save window will be displayed.

NMR_Save					
ave installation files Restore insta	allation files	Save user files	Restore user files		
Restore installation specific files.					
Installation specific files are restor can be used to copy the files from restore a backup of the installatior	ed from a p a previous n specific fil	previously created installation to a r les.	I backup file. This bac new installation or to	kup file	
Note:					
You can only restore files that are	named cor	rrectly (nmr_back	up_"date").		
To restore user specific files use t	he "Restor	e user files" tab.			
Location of backup file:	C:\Bru	uker\TopSpin <ve< td=""><td>rsion>\nmr_backup</td><td>Browse</td><td></td></ve<>	rsion>\nmr_backup	Browse	
Name of backup file				~	
Restore destination (TopSpin hor	me): C:\Bru	uker\TopSpin <ve< td=""><td>sion></td><td>Browse</td><td></td></ve<>	sion>	Browse	
Display default information:	۲				
Display additional information:	0				
Log:					
					^
					~
				Restore C	lose

- 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
- Enter the location of the Restore destination, the default is: <TOPSPINHOME>
- Click **Restore** and enter the NMR administration password in the upcoming Password request window.
- Execute the command cf

6 Deinstallation of TopSpin

6.1 Deinstallation on Windows

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

- Click the Windows Start button.
- Open the Control Panel.
- Click Programs and Functions.
- Select the TopSpin Version to uninstall and click Uninstall/Change.

This will cleanly shut down running services and deinstall the software package. On the other hand, configuration files and acquired data will be left on the disk.

The following window will be displayed:

== Uninstalling TopSpin <version></version>	= =
	= =
Installed in C:\Bruker\TopSpin <version></version>	= =
= Installed at: 2010-12-16 13:36:13 +0100	= =
Do you want to uninstall this program? (yes/no)	

• Enter yes.

The deinstallation starts and might take a few minutes. When the deinstallation is finished, all programs and icons of the TopSpin version are removed from the Workstation.

6.2 Deinstallation on Linux

During the installation of TopSpin also a deinstallation routine is copied into the sub folder uninstall.

- Open a file browser like konqueror or a shell window.
- · Open the program directory.
- Open 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/topspin<version>/uninstall/uninstall-topspin.sh
- To deinstall SpectrOS only, run /opt/Bruker/spectros/uninstall/uninstall-spectros.sh

7 Contact

Manufacturer

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Bruker BioSpin Hotlines

Contact our Bruker BioSpin service centers.

Bruker BioSpin provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the service center or hotline you wish to contact from our list available at:

https://www.bruker.com/service/information-communication/helpdesk.html

H9168SA2_3_003

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