

TopSpin

- Acquisition
Commands and Parameters
Version 017



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1 Introduction

1.1 About This Manual

This manual is a reference to TopSpin acquisition or acquisition related commands and parameters. Every command is described on a separate page with its syntax and function as well and its main input/output files and parameters. Although file handling in TopSpin is completely transparent to the user, it is sometimes useful to know which files are involved and where they reside. For example, if you have permission problems or if you want to process or interpret your data with third party software.

Some of the commands referred to in this manual are processing commands. They are all described in the Processing reference manual.

1.2 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	<i>\$tshome/exp/stan/nmr/</i> <i>lists</i> <i>expno, procno,</i>
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

File/Directory Conventions

<tshome> - the TopSpin home directory (default C:\Bruker\Topspin under Windows or /opt/Topspin under Linux)

Header Conventions

SYNTAX - only included if the command described requires arguments

USED IN AU PROGRAMS - only included if an AU macro exists for command described

1.3 About Dimensions

TopSpin can acquire up to 8 D dimensional data. The directions of a dataset are indicated with the terms F1, F2, F3 etc. which are used as follows:

1D Data:

F1 - acquisition direction

2D Data:

F2 - acquisition or direct direction

F1 - indirect direction

3D Data:

F3 - acquisition or direct direction

F2 - indirect direction

F1 - indirect direction

In 3D processed data, F2 is always the second and F1 the third direction. In 3D raw data, this order can be the same or reversed, depending on the value of AQSEQ (see the description of this acquisition parameter).

1.4 About Digitally Filtered Avance Data

The first points of the raw data measured on an Avance spectrometer are called group delay. These points represent the delay caused by the digital filter and do not contain spectral information. However, they contain information about the digital filtering and are required for processing. The first couple of points of the group delay are always zero. The group delay only exists if digital filtering is actually used, i.e. if the acquisition parameter DIGMOD is set to digital.

1.5 Usage of Acquisition Commands in AU Programs

Many acquisition commands described in this manual can also be used in AU programs. The description of these commands contains an entry USAGE IN AU PROGRAMS. This means an AU macro is available which is usually the name of the command in capitalized letters.



Note that IconNMR automation automatically calls acquisition AU programs. If, in this manual, the entry USAGE IN AU PROGRAMS is missing, no AU macro is available.

Usually, such a command requires user interaction and it would not make sense to put it in an AU program. However, if you still want to use such a command in AU, you can do that with the XCMD macro which takes a TopSpin command as argument. Examples are:

```
XCMD("eda")
```

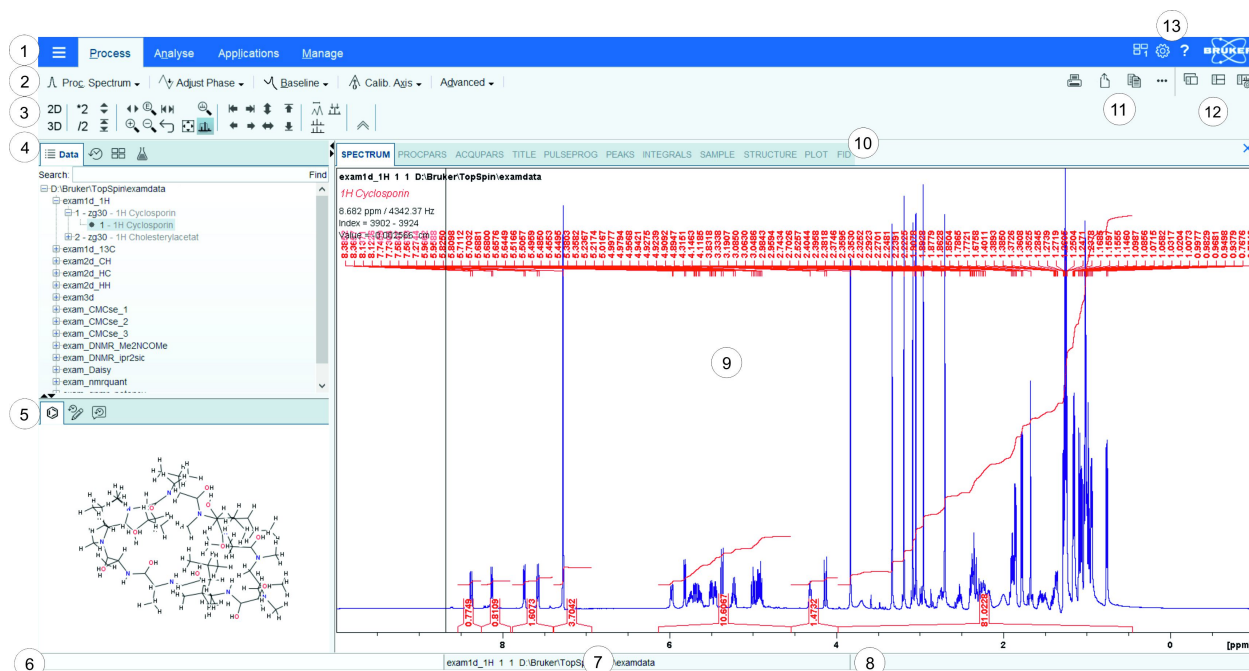
```
XCMD("setdef ackn no")
```

AU programs can be set up with the command **edau**.

Acquisition commands can also be used in an TopSpin macro. These are scripts created with **edmac** containing a sequence of TopSpin commands or Python commands.

1.6 Starting Commands from the TopSpin Menu

The TopSpin graphical user interface is shown in the following figure.

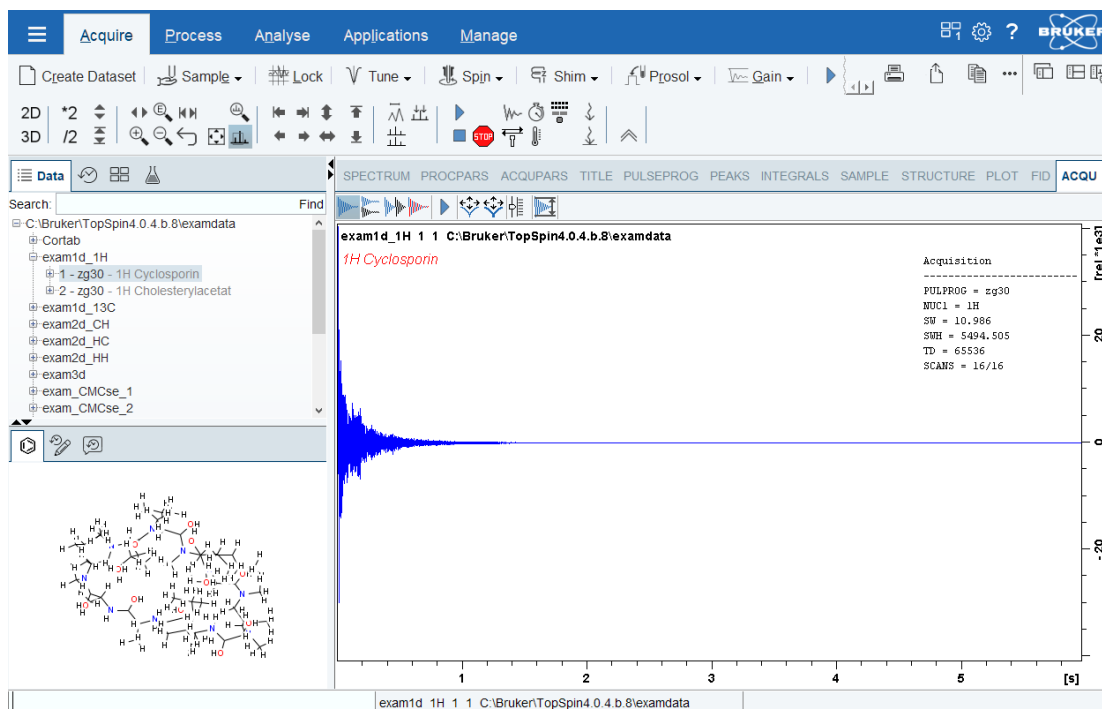


1	Menu bar	8	Status display bar
2	Workflow button bar	9	Dataset window
3	Tool bar	10	Dataset window tabs
4	Browser and search window	11	Print, export, copy and publish
5	Structure window, command line history, status line history	12	Viewing options
6	Command line	13	Window switcher, setup preferences and help
7	Current dataset bar		

A general overview of the TopSpin functionalities and commands is provided in the following manuals:

- Avance Beginners Guide
- Basic NMR Experiments Manual
- TopSpin User Manual

This manual describes all acquisition commands as they can be entered on the command line. However, they can also be clicked from the upper toolbar or from the TopSpin popup menus. Most acquisition commands can be found in the TopSpin menu bar when the **Acquire** workflow button is enabled (see figure below). In addition, spectrometer management commands are available under **Manage | Spectrometer**.



The buttons of the ACQU window have the following functions:



Show FID in shuffled mode.



Show FID in unshuffled mode, horizontally arranged.



Show FID in unshuffled mode, vertically arranged.



Show FID in unshuffled mode, interleaved.



Start acquisition [**zg**]



Start wobble [**wobb**]



Start wobble (thick lines) [**wobb thick**]



Start gs [**gs**]



Use current FID as reference for scaling [**noscale**]

Once an acquisition has been started additional and/or different buttons become available, depending on which acquisition command has been started. See commands like **zg**, **wobb** and **gs**.



Note that the Acquire menu is only available after TopSpin has been configured as a spectrometer (command **cf**).

1.7 Command Queuing

In TopSpin 2.1 and newer, command spooling has been implemented. Acquisition commands like **zg**, **rga**, **atma** and **go** are automatically queued, if this feature is **on** (default **off**, can be set with the command **set**). All other commands can be queued with the command **qu**, e.g. **qu xfb**.

Queued commands can be viewed in the Spooling field of the acquisition status bar.



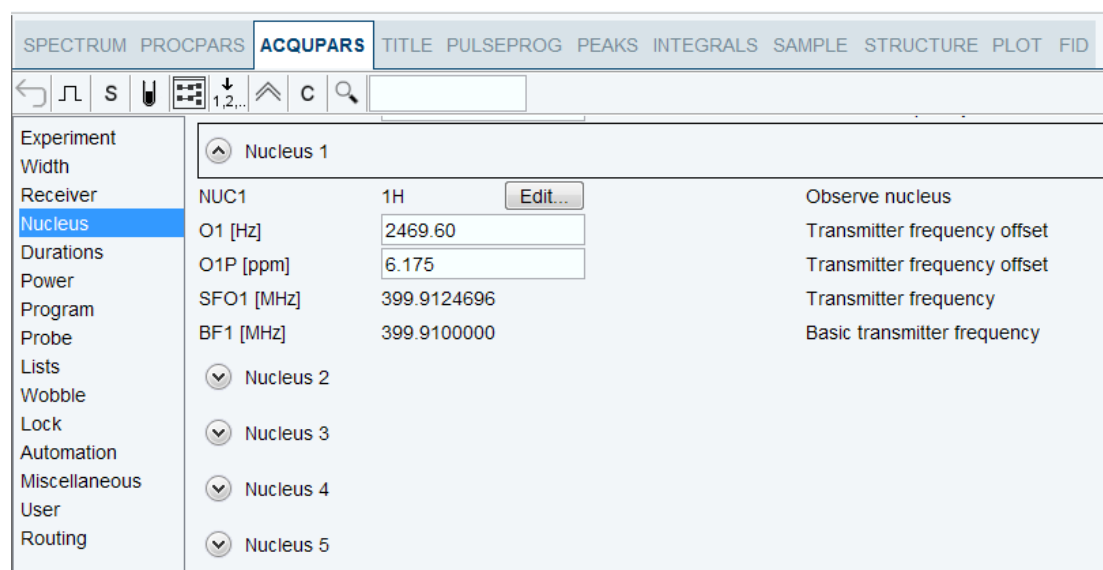
Note that the spooling field must be activated in the User Preferences window (command **set**).

2 TopSpin Parameters

2.1 About TopSpin Parameters

TopSpin parameters are divided in acquisition and processing parameters. In this manual, we will mainly concern ourselves with acquisition parameters. Furthermore, we will discuss the acquisition related lock and prosol parameters.

For each parameter we will indicate the location where it can be found, for example parameter **O1**. For instance to jump to the parameter **O1** click on the navigation bar on **Nucleus**:



The following terms will be used:

Acquisition Parameters

Parameters that must be set by the user, for example with **eda**, and that are interpreted by acquisition commands, for example **zg**.

Acquisition Status Parameters

Parameters that are set by acquisition commands like **zg**. They represent the status of the raw data and can be viewed, for example with **dpa**. Some acquisition status parameters are used as input by processing commands.

Lock Parameters

Parameters that are used for locking the magnetic field. They can be set up with the **edlock** command and are interpreted when you lock in, either with the **lock** command or from the BSMS display.

Prosol Parameters

Probe and solvent dependent parameters, mainly pulse lengths and power levels. They can be set up with the **edprosol** command. The **getprosol** command reads the prosol parameters and copies them to the corresponding acquisition parameters.



Note that entering **getprosol** is equivalent to clicking the **AcquPars** tab and then clicking the button.

Input Parameters

Parameters that are interpreted by the commands described in this manual. They can be:

- Acquisition parameters (input of, for example, **zg**)
- Lock parameters (input of **edlock**, **lock** and **lopo**)
- Prosol parameters (input of **edprosol** and **getprosol**)

Output Parameters

Parameters that are set or modified by commands described in this manual. They can be:

- Acquisition status parameters (output of, for example, **zg**)
- Lock parameters (output of **edlock**)
- Prosol parameters (output of **edprosol**)

Temporary Parameters

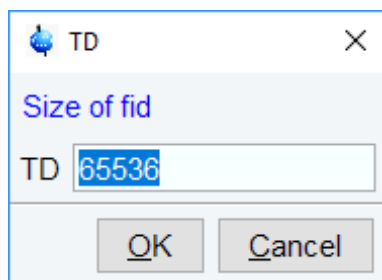
Parameters that are not stored in parameters files and not interpreted directly by acquisition commands. They are related to other parameter that are directly interpreted by acquisition commands. If you change a temporary parameter, for example in **eda**, the related parameters will be automatically adjusted. An example of a temporary parameter is AQ that is determined by the equation:

$$AQ = TD / (2 * SW * SFO1)$$

Acquisition parameters can be set with the parameter editor **eda** and acquisition status parameters can be viewed with **dpa**. Alternatively, each parameter can be set or viewed by entering its name in lowercase letters on the command line. For example, for the parameter TD:

- **td** - set the parameter TD
- **s td** - view the status parameter TD

The dimensionality of the dataset is automatically recognized. For example, for a 2D dataset the following dialog box is offered:



Although status parameters are normally not changed by the user, a command like **s td** allows you to do that. This, however, would make the dataset inconsistent.

Before an acquisition has been performed, the acquisition status parameters of a dataset do not contain significant values. After the acquisition, they represent the status of the raw data.

Most acquisition status parameters are set to the same values as the corresponding acquisition parameters. In other words, the acquisition command has done what you told it to do. There are, however, some exceptions:



- When an acquisition was interrupted, the acquisition status parameters might not have been updated yet.
- Some acquisition parameters are automatically adjusted by the acquisition command, e.g. RG and FW.

- The values of some parameters are a result of the acquisition. They cannot be set by the user (they do not appear as acquisition parameters) but they are stored as acquisition status parameters. Examples are AQSEQ, YMAX_a and NC.

2.2 Parameter Value Types

With respect to the type of values they take, acquisition parameters can be divided into four groups:

- Parameters taking integer values, e.g. NS, TD, DR
- Parameters taking real (float or double) values, e.g. SW, O1, DE
- Parameters using a predefined list of values, e.g. AQ_mod, DIGTYP
- Parameters specifying file names, e.g. GRADIENT, SHAPE

Please note that these parameters can be selected with this button  and can be edited with this button .

You can easily see to which group a parameter belongs from the parameter editor opened with the command **eda**.



Note that the values of parameters which use a predefined list are stored in the parameter file as integers.

The first value of the list is always stored as 0, the second value as 1 etc. The next table shows the values of the parameter DSPFIRM_mod as an example:

Parameter value	Integer stored in the proc(s) file
sharp(standard)	0
smooth	2
medium	3
rectangle	4

Table 2.1: Parameter value types

2.3 Parameter Files

TopSpin parameters are stored in various files in the dataset directory tree.

In a 1D Dataset:

- <dir>/data/<user>/nmr/<name>/<expno>/
 - *acqu* - acquisition parameters
 - *acqu*s - acquisition status parameters

In a 2D Dataset:

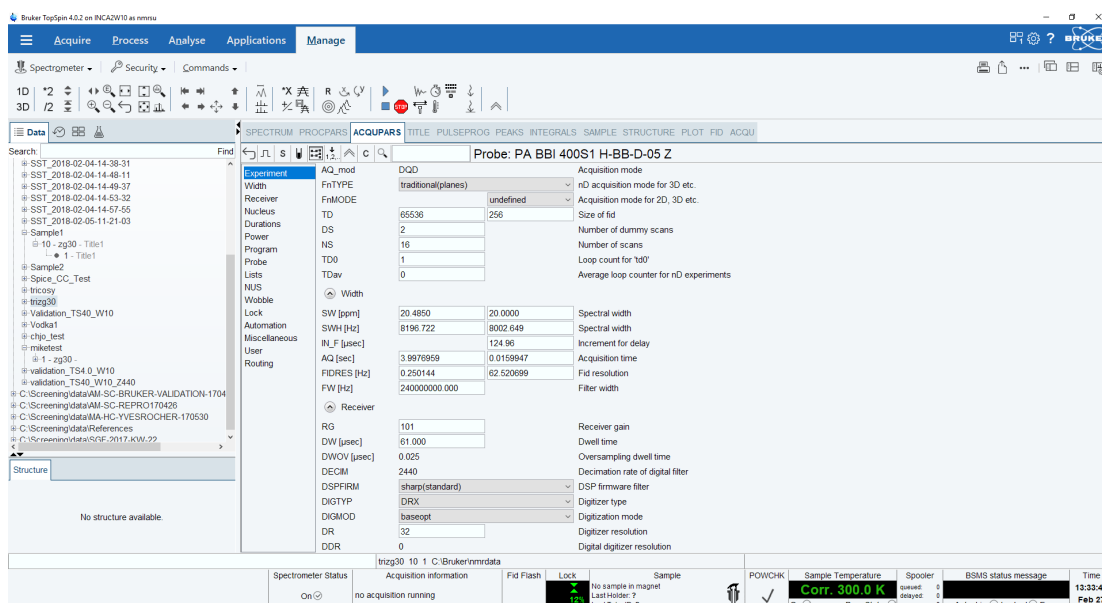
- <dir>/data/<user>/nmr/<name>/<expno>/
 - *acqu* - F2 acquisition parameters
 - *acqu*2 - F1 acquisition parameters
 - *acqu*s - F2 acquisition status parameters
 - *acqu*2s - F1 acquisition status parameters

In a 3D Dataset:

- `<dir>/data/<user>/nmr/<name>/<expno>/`
 - *acqu* - F3 acquisition parameters
 - *acqu2* - F2 acquisition parameters
 - *acqu3* - F1 acquisition parameters
 - *acquS* - F3 acquisition status parameters
 - *acqu2s* - F2 acquisition status parameters
 - *acqu3s* - F1 acquisition status parameters

2.4 Acquisition (eda) Parameters

This paragraph contains a list of all acquisition parameters with a description of their function. Most of them are interpreted by various acquisition commands like **zg**, **go**, **ii**, **gs** and **rga**. Some, however, are only interpreted by specific commands which are then specified in the list below. Acquisition parameters can be set by entering **eda** on the command line, clicking the AcqPars tab of a data window or by typing the parameter names in lowercase letters on the command line.



AQ - Acquisition Time In Seconds

- Takes a float value
- Temporary parameter calculated from the equation:

$$AQ = TD / (2 * SW * SFO1)$$
- AQ represents the time to acquire one scan. If you change AQ, TD is changed accordingly. With AVANCE NEO only DIGTYP=DRX is available. Note that extra dwell times are automatically added.

AMP[%] - Amplitude Of Pulses

- Takes float values in percent
- Array range [0-31]

- Can be set from **eda** in the submenu **Durations**
- Can also be set by entering **amp0**, **amp1** etc. on the command line
- Can also be set from the **gs** window
- Interpreted by the pulse program statements **amp0**, **amp1**, **amp2** etc.

AQ_mod - Acquisition Mode

- Takes value **DQD**
- Can be set from **eda** in the submenu **Durations**
- **aq_mod** shows the actual Acquisition mode
- The values of AQ_mod have the following meaning:
DQD = digital quadrature detection. Simultaneous mode that eliminates quad images and O1 spikes. AQ_mod can only be set to DQD when the parameter DIGMOD is set to *digital*. When you set DIGMOD to analog, AQ_mod automatically changes to **qsim**. Furthermore, DQD can only be used up to a certain spectral width as is shown in table Fragment Table Maximum SW (kHz) for AQ_mod = DQD. Above this value, acquisition commands automatically switch the acquisition mode to qsim. In that case, the acquisition parameter AQ_mod = DQD.

AUNM - Name Of An Acquisition Au Program

- Takes a character array value
- Can be set from **eda** in the submenu **Automation** or by entering **aunm** on the command line
- Interpreted by **xaua**
- The command **xaua** executes the AU program specified by AUNM. Although this can be any AU program, AUNM is normally used to specify an AU program that performs an acquisition. For example, in several standard parameter sets, AUNM is set to **au_zg**. The command **xaua** can be entered on the command line or called from AU program with its macro XAUA.

BF1 - BF8 - Basic Frequency For Frequency Channel f1 to f8

- Take a double value (MHz).
- Are automatically set when NUC1, NUC2 etc. are selected from **edasp**.
- When you set up an experiment and define NUC1 in the routing table, BF1 is automatically read from the nucleus table. In the same way, BF2 is automatically read when NUC2 is defined etc. The routing table can be opened with **edasp** or by clicking the **Edit** button close to NUC1 in **eda**. The nucleus table is created with the command **cf** that can be executed by the NMR Superuser. This command prompts you for the 1H basic frequency and then automatically calculates the basic frequencies for all other nuclei. For each nucleus, **cf** sets the basic frequency such that the most common reference substance for that nucleus would resonate at about 0 ppm. If you want to change the nuclei table, you can do that with the command **ednuc**. This is, for example, necessary if you are using a different reference substance for a certain nucleus.



Note, that if you execute **cf** and change the 1H basic frequency, you must click RESTORE in the nuclei table (**ednuc**).

CNST- Array Of Constants Used In Pulse Programs

- Takes float values
- Array range [0-63]
- Can be set from **eda** in the submenu **Program parameters**

- Can also be set by entering **cnst0**, **cnst1** etc. on the command line.
- Interpreted by the pulse program statements `cnst0`, `cnst1`, `cnst2` etc.
- The values of the parameter array CNST can be used as constants in a pulse program. For example, the pulse program line:

```
"d2 = 1s/cnst2*2"
```

Uses the value of CNST2 as a coupling constant. Note the difference between the pulse program statement `cnst2` and the TopSpin command **cnst2**. The latter is actually not a command but a way of setting the value of CNST[2].

CPDPRG1 - CPDPRG8 - Names of CPD Programs

- Take a character string value
- Can be set from **eda** (submenu **Program parameters**) by entering a name or by clicking the down arrow and then selecting a CPD program from the appearing list
- Can also be set by entering **cpdprg1**, **cpdprg2** up to 8 on the command line
- Interpreted by the pulse program statements `cpd1` - `cpd8`, `cpds1`- `cpds8` and `cpdngs1` - `cpdngs8`
- The values of CPDPRG1 - CPDPRG8 are the names of composite pulse decoupling (CPD) programs. The pulse program statements `cpd1` executes the CPD program defined by CPDPRG1, `cpd2` executes the CPD program defined by CPDPRG2 etc. In several Bruker CPD type parameter sets, the CPD program is specified by CPDPRG2 and executed on frequency channel f2. For example, the parameter set C13CPD contains the following settings:

```
CPDPRG2 = waltz16
```

```
PULPROG = zgpg30
```

And the pulse program *zgpg30* contains the following line:

```
d1 cpd2:f2
```

The statements `cpd3` and `cpd4` which execute the CPD programs specified by CPDPRG3 and CPDPRG4, respectively, are often used in 3D experiments. Note, however, that the `cpd1` - `cpd8` commands are equivalent and can be used to run any CPD program on any frequency channel.

`cpds1` works like `cpd1`, except that it will execute the CPD program synchronously with the pulse program. This means `cpds1` always starts the CPD program at the beginning, whereas `cpd1` continues the CPD program where it was last stopped by the `do` statement. The difference between `cpds2` and `cpd2`, `cpds3` and `cpd3` etc. is equivalent.

`cpdng1` works like `cpd1`, except that the transmitter gate for channel f1 will not be opened. `cpdngs1` works like `cpds1`, except that the transmitter gate for channel f1 will not be opened. For the channels f1, f2 ect. the statements `cpdng2`, `cpdng3` etc are available.

The list of CPD programs which appears when you click the down arrow in **eda**, contains both Bruker and user defined CPD programs. Bruker CPD programs must be installed, once, with **expinstall**. You can set up your own CPD programs with the command **edcpd**.

D- Array Of Delays

- Takes float values (sec)
- Array range [0-63]
- Can be set from **eda** in the submenu **Durations**
- Can also be set by entering **d0**, **d1**, **d2** up to 63 on the command line

- Interpreted by the pulse program statements `d0 - d31`, `id0 - id31`, `dd0 - dd31`, `rd0 - rd31`
- The pulse program statement `d0` causes a delay of D0 seconds, `d1` causes a delay of D1 seconds etc. In principle, all delays can be used for any purpose. In Bruker pulse programs, however, some conventions are followed. These are listed in the file `Param.info` that can be viewed with **edpul**. For example, D1 is used as a relaxation delay, D0 is used in combination with IN0 and ND0 as incrementable delay in 2D experiments. D0 and D10 are used as incrementable delays in 3D experiments. Note however, that all delays D1 – D63 are incrementable, not only D0 and D10. For more information click:

Help | Manuals | Programming Manuals | Pulse Programming

DDR - Digital Digitizer Resolution

- Takes an integer value
- Temporary parameter calculated according to the equation:

$$DDR = 2^{\log(DECIM)} + 1$$

- Cannot be set by the user
- DDR expresses the enhancement of the digitizer resolution by digital filtering. The total digitizer resolution, as defined by DR, is the sum of the hardware resolution (see table Gradient Parameters) and DDR.

DE - Pre-Scan Delay

- Takes a float value (microseconds)
- Can be set from **eda** (submenu **Receiver**) or by entering **de** on the command line
- DE is executed as a part of the `go` statement. DE consists of 4 pre-scan subdelays DEPA, DERX, DE1 and DEADC. These subdelays end simultaneously at the end of DE (i.e. the beginning of the data sampling), and at the beginning of each subdelay a certain action is performed:
 - DEPA: the preamplifier is switched from transmit to observe mode (default 4,5 µsec)
 - DERX: the receiver gate is opened (default 1,5 µsec)
 - DE1: the intermediate frequency is added to the frequency of the observe channel. This corresponds to the execution of the `syrec` statement (default 4,5 µsec).
 - DEADC: the digitizer is enabled (default 0,5 µsec)

DE can be set from **eda** or from the command line. The subdelays can be set with the command **edscon**. Their maximum value is DE - 1 µsec.

After DE, the digitizer starts to sample the data points.

DECIM - Decimation Factor Of The Digital Filter

- Takes an integer value
- Cannot be set by the user
- Advance spectrometers use the concept oversampling which means that the data points are sampled much faster than specified by DW. This results in a larger number of points than specified by the user; a multiple of TD. Before the data are written to disk, they are digitally filtered which reduces (decimates) their number to TD. The decimation factor is defined by the following equation:

$$DECIM = DW/DWOV$$

where DWOV is the oversampling dwell time.



Note that DECIM can only take an integer value and DWOV must be greater than the minimum value for the current digitizer (see table Gradient Parameters). See also the acquisition status parameter DECIM.

DIGMOD - Digitizer Mode

- Takes one of the values digital, **baseopt**
- Can be set from **eda** (submenu **Receiver**) or by entering **digmod** on the command line
- In most standard parameter sets, DIGMOD is set to **digital** which means that oversampling and digital filtering is used. Oversampling means that the data points are sampled much faster than specified by DW. This results in a larger number of points than specified by the user; a multiple of TD. Before the data are written to disk, they are digitally filtered during which their number is reduced (decimated) to TD.

In TopSpin 2.0 and newer, DIGMOD can also be set to **baseopt** (for a description of this value, see parameter DSPFIRM).

DIGTYP - Digitizer Type

- Takes only DRX for AVANCE NEO. No other digitizer is available.

DQDMODE - Sign Of The Frequency Shift During Digital Quadrature Detection

- Takes one of the values **add** or **subtract**.
- Can be set from **eda** (submenu **Receiver**) or by entering **dqdmode** on the command line.
- DQDMODE defines the frequency shift applied in Digital Quadrature Detection mode as positive (add) or negative (subtract).

DR - Digitizer Resolution

- Takes an integer value.
- DR is the sum of the hardware resolution (see table Gradient Parameters) and the digital digitizer resolution DDR. It is automatically set to the maximum resolution of the current digitizer (DIGTYP). Because Avance spectrometers use the principle of oversampling, this value can be higher than the resolution of the digitizer.

Usually, you want to use maximum resolution and keep this value of DR. In some cases, however, it is useful to set DR to a lower value. For example, if you want to acquire a large number of scans which might cause overflow for the maximum value of DR. However, to solve this problem, you can also set the parameter OVERFLW to **check** to halt the acquisition as soon as data overflow would occur.

DS - Number Of Dummy Scans

- Takes an integer value.
- Interpreted by the pulse program statement `go=n`, `gonp=n` and `rcyc=n`.
- Can be set from **eda** (submenu **Experiment**) or by entering **ds** on the command line.
- Dummy scans are scans during which no fid is accumulated. Other than that, they are identical to normal scans, which means they take the same time (AQ) and perform phase cycling. Dummy scans are used to reach steady state conditions concerning T1 relaxation. This is necessary whenever the recycle delay of the experiment is shorter than 4 times the T1 value of the measured nucleus. Furthermore, they are used to establish a stable temperature. This is especially important in decoupling and TOCSY experiments where the irradiation high power increases the sample temperature. Dummy scans are performed if DS > 0 and the pulse program contains a `ze` statement before the `go=n` or `rcyc=n` loop. If a `zd` is used instead of `ze`, dummy scans are omitted.

DSPFIRM - Firmware Used For Digital Filtering

- Takes one of the values **sharp**, **smooth**, **medium**, **rectangle**.
- Can be set from **eda** (submenu **Receiver**).
- DSPFIRM defines the filter function used for digital filtering. This determines the maximum spectral width that can be used. For high resolution experiments, DSPFIRM is usually set to **sharp**. The values **medium** and **smooth** are used for other applications.

In TopSpin 2.0 and newer, DSPFIRM can also be set to **rectangle**. The oversampled data are then filtered in such a way that the initial points of the FID are corrected. Setting DSPFIRM to **rectangle** will automatically set the parameter DIGMOD to **baseopt** and vice versa. In order to be able to correct the first points at the start of the FID, the exact position of the time 0 point must be known. This point is normally somewhere within the excitation pulse; for instance, for a normal 1-pulse-experiment with a 90° excitation pulse p0, it is at $p0 * (1 - 2 / \pi)$. However, this depends on the experiment. Therefore, a new parameter ACQT0 was introduced in TopSpin 2.0, which can only be set within the pulse program. It measures the zero time from the beginning of the delay DE which is also the start of the go macro or the end of the excitation pulse. For the example given above, the following line has to be added at the beginning of the pulse program zg:

```
acqt0=-p0*2/3.14159;
```

This information enables the alignment of the data acquisition relative to the time 0 point of the FID. As always, the time is measured from left to right, and since this time is before the start of the FID, a negative time results. If this statement is missing, it is not possible to use the rectangle filter. As a result, the value of DE chosen by the operator may be temporarily prolonged by the program. The effects of this filter are:

- No first order phase distortion, so first order phase correction is not necessary.
- No so-called smilies (distortions of the spectrum at the left and right edges of the spectrum).
- The baseline of the resulting spectrum will be exactly 0 provided that no other effects distort the FID and that a correct zero order phase correction has been done.
- Signals at the very edge of the spectrum are not attenuated or distorted nor are they folded in.

This method requires more resources on the internal computer of the spectrometer than a non-baseopt acquisition, therefore performance can be a limiting factor here.

Among other things, 16 times more data points are internally processed in order to guarantee a good and reliable correction of the TD points of the FID. This is also the reason why the acquisition window shows a FID with 16*TD points in case of **baseopt**, even if only TD points are later on stored on disk.

DW - Dwell Time

- Takes a float value.
- Can be set from **eda** (submenu **Receiver**) or by entering **dw** on the command line.
- Temporary parameter, calculated from the equation:

$$DW = 10e6 / (2 * SW * SFO1)$$
- The dwell time is the time between the acquisition of two successive data points. Although it is normally calculated from SW, you can also set **dw**. In that case, the spectral width is adjusted according to the equation:

$$SW = 10e6 / (2 * (0.05 + DW) * SFO1)$$

When you set DW, you will often notice that the value you enter is slightly adjusted. The reason is that, when oversampling is used, the relation.

$$DW = DWOV * DECIM$$

Must be fulfilled and DECIM can only take integer values.

DWOV - Oversampling Dwell Time

- Cannot be set by the user.
- Automatically set according to DIGTYP and DW.
- Has a minimum value which depends on the digitizer (see table Gradient Parameters).
- The parameter DWOV reflects the principle of oversampling. This is used when DIGMOD = digital and means that the data are sampled much faster than specified by the user. In other words, a data point is sampled every DWOV μ s rather than every DW μ s where DWOV is only a fraction of DW. DWOV is set to the minimum value that can be handled by the digitizer or DSP-firmware (see table Gradient Parameters). Actually the value of DWOV is often a little above the minimum because the following relation must be fulfilled:

$$\text{DWOV} = \text{DW}/\text{DECIM}$$

Here, DECIM is the decimation factor that can only take integer values.

EXP - Experiment Performed

- Takes a character array value.
- Is set by IconNMR.
- IconNMR sets EXP to the value of the parameter set that was used for the experiment.

FCUCHAN - Routing Between Logical Frequency Channels and FCU's (i.e. TRX 2)

- Array of integer values.
- Can be set from **eda** (submenu **Routing**) but is normally set graphically from the **edas** window (see this command for more information).
- The values of FCUCHAN define the relation of the FCU's (i.e. TRX 2) to the logical frequency channels. For example, FCUCHAN[1] = 2 means that FCU 2 (i.e. TRX 2) is used for logical channel f1.

FIDRES - FID Resolution

- Takes a float value (Hz).
- A temporary parameter calculated from the equation:
$$\text{FIDRES} = \text{SW} * \text{SFO1} / \text{TD}.$$
- Although FIDRES is normally calculated from SW, you can also set FIDRES. In that case, TD is adjusted while SW remains the same.



Note that the value that you enter for FIDRES is often adjusted a little. The reason is that TD is recalculated according to $\text{TD} = \text{SW} * \text{SFO1} / \text{FIDRES}$ and rounded to the nearest power of two. FIDRES is then adjusted to fulfill the same equation.

FnMODE - Acquisition Mode Of The Indirect Directions (data \geq 2D)

- Takes one of the values described below.
- Can be set with **eda** (submenu **Experiment**) or by entering **fnmode**.
- Interpreted by the pulse program statement **mc**.

The parameter FnMODE defines the acquisition mode of the indirect directions in a multi-dimensional experiment. Compared to **wr**, the **mc** statement simplifies the switching of the acquisition mode and allows you to use the same pulse program for various experiments. FnMODE can take the following values:

- **undefined**

This value must be used if the pulse program contains no **mc** statement.

- **QF**

Successive fids are acquired with incrementing time interval without changing any phase program. This corresponds to the `mC` clause F1QF or F2QF.

– **QSEQ**

Successive fids will be acquired with incrementing time interval and phases 0 and 90°. This corresponds to the `mC` clause F1PH or F2PH.

– **TPPI**

Successive fids will be acquired with incrementing time interval and phases 0°, 90°, 180° and 270°. This corresponds to the `mC` clause F1PH or F2PH.

– **States**

Successive fids will be acquired incrementing the time interval after every second fid and phases 0° and 90°. This corresponds to the `mC` clause F1PH or F2PH.

– **States-TPPI**

Successive fids will be acquired incrementing the time interval after every second fid and phases 0°, 90°, 180° and 270°. This corresponds to the `mC` clause F1PH or F2PH.

– **Echo-Antiecho**

Special phase handling for gradient controlled experiments. This corresponds to the `mC` clause F1EA or F2EA.

For more information on the `mC` statement and the use of `FnMODE` click:

Help | Manuals | Programming Manuals | Pulse Programming

FQ1LIST - FQ8LIST - Irradiation Frequency Lists

- Take a character array value.
- Can be set from **eda** (submenu **Lists**) by entering a name or by clicking the down arrow and selecting a name from the appearing list.
- Can also be set by entering **fq1list**, **fq2list** etc. on the command line.
- Interpreted by the pulse program statements `fq1` to `fq8`.
- The parameters FQ1LIST to FQ8LIST define the names of frequency lists and are interpreted by the pulse program statement `fq1` to `fq8`. For example, the first time `fq1` is executed, the first value in the frequency list defined by FQ1LIST is read. The second time `fq1` is executed, the second value in this list is read etc. At the end of the frequency list, the list position is set back to the first value. Note that `fq1` can be executed multiple times because it occurs on several lines of the pulse program or because it occurs on a line that is part of a loop. In the same way `fq2` reads the list defined by FQ2LIST etc. The `fq1` to `fq8` statements must be preceded with a delay and followed by the frequency channel on which the pulse will be executed, for example:

```
d1 fq2:f2
```

In Bruker pulse programs, `fq1` is normally used on channel f1, and `fq2` on channel f2 but any combination is allowed. The delay must be greater than 2 µs. The frequency lists can be created or modified with the command **edlist**.

FW - Analog Filter Width

- Takes a float value.
- Can be set from **eda** (submenu **Width**) or by entering **fw** on the command line.
- For digitizer type DRX FW ist set to 240 MHz.

GRADIENT - Gradient Parameter Table

- Takes a list of real values (gradients) and character strings (filenames).

Index	GPX [%] (GPX)	GPY [%] (GPY)	GPZ [%] (GPZ)	Filename (GPNAM)
0	0	0	0	SMSQ10.100
1	0	0	50	SMSQ10.100
2	0	0	-10	SMSQ10.100
3	0	0	0	SMSQ10.100
4	0	0	0	SMSQ10.100
5	0	0	0	SMSQ10.100
6	0	0	0	SMSQ10.100
7	0	0	0	SMSQ10.100
8	0	0	0	SMSQ10.100
9	0	0	0	SMSQ10.100
10	0	0	0	SMSQ10.100
11	0	0	0	SMSQ10.100
12	0	0	0	SMSQ10.100
13	0	0	0	SMSQ10.100
14	0	0	0	SMSQ10.100
15	0	0	0	SMSQ10.100
16	0	0	0	SMSQ10.100

Figure 2.1: Gradient Parameters

- Can be set from **eda** in the submenu **Power | GRADIENT**.
- The gradients are interpreted by pulse program statements `gron0 - gron31` and `:gp0 - :gp31`.
- The filenames are interpreted by pulse program statements `:gp0 - :gp31`.
- TopSpin allows you to use static gradients and shaped gradients. Static gradients have a constant strength during the time they are on. They are switched on by the pulse program statements `gron0 - gron31`. These read the gradient strength for each direction from the GP031 table. The `groff` command switches the static gradients off. According to table Gradient Parameters, the pulse program section

```
d21 gron2
d22
d23 groff
```

would switch the X, Y and Z gradient on during the time D1+D2 with gradient strengths 75.0, 75.0 and 75.0, respectively. The gradient strength is expressed as a percentage of the maximum strength and runs from -100.0 to 100.0%. Static gradients do not use the **Filename** entry of the GP031 table.

Shaped gradients have a strength that varies in time. They are switched on by the pulse program statements `gp0 - gp31`. These interpret the **Filename** field of the gradient table. A file which is defined here contains a list of values between -1 and 1. Each value represents the relative gradient strength for a given time interval. They are multiplied with the values of GPX, GPY and GPZ to give the percentage of the maximum gradient strength for the respective direction. According to the table Gradient Parameters, the statement `p16:gp2` would switch on the X, Y and Z gradient on during the time P16 with

gradient strengths 75.0, 75.0 and 75.0, respectively. The strength of each gradient would then vary in time according to the list of values in the file *gradrec5m*. When you click the down arrow to the right of each **Filename** field, a list of available files will appear. Such a list contains both Bruker and user defined gradient files. The former must be installed once with **expinstall**, with the option **Install Library Gradient Files** selected. The latter can be created with the *ShapeTool* (command **stdisp**). The gradient files reside in the directory:

```
<tshome>/exp/stan/nmr/lists/gp
```

The gradient parameters can also be set from the keyboard. For example, entering **gpx2**, **gpy2**, **gpz2** allows you to set the gradient strength for the three respective directions. With **gpnam2** you can set the shaped gradient file name.

GRDPROG - Gradient Program Name

- Takes an ascii string value.
- Interpreted by the pulse program statement `ngrad`.
- Standard gradient programs are delivered with TopSpin. They must be installed once, with the command **expinstall** with the option **Install Library Gradient Files** selected.

HDDUTY - Homodecoupling Duty Cycle (in percent)

- Takes a float value.
- Can be set from **eda** (submenu **Durations**) or by entering **hdduty** on the command line.
- HDDUTY describes the ratio between the time used for homodecoupling and the time used for actual signal detection.

HDRATE – Oversampling during Homodecoupling

- Can be set from **eda** (submenu **Durations**) or by entering **hdrate** on the command line.
- Determines how many pulse/acquire cycles are executed per dwelltime in case of homodecoupling.
- HDRATE is in units of [25ns], i.e. a HDRATE of 480 means that the length of one pulse/acquire-element takes 12usec.
- HDRATE is limited by certain hardware capabilities because there is a maximum possible frequency for switching between pulse and observe mode.

HPMOD - Routing Between High Power Amplifiers And Preamplifier Modules

- Array of integer values.
- Can be set from **eda** (submenu **Routing**) but is normally set graphically from the **edasp** window (see this command for more information).

HPPRGN - High Power Preamplifier Gain

- Takes one of the values normal or plus.
- Gain selection for spectrometers equipped with HPPR preamplifiers. By default, HPPRGN is set to **normal** (**eda** submenu **Receiver**). The value **plus** is only used for test purposes and should not be used for experiments.

INP[μsec] - Array Of Increments For Pulses ; P[μsec]

- Takes double values (μsec).
- Array range [0-63]
- Can be set from **eda** (submenu **Durations**)
- Can also be set by entering **inp0**, **inp1**, **inp2** etc. on the command line.

- Interpreted by the pulse program statements `ipu0 – ipu63` and `dpu0- du63`.
- The pulse program statement `p0` executes a pulse with a length specified by `P0`. This length can be modified by the following pulse program statements:

`ipu0` increments the pulse length by `INP[0]`

`dpu0` decrements the pulse length by `INP[0]`

`rpu0` resets the pulse length to the value of `P[0]`

In the same way, you can modify the length of the pulses executed by `p1` to `p63` with `INP[1]` to `INP[63]`, respectively.

IN[sec]- Array Of Increments For Delays D[sec]

- Takes double values (sec).
- Array range [0-63]
- Can be set from **eda** (submenu **Durations**)
- Can also be set by entering **in0**, **in1**, **in2** etc. on the command line.
- Interpreted by the pulse program statements `id0 – id63` and `dd0- dd63`.
- The pulse program statement `d0` causes a delay with a length specified by `D[0]`. This length can be modified by the following pulse program statements:

`id0` - increments the delay by `IN[0]`

`dd0` - decrements the delay by `IN[0]`

`rd0` - resets the delay to the value of `D[0]`

In the same way, you can modify the length of the delays caused by `d1` to `d63` with `IN[1]` to `IN[63]`, respectively.

In 2D dataset, `IN[0]` and `ND[0]` play a special role. In **eda** (submenu **Durations**), they appear as the single parameters `IN0` and `ND0` in the F1 direction. They are determined by the following equation:

$$SW(F1) = 1/(SFO1 * IN0 * ND0)$$

Where `IN0` is the spectral width and `ND0` the number of occurrences of `d0` in the pulse program. If you change `IN0` or `ND0`, `SW` is automatically recalculated. If you change `SW`, `IN0` is recalculated and `ND0` remains the same. You can set these parameters in **eda** or, from the command line, with:

in0

nd0

sw

Note that `IN0` and `ND0` only exist in the F1 direction but `SW` exists in F2 and F1.

In a 3D dataset, `IN0` and `ND0` play the same role in F1 indirect direction as they do in the 2D dataset. F1, however, is the third direction now. For the F2 indirect direction F2, the parameters `IN10` and `ND10` are used. In 3D, the following equations hold:

$$SW(F1) = 1/(SFO1 * IN0 * ND0)$$

$$SW(F2) = 1/(SFO1 * IN10 * ND10)$$

You can set these parameters in **eda** or, from the command line, with:

in0

nd0

in10

nd10

SW

Note that IN0 and ND0 only exist in F1, IN10 and ND10 only in F2 but SW exists in F3, F2 and F1.

L - Array Of Loop Counters

- Takes integer values.
- Can be set from **eda** (submenu **Program parameters**)
- Can also be set by entering **I0, I1, I2** etc. on the command line.
- Interpreted by pulse program statements **l0-l31, iu0-iu31, du0-du31** and **ru0-ru31**.
- The parameters **L[0] - L[31]** are read by the pulse program statements **l0 - l31**. These are mainly used in loop structures like **l0 to x times l0** where **x** is a pulse program label; a number or a string which labels a previous line in the pulse program. An example of such a structure is:

```
4 (p1 ph1)
d2
..
l0 to 4 times l3
```

The loop counter values can be varied as follows:

```
iu0 - iu31 increment the loop counter used l0 - l31 by 1.
du0 - du31 decrement the loop counter used l0 - l31 by 1.
```

Note that these increments and decrements only count during the execution of the current pulse program. They are not stored in the parameters **L[0] - L[31]**. Furthermore,

```
ru0 - ru31 reset the loop counter used l0 - l31 to L[0] - L[31]
```

The statements **l0 - l31** are also used in **if** structures (conditions). Two simple conditions are:

```
if "(l3 != 0)" : true if l3 is unequal zero
if "(l3 == 0)" : true if l3 equals zero
```

Further conditions are:

```
if "(l3 operand expression)"
```

where operand can be: **==, !=, >, <, >=** or **<=** and expression can be a number or an arithmetic expression built from pulses, delays and/or loop counters. The statements effected by a certain condition must be put between curly brackets. Furthermore, you can use the **else** structure for statements which must be executed if the condition is not true. An example is:

```
if "(l5 > 2)"
{
    p1 ph1

}
else
{
}
```



Note that the syntax of the conditional statements is similar to C language syntax. However, you cannot use the C "else if" statement.

LOCNUC - Lock Nucleus

- Takes a character string value.
- Can be set from **eda** (submenu **Lock**) by entering a name in the **LOCNUC** field or by clicking the down arrow and selecting a nucleus from the appearing list.
- Can also be set by entering **locnuc** on the command line.
- Is interpreted by **edlock**, **lock**, **lopo**, **sref**.
- High resolution samples are usually locked on 2H or 19F. For these two nuclei, standard lock parameter files are delivered with TopSpin. These can be edited with the command **edlock**.

NBL - Number Of Blocks (Of Acquisition Memory)

- Takes an integer value.
- Interpreted by the pulse program statements **st**, **st0**, **ze**, **zd**, **wr**, **if**.
- The parameter NBL is used to acquire FID's in multiple memory blocks, for example in NOE difference experiments. For NBL = 1 (the default value), one FID (NS averages) is written to disk at the end of the acquisition. For NBL > 1, multiple FIDs are acquired in the acquisition memory before these are written to disk. The **st** statement increments the memory pointer by TD in order to use the next block. The statement **wr #0** will write NBL FIDs to disk. The following pulse program statements interpret NBL:

st - increment the memory pointer by TD

wr - write NBL blocks to disk

st0 - set the memory pointer to the position of the first FID

ze, **zd** - clear the acquisition memory of all NBL blocks

if - increment the file pointer in the raw data file by NBL*TD

df - decrement the file pointer in the raw data file by NBL*TD

nbl - loop counter specifying the number of blocks

If TD is not a multiple of 256 (1024 bytes), successive FIDs will still begin at 1024 byte memory boundaries. This is so for the FIDs in the acquisition memory as well as on disk. The size of the raw data file (**ser**) is therefore always a multiple of 1024 times NBL.

ND0 - Number Of Delays D0

- Takes an integer value.
- Temporary parameter.
- Only used in 2D and 3D datasets in the F1 direction.
- Number of **d0** statements in the increment loops of a pulse program for 2D or 3D experiments. Used to calculate the spectral width in the F1 direction according to:

$$SW = 1 / (SFO1 * ND0 * IN0)$$

N0 is set to 2, if the evolution time contains a 180° pulse (e.g. HMQC, HMBC, HSQC). Otherwise, it is set to 1 (e.g. NOESY, COSY, ROESY, TOCSY).

ND10 - Number Of Delays D10

- Takes an integer value.
- Temporary parameter.
- Only used in 3D datasets in the F2 direction.
- Number of **d10** commands in the increment loops of a pulse program for 3D experiments. Used to calculate the spectral width in the F2 direction according to

$$SW = 1 / (SFO1 * ND10 * IN10)$$

ND10 is typically set to 2, if the evolution time contains a 180° pulse. Otherwise, it is set to 1. Usually this is described in the pulse program comment section.

NS - Number Of Scans

- Takes an integer value.
- Interpreted by the pulse program statement `go=n`, `gonp=n` and `rcyc=n`.
- Can be set from **eda** (submenu **Experiment**) or by entering **ns** on the command line.
- The pulse program statements `go=n` and `rcyc=n` loop NS times to the line which the label `n`. In Bruker pulse programs, the label `n` is usually 2. The acquired data are accumulated in memory. After NS scans, the pulse program continues with the next statement which is often `wr #0`. This statement writes the accumulated data to disk.

After setting NS, you can calculate the resulting experiment time with the command **expt**. Then you can adjust NS such that the available time is properly used. Alternatively, you can set NS to a high value and halt the experiment (with the command **halt**) when time is up (see also DS).



NUC1 - NUC8 - Nucleus For Frequency Channel f1 - f8

- Take a value from a predefined list of nuclei.
- Can be set from **eda** (submenu **Nucleus**) by clicking **Edit** (o1 to o8).
- Can also be set from **edasp**.
- The parameter NUC1 assigns a nucleus to the frequency channel f1, NUC2 assigns a nucleus to the frequency channel f2 etc. In most routine experiments, only NUC1, NUC2 and NUC3 are used. For example:
 - 1D PROTON experiment without decoupling:
 - NUC1 = 1H
 - NUC2 = off
 - NUC3 = off
 - 1D C13 experiment with 1H decoupling:
 - NUC1 = 13C
 - NUC2 = 1H
 - NUC3 = off
 - 2D 1H experiment with 13C and 15N coupling:
 - NUC1 = 1H
 - NUC2 = 13C
 - NUC3 = 15N


In 2D datasets, NUC1 in the indirect direction (F1) must be set by selecting a nucleus from the listbox. In 3D datasets, this principle holds for both indirect directions, F2 and F1.


O1 - O8 -Irradiation Frequency Offset For Frequency Channel f1 - f8 in Hz

- Take a double value (Hz).
- Can be set from **eda** (submenu **Nucleus**) or by entering **o1**, **o2** etc. on the command line.
- Can also be set from **edasp** by adjusting OFSH1, OFSX1, OFSH2 etc.
- Can also be set from **gs** by adjusting **Offset** (FID display).

- O1 - O3 can be set by clicking the button  in the upper toolbar.
- O1 can be set by clicking the button  in the upper toolbar.
- The parameter O1 represents the irradiation (carrier) frequency offset. It is the center of the spectral region to be acquired. O1 is related to the basic frequency and the carrier frequency according to:

$$O1 = SFO1 - BF1$$

The button  can be used if you are setting up your experiment from an existing spectrum. It sets O1 to the center of the currently displayed spectral region. The button

 puts the cursor on the spectrum. You can then set the corresponding frequency offset by moving the mouse and clicking the left mouse button on a certain position. Because most Avance spectrometers are equipped with a maximum of four channels, O5 to O8 are normally unused. Therefore, they appear at the end of the **eda** table. See also O1P - O8P.

O1P - O8P - Irradiation Frequency Offset For Frequency Channel f1 - f8 in ppm

- Take a double value (ppm).
- Temporary parameters calculated from the equations:

$$O1P = O1/BF1$$

$$O2P = O2/BF2$$
 etc.
- Can be set from **eda** (submenu **Receiver**) or by entering **o1p**, **o2p** etc. from the command line.
- Can be set by setting O1 - O8 (see these parameters).
- The parameter O1P represents the irradiation (carrier) frequency offset in ppm. Because chemical shift values are expressed in ppm, it is usually more convenient to set O1P rather than O1.

OVERFLW - Data Overflow Check


- Takes one of the values **check** or **ignore** (default is **ignore**).
- Can be set from **eda** (submenu **Receiver**) or by entering **overflow** on the command line.
- For OVERFLW = **check**, acquisition commands check for possible data overflow.

P[μsec] - Array Of Pulse Lengths

- Takes float values (μsec).
- Array range [0-63]
- Can be set from **eda** (submenu **Durations**)
- Can also be set by entering **p0**, **p1**, **p2** etc. on the command line.
- Interpreted by the pulse program statements **p0** – **p63**, **ipu0** – **ipu63**, **dpu0** – **dpu63**, **rpu0** – **rpu63**.
- The pulse program statement **p0** executes a pulse of P[0] μseconds, **p1** executes a pulse of P[1] μseconds etc. In principle, all pulses can be used for any purpose. In Bruker pulse programs, however, certain conventions are used. You can view the file that contains these conventions by entering the command **edpul param.info**.

PARMODE - Dimensionality Of The Raw Data

- Takes one of the values 1D, 2D,..., 8D.
- Array range [0-9]

- Can be set by changing the dimension from the parameter editor (**eda**) toolbar .
- Interpreted by **zg**, **rpar** and by all processing commands which access raw data (see Processing Reference Manual).
- The parameter PARMODE defines the dimensionality of the raw data. 1D-8D. It is interpreted by acquisition commands like **zg** and cross checked with the current pulse program. If the dimensionality of PARMODE and the pulse program are different, a warning will appear. If you want, you can still continue the acquisition.

PARMODE is also interpreted by processing commands which access the raw data. If, for example, you enter **ft** on a 1D dataset, it is simply Fourier transformed. If however, you enter **ft** on a 2D dataset, you are first prompted to enter the FID number you want to Fourier transform. Processing commands which access processed data, like **abs**, interpret the processing parameter PPARMOD rather than the acquisition parameter PARMODE.

If you change PARMODE and set it to a lower dimension, the unnecessary files are deleted. For example, if you change it from 2D to 1D the files *acqu2* and *proc2* are deleted. Furthermore, the processing status parameter PPARMOD is automatically set the chosen lower dimension. However, you are warned before this actually happens and you have the possibility of keeping all files.

If you enter **rpar** to read a parameter set with a different dimensionality then the current dataset, a warning about this will appear. If you click OK, the data files and superfluous parameters files will be deleted. However, if you enter **rpar** with two arguments on the command line, i.e. **rpar <name> <type>**, this will happen without a warning. The reason is that **rpar** is often used in automation.

PHCOR[degree] - Array Of Correction Angles For Phase Programs

- Takes float values (degrees).
- Can be set from **eda** (submenu **Program parameters**)
- Can also be set by entering **phcor0**, **phcor1** etc. on the command line.
- Interpreted by the pulse program statements **ph0:r** - **ph31:r**.
- The option **:r** after a phase program statement in a pulse program adds phase correction factor to the phase. For example, the statement:

```
p1 ph8:r
```

executes a pulse with the current phase from phase program **ph8** plus the value of PHCOR[8]. For **ph8** = 0 1 2 3 and PHCOR[8] = 2, the phase cycle would be 2° 92° 182° 272°.

PCPD[μsec] - Array of CPD Pulse Lengths

- Takes float values (μsec).
- Array [0-9]
- Can be set from **eda** (submenu **Durations**)
- Can also be set by entering **pcpd1**, **pcpd2** etc. on the command line.
- Interpreted by the CPD program command **pcpd**.
- The PCPD parameters represent pulse lengths for CPD decoupling. They are interpreted by the CPD command **pcpd**. Which PCPD pulse is used depends on the frequency channel on which the CPD program runs. For example, the pulse program statement:

```
d1 cpd2:f2.
```

Runs the CPD program defined by CPDPRG2 on channel f2. Therefore, a `pcpd` command in this CPD program will execute a pulse of length PCPD[2].



Note that the element PCPD[0] exists but cannot be used because there is no channel that corresponds to it.

PH_ref - Receiver Phase Correction

- Takes a float value (degrees).
- Could be reached by entering **PH_ref** on the command line or can be set in **eda** (submenu **Experiment**).
- Interpreted by the pulse program statement `go=n phxx:r`.
- PH_ref adds a value to the receiver phase. For example, the pulse program statement:

```
go=2 ph30:r
```

starts the acquisition with receiver phase:

`ph30 + PH_ref`

The AU program **phtran** calculates the value of PH_ref for a 2D dataset from the spectrum phase correction values of a 1D row (for more information, type **edau phtran** and view the header of the AU program).

PLW[W] - Array Of Power Levels

- Takes float values (Watts)
- Array [0-63]
- Can be set from **eda** (submenu **Power**)
- Interpreted by the pulse program statements **plw0**, **plw1**, **plw2** etc.
- Can also be set from the **gs** dialog window.
- Interpreted by the pulse program statements `p10`, `p11`, `p12` etc.
- The power levels PLW[0] to PLW[63] can be used to set the power for the frequency channels. The default power for channel fn is PLW[n] (PLW[1] for f1, PLW[2] for f2 etc.) You can, however, explicitly assign a certain power level to a certain channel in the pulse program. For example, the pulse program statements:

```
p11:f2
```

```
p13:f4
```

Set the power of channel f2 to PLW[1] and the power of channel f4 to PLW[3]. The parameters PLW[0-63] can also be used to set the power of hard or shaped pulses in CPD programs. For example, the CPD program statement:

```
p31:sp1:180 pl=p11
```

Sets the power of the shaped pulse `sp1` to PLW[1].

PLdb[dB] - Array Of Power Levels

- Takes float values (dB).
- Array [0-63]
- Can be set from **eda** (submenu **Power**)
- Can also be set by entering **pldb0**, **pldb1** etc. on the command line.
- Can also be set from the **gs** dialog window.
- Interpreted by the pulse program statements `p10`, `p11`, `p12` etc.

- The power levels PLdB[0] to PLdB [63] can be used to set the power for the frequency channels. The default power for channel fn is PLdB [n] (PLdB [1] for f1, PLdB [2] for f2 etc.) You can, however, explicitly assign a certain power level to a certain channel in the pulse program. For example, the pulse program statements:

```
p11:f2
```

```
p13:f4
```

Set the power of channel f2 to PLdB [1] and the power of channel f4 to PLdB [3]. The parameters PLdB [0-63] can also be used to set the power of hard or shaped pulses in CPD programs. For example, the CPD program statement:

```
p31:sp1:180 p1=p11
```

Sets the power of the shaped pulse `sp1` to PLdB [1].

PRECHAN - Routing Between Switchbox Outputs And Preamplifier Modules

- Array of integer values; array range [0-32].
- Can be set from **eda** (submenu **Routing**) but is normally set graphically from the **edasp** window (see this command for more information).
- The values of PRECHAN define the connection between the switchbox outputs and the HPPR preamplifier modules. For example:

```
PRECHAN[1] = 0 : Output 1 is connected to HPPR module 0
```

```
PRECHAN[3] = 1 : Output 3 is connected to HPPR module 1
```

```
PRECHAN[1] = 2 : Output 1 is connected to HPPR module 2
```

```
PRECHAN[2] = 3 : Output 2 is connected to HPPR module 3
```

PULPROG - Pulse Program Used For The Acquisition

- Takes a character string value.
- Can be set from **eda** (submenu **Experiment**) by entering a name or by clicking the down arrow and selecting a pulse program from the appearing list.
- Can also be set by entering **pulprog** on the command line.
- Also set by the command **edcpul <name>**
- Acquisition commands run the pulse program defined by PULPROG. If you set the pulse program in **eda**, you can click the down arrow to the right of the PULPROG field. A list of Bruker and user defined pulse programs will appear and you can click the one you need.



Note that Bruker pulse programs must be installed once with **expinstall**. If you start your experiment by reading a standard parameter set (with **rpar**), PULPROG is usually set to the appropriate pulse program. The pulse programs from the Bruker library cannot be modified and saved under the same name. Users can write their own pulse programs that other user cannot modify (except the nmrsu).

RECCHAN - Array Of Receiver Channels

- Takes integer values.
- Can be set from **eda** (submenu **Routing**).
- Array [0-15]

RG - Receiver Gain

- Takes an integer value.

- RG controls the amplitude of the FID signal before it enters the digitizer. It is usually determined automatically with the command **rga**. This command performs an automatic determination of the optimum receiver gain. It runs several acquisitions with varying receiver gain until the maximum value is found that does not cause overflow. The parameter RG is then set to this value. If the RG value is already known from previous experiments, it can be set from **eda** (submenu **Receiver**) or by entering **rg** on the command line. RG can also be set from the **gs** dialog.

On AVneo spectrometers, the maximum RG value is 101. If you enter a larger value is entered it is automatically reduced to the maximum allowed value.

RO - Sample Rotation Frequency in Hz

- Takes an integer value.
- Can be set from **eda** (submenu **Probe**) or by entering **ro** or **ro <value>**.
- Interpreted by **ro acqu**.
- The command **ro acqu** will set sample rotation to the value of RO. It will wait for 60 seconds and then check if the specified rate has been reached. If this is not the case, an error message is displayed.

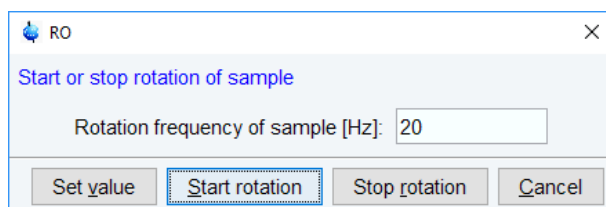


Figure 2.2: RO

RSEL - Routing between FCU's and Amplifiers

- Array of integer values, array range [1-24].
- Can be set from **eda** (submenu **Routing**) but is usually set graphically from the **edasp** window (see this command for more information).
- The values of RSEL define the connections between the TRX's and the amplifiers. For example:

RSEL[1] = 2 : TRX 1 is connected to amplifier 2

RSEL[2] = 0 : TRX 2 is not connected to any amplifier


RSEL[0] is unused

SFO1 - SFO8 - Irradiation (carrier) Frequencies For Channels f1 to f8

- Take a double value (MHz).
- Are automatically calculated from the equation:

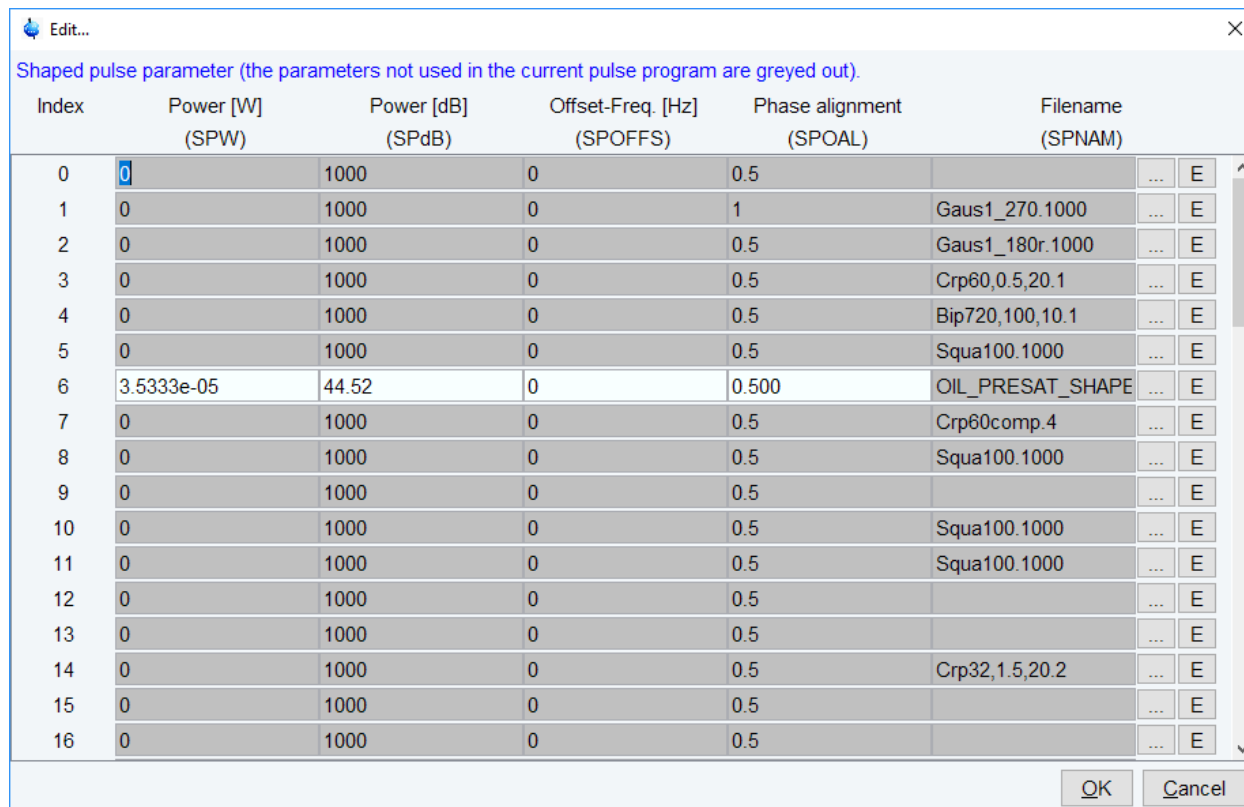
$$\text{SFO1} = \text{BF1} + \text{O1}$$

$$\text{SFO2} = \text{BF2} + \text{O2}$$
 etc.
 where O1, O2 etc. are set from **edasp** or **eda** (submenu **Nucleus**)
- can also be set with **gs** by adjusting **Frequency** (FID display)

- SFO1 can be set by clicking  in the upper toolbar.
- The parameter SFO1 represents the irradiation (carrier) frequency for channel f1. It is usually set from the by defining the nucleus and frequency offset for channel f1 in the routing table (opened with **edasp**).

SHAPE - Shaped Pulse Parameter Table

- Can be set from **eda** (submenu **Power**)
- Allows you to set power level, frequency offset, phase alignment and filename for 64 shaped pulses.
- Interpreted by pulse program statements like `sp0 – sp63`



Index	Power [W] (SPW)	Power [dB] (SPdB)	Offset-Freq. [Hz] (SPOFFS)	Phase alignment (SPOAL)	Filename (SPNAM)
0	0	1000	0	0.5	
1	0	1000	0	1	Gaus1_270.1000
2	0	1000	0	0.5	Gaus1_180r.1000
3	0	1000	0	0.5	Crp60,0.5,20.1
4	0	1000	0	0.5	Bip720,100,10.1
5	0	1000	0	0.5	Squa100.1000
6	3.5333e-05	44.52	0	0.500	OIL_PRESAT_SHAPE
7	0	1000	0	0.5	Crp60comp.4
8	0	1000	0	0.5	Squa100.1000
9	0	1000	0	0.5	
10	0	1000	0	0.5	Squa100.1000
11	0	1000	0	0.5	Squa100.1000
12	0	1000	0	0.5	
13	0	1000	0	0.5	
14	0	1000	0	0.5	Crp32,1.5,20.2
15	0	1000	0	0.5	
16	0	1000	0	0.5	

Figure 2.3: Shaped pulse parameter

- When you open **eda** and click on **SHAPE edit**, a list of shaped pulse parameters will appear as displayed in the table above.

The table has 64 entries (index 0-63) which are interpreted by the pulse program statements `sp0 - sp31`. These occur on pulse program lines like:

```
p1:sp2:f1
```

This line interprets entry 2 of the table and execute a Q3.1000 shaped pulse on channel f1 with length P1, Power 120.0, Offset 0.0 and Phase 0.55. When you click the down arrow to the right of a **Filename** entry, a list of available shape files will appear. This lists contains both Bruker and user defined shape files. The former must be installed once with **expinstall**. The latter can be created with the *ShapeTool* (command **stdisp**).

The Shaped Pulse Parameter Table entries are also available as acquisition parameters. They do not appear individually in **eda** but they can be set from the command line (see the next table).

They also appear as acquisition status parameters when you enter **dpa**.

Description	Acquisition parameters	Commands
power level	SPW[0-63]	spw0 – spw63
	SPdB[0-63]	Spdb0-spdb63
frequency offset	SPOFFS[0-63]	spoffs0 – spoffs63

Description	Acquisition parameters	Commands
phase alignment	SPOAL[0-63]	spoal0 – spoal63
file name	SPNAM[0-63]	spsnam0 – spsnam63

Table 2.2: Acquisition Status Parameters

SOLVENT - the Sample Solvent

- Takes a character string value.
- Can be set from **eda** (submenu **Lock**) by entering a name or by clicking the down arrow and selecting a solvent from the appearing list.
- Can also be set by entering **solvent** on the command line.
- Interpreted by **getprosol** and IconNMR automation.
- Also interpreted by **lock -acqu**, **lopo** and **sref**.
- The parameter SOLVENT must be set to the name of the solvent used in the current sample. Some acquisition parameters like pulse length and power level are dependent on the probe and the solvent. The command **getprosol** interprets SOLVENT and PROBHD and sets all dependent parameters accordingly. These parameters must be defined once, with **edprosol**, for all probes and solvents. In IconNMR automation, **getprosol** is automatically performed after a standard experiment has been read.


SUBNAM – Name of subroutine

- Can be set from **eda** (submenu **Program parameters**) or by entering **subnam** on the command line.
- Different subroutines can be called from a pulse program without changing the pulse program itself by using the parameters SUBNAM 1-16
`Subr <${SUBNAM1}>(dl, pl, fl)`
- The compiler will insert the subroutine whose name is in SUBNAM1 at this place.
- The precompiled pulse program `pulseprogram` in the raw data directory always shows the expanded subroutine together with lines which mark its begin and end.

SPINCNT – Counter for spinning sample

- Can be set from **eda** (submenu **Probe**) or by entering **spincnt** on the command line.
- Defines the number of sample rotor periods for which the pulse program execution is halted if a `spin_wait` instruction is used (for further information please look up **Help | Manuals | Programming Manuals | Pulse Programming**).


SW - Spectral Width in ppm

- Takes a double value (ppm).
- Can be set from **eda** (submenu **Width**) or by entering **sw** on the command line.
- SW can be set by clicking the button  in the upper toolbar.
- The spectral width should be set to such a value that all relevant peaks are expected to fall within that range. This means, for an unknown sample, SW should be set to a large value, like 50 ppm for a proton spectrum. The spectral width determines the dwell time according to the following equation:

$$DW=1/(2*SW*SFO1)$$

Where DW is expressed in μ sec.

When you enter a certain value for SW, you may notice that it is slightly adjusted by TopSpin. The reason is that the digitizer hardware can only handle discrete values of DW. For DIGMOD = baseopt the DSP firmware is automatically set to rectangle limiting the maximum allowed spectral width (see the next table).

Clicking the button  in the upper toolbar will set SW to the region currently displayed on the screen. It will also set SFO1 to the frequency of the center of that region. For 2D and 3D experiments, SW as it is described above corresponds to the width in the acquisition direction. In the indirect directions, the spectral width are calculated from the parameters IN0, IN10, ND0, and ND10. In 2D, the following relations count:

$$SW(F1)=1/(SFO1*ND0*IN0)$$

$$SWH(F1)= 1/(ND0*IN0)$$

In 3D, the following relations count:

$$SW(F2)=1/(SFO1*ND10*IN10)$$

$$SWH(F2)= 1/(ND10*IN10)$$

$$SW(F1)=1/(SFO1*ND0*IN0)$$

$$SWH(F1)= 1/(ND0*IN0)$$

DSPFIRM					
DIGMOD		sharp	smooth	medium	rectangle
	digital	5000	5000	5000	n.a.
	baseopt	n.a.	n.a.	n.a.	625

Table 2.3: Maximum SW (kHz) for DIGTYP = DRX

SWH - Spectral Width in Hz

- Takes a double value.
- Can be set from **eda** (submenu **Width**) or by entering **swh** on the command line.
- Is related to SW according to the following equation:

$$SWH = SW * SFO1$$

During experiment setup, SW is usually defined and SWH is automatically calculated from it. The maximum values depend on the digitizer, the acquisition mode and the DSP firmware as it is shown in table Maximum SW (kHz) for DIGTYP = DRX above.



Note that SWH is stored in the parameter file *acqu* as SW_h.

SWIBOX - Routing between Switchbox Inputs and Switchbox Outputs

- Array of integer values [0-63].
- Can be set from **eda** (submenu **Routing**) but is normally set graphically from the **edasp** window ([see this command for more information \[47\]](#)).
- The values of SWIBOX define the connection between the switchbox inputs and switchbox outputs. For example, SWIBOX[1] = 3 means that Input 1 is connected Output 3.

TD - Time Domain; Number Of Raw Data Points

- Takes an integer value.

- The parameter TD determines the number of raw data points to be acquired. A large value of TD enhances the spectrum resolution, but also increases the acquisition time AQ. TD is usually set to a power of 2, for example 64k for a 1D spectrum, which corresponds to 65536 points. The FID resolution is related to the number of data points according to:

$$\text{FIDRES} = \text{SW} * \text{SFO1} / \text{TD}$$

In a 2D experiment, TD in the acquisition direction (F2) has the same meaning as in 1D. In the indirect direction (F1), it represents the number of increments. As such, it is interpreted by pulse program statements like:

```
lo to n times td1
```

In a 3D experiment, TD in the acquisition direction (F3) has the same meaning as in 1D. In the indirect directions (F2 and F1), it represents the number of increments. As such, they are interpreted by statements like:

```
lo to n times td1 ; F1 loop in 2D or 3D experiments
```

```
lo to n times td2 ; F2 loop in 3D experiments
```

As an alternative to `lo to n times td1`, you can also use the `mc` statement. Do not confuse this with the TopSpin processing command `mc` that performs magnitude calculation.

TD0 - Loop Counter For One-Dimensional Experiments

- Takes an integer value.
- Interpreted by the pulse program statement `mc`.
- TD0 is normally used as a loop counter for multiple 1D experiments that are measured under varying conditions (for example varying temperature or pressure) and that are stored as 2D data. Similarly, it can be used for multiple 2D experiments that are stored as 3D data.

TE - Demand Temperature On The Temperature Unit

- Takes a float value.
- Can be set from **eda** (submenu **Probe**) or by entering **te** on the command line.
- Interpreted by **teset**.
- The command **teset** sets the temperature on the temperature unit to the value of TE. It be entered on the keyboard, or called from AU program with its macro TESET.

V9 - Maximum Variation Of A Delay

- Takes a float value (between 0.0 and 100.0 percent).
- Can be set from **eda** (submenu **Nucleus**) or by entering **v9** on the command line.
- Interpreted by pulse program statements like `d1:r, p1:r`.
- The pulse program statement `d1` causes a delay D1. The statement `d1:r`, however, causes a delay D1 plus a random value. As such, the delay is a different every time the statement `d1:r` is executed. The parameter V9 specifies, in percent, the maximum amount which is added to or subtracted from D1. As such, the effective delay varies between 0 and 2*D1. The `:r` option can be used for any of the statements `d0 – d63` and `p0 – p63` to vary D[0-63] and p[0-63], respectively.



Note that the command **gs** ignores the `:r` option.

VALIST - Variable Amplitude (Power) List

- Takes a character array value.
- Can be set from **eda** (submenu **Lists**) by entering a name or by clicking the down arrow and selecting a name from the appearing list.
- Can also be set by entering **valist** on the command line.
- Interpreted by user defined pulse program statements.
- The parameter VALIST defines the name of variable amplitude (power) list. Such a list can be created with **edlist va** and has entries like:

```
-6.0
0.0
3.0
6.0
```

that represent attenuation values in dB.

The usage of a VA list is different from pulse and delays lists. You must define the statement by which a VA list is accessed in the pulse program. Such a statement can have any name, for example the name `vanam` is used in the examples below. The suffixes `.inc`, `.dex` and `.res` can be used to increment, decrement and reset the lists position, respectively. Furthermore, the caret operator (^) allows you to read a list value and increment the list position with one statement. The following pulse program entries illustrate the use of a variable amplitude list:

```
define list<power> vanam = <$VALIST>
definition of the power list

d1 vanam:f2 vanam.dex
set the power to the current value of the list and decrement the index

d1 vanam[2]:f3
set the power to the second value of the list

"vanam.idx = vanam.idx + 3"
increment the list index by 3

d1 vanam^:f4
set power to the current value of the list increment the index
```

As an alternative to using a list defined by the parameter VALIST, you can explicitly define a variable amplitude (power) list filename or even the list values in the pulse program. The following examples illustrate such definitions:

```
define list<power> vanam=<my_filename>
define list<power> vanam={10 30 50 70}
```



Note that the second definition does not require a list file. For more information on using variable amplitude lists click:

Help | Manuals | Programming Manuals | Pulse Programming

VCLIST - Variable Counter List

- Takes a character array value.

- Can be set from **eda** (submenu **Lists**) by entering a name or by clicking the down arrow and selecting a name from the appearing list.
- Can also be set by entering **vclist** on the command line.
- Interpreted by the pulse program statements `lo to x times c, ivc, vcidx`.
- The parameter VCLIST defines the name of variable counter list. Such a list can be created with **edlist => List type : vc** and has entries like:

4
7
20

The currently defined list is interpreted by the pulse program statement: `lo to x times c`

Where `x` is a pulse program label and `c` is the value at the current position of the counter list. When this statement is executed for the first time, the current position is the first entry in the list. The position is incremented by the statement `ivc`.

VDLIST - Variable Delay List

- Takes a character array value.
- Can be set from **eda** (submenu **Lists**) by entering a name or by clicking the down arrow and selecting a name from the appearing list.
- Can also be set by entering **vdlist** on the command line.
- Interpreted by the pulse program statements `vd, ivd` and `vdidx`.
- The parameter VDLIST defines the name of variable delay list. Such a list can be created with **edlist => List type : vd** and has entries like:

10m
50m
2s

Where `m` = milliseconds and `s` = seconds. The currently defined list is interpreted by the pulse program statement `vd` that reads the delay value at the current position. When `vd` is executed for the first time, the current position is the first entry in the list. The position is not incremented by `vd`; this is done by the statement `ivd`. As such, `vd` is normally used in combination with `ivd`. The statement `"vdidx=n"` sets the index to position `n` in the list.

VPLIST - Variable Pulse List

- Takes a character array value.
- Can be set from **eda** (submenu **Lists**) by entering a name or by clicking the down arrow and selecting a name from the appearing list.
- Can also be set by entering **vplist** on the command line.
- Interpreted by the pulse program statements `vp, ivp` and `vpidx`.
- The parameter VDLIST defines the name of variable pulse list. Such a list can be created with **edlist => List type : vp** and has entries like:

10u
50m
2s

Where `u` = microseconds, `m` = milliseconds and `s` = seconds. The currently defined list is interpreted by the pulse program statement `vp` that reads the pulse length value at the current position. When `vp` is executed for the first time, the current position is the first

entry in the list. The position is not incremented by `vp`; this is done by the statement `ivp`. As such, `vp` is normally used in combination with `ivp`. The statement "`vpidx=n`" sets the index to position `n` in the list. A variable pulse list can only be used for hard pulses, not for shaped pulses or shaped gradients. As an alternative to a VP list, you can also specify a list of pulse values within the pulse program using a `define` statement. For more information on this topic click:

[Help](#) | [Manuals](#) | [Programming Manuals](#) | [Pulse Programming](#)

VTLIST - Variable Temperature List

- Takes a character array value.
- Can be set from **eda** (submenu **Lists**) by entering a name or by clicking the down arrow and selecting a name from the appearing list.
- Can also be set by entering **vtlist** on the command line.
- Interpreted by the AU program macros RVTLIST, VT, IVTLIST, DVTLIST.
- The parameter VTLIST defines the name of variable temperature list. Such a list can be created with **edlist => List type : vt** and has the following format:

```
300
320
340
```

Where each entry is a temperature value in Kelvin.

Temperature lists are interpreted by the AU program macros:

RVTLIST - open the temperature list defined by VTLIST

VT - read the current value from the list and set it on the temperature unit


IVTLIST - increment the current position in the list to the next value

DVTLIST- decrement the current position in the list to the previous value




Note that temperature lists are only interpreted by AU program macros, not by pulse program statements.

WBST - Number Of Wobble Steps

- Takes an integer value between 64 and 4096 (default 1024).
- Can be set from **eda** (submenu **Wobble**) or by entering **wbst** from on the command line.
- Can also be set by clicking  in the wobb window.
- Interpreted by **wobb**.
- The parameter WBST determines the number of steps (frequencies) used for tuning and matching a probe (wobbling). A probe is correctly tuned when the dip of the wobble curve is exactly at the center of the display. Normally, the default value of WBST (256) is high enough for exact tuning. If necessary, you can set WBST to a higher value for a better resolution.

WBSW - Wobble Sweep Width

- Takes a double value between 1 KHz and 4 MHz.
- Can be set from **eda** (submenu **Wobble**) or by entering **wbsw** from on the command line.
- Can also be set by clicking  in the wobb window.
- Interpreted by **wobb**.

- The parameter WBSW sets the frequency range for tuning and matching a probe (wobbling). The center of the wobble region is determined by SFO1. When you change WBSW from the command line, **wobb** is automatically restarted. The command **atma** automatically calculates the optimum sweep width and does not interpret WBSW. During tuning/matching **atma** temporarily sets the parameters WBST and WBSW to the calculated values and then resets them to their original values.

ZGOPTNS - Acquisition (zg) Options

- Takes a character array value.
- Can be set from **eda** (submenu **Program parameters**) by entering **zgoptns** on the command line.
- The parameter allows you to set an option to acquisition commands like **zg** and **go**. As an alternative, acquisition options can also be specified on the command line or in the pulse program. For example, the option DQF can be set in the following three ways:
 - By setting the parameter ZGOPTNS to DQF
 - By specifying the option as an argument, e.g.: **zg -DDQF**
 - By defining the option in the pulse program, e.g.: `#define DQF`

2.5 Acquisition Status (dpa) Parameters

This paragraph contains a list of all acquisition status parameters with a description of their function. They are stored for each dataset in the file:

- `<dir>/data/<user>/nmr/<name>/<expno>/`

acqus - acquisition status parameters

These can be viewed by entering **dpa** on the command line or clicking AcquPars tab in the data window and then clicking the **S** button. Some acquisition status parameters are interpreted by processing commands that work on raw data. Others are only stored as information for the user.

After an acquisition has finished, most acquisition status parameters have been set to the same value as the corresponding acquisition parameter. Sometimes, however, this is different. For example:

- Some parameters are continuously updated during the acquisition, e.g. NS, F1-TD (in 2D). When the acquisition is halted with **halt**, the current values are stored as acquisition status parameters.
- Some acquisition parameters are adjusted at the beginning of the acquisition, e.g. RG, FW, DR, SW. The modified values are stored as acquisition status parameters.
- The values of some parameters are a result of the acquisition. They cannot be set by the user (they do not appear as acquisition parameters) but they are stored as acquisition status parameters. Examples are AQSEQ, YMAX_a, LOCSHFT, NC.

The acquisition status parameters which are a result of or adjusted by the acquisition are listed below.

AQ_mod - Acquisition Mode

- Takes one of the values **qf**, **qsim**, **qseq** or **DQD**.
- Can be viewed from **dpa** or by entering **s aq_mod** on the command line.
- Normally, the acquisition status parameter AQ_mod is set to the same value as the acquisition parameter AQ_mod. If, however, AQ_mod = DQD but DIGMOD = analog, **zg** performs an acquisition in simultaneous mode and sets the status parameter AQ_mod to qsim. The same thing happens if your spectrometer is not equipped for DQD (see also the description of AQ_mod in chapter [Acquisition \(eda\) Parameters](#) [16]).

AQSEQ - Acquisition Order

- Used for datasets with dimension $\geq 3D$.
- Takes one of the values **321**, **312** for 3D data.
- Takes one of the values **4321**, **4312**, **4231**, etc. for 4D data.
- Can be viewed with **dpa** or by entering **s aqseq** on the command line.
- Interpreted by the processing command **tf3** and **ftnd**.
- AQSEQ describes the order in which the directions have been acquired. It is automatically set according to the loop structure in the pulse program. For example, a 3D pulse program usually contains a double nested loop with loop counters **td1** and **td2**. If **td1** is used in the inner loop and **td2** in the outer loop, AQSEQ is set to 312. Otherwise it is set to 321.

AQSEQ is evaluated by commands which process raw nD data, like **ftnd** or **tf3**. If the acquisition status parameter AQSEQ is not set, the processing parameter AQORDER is evaluated to determine the acquisition order.

BYTORDA - Byte Order of the Raw Data

- Takes one of the values **big** or **little**.
- Can be viewed with **dpa** or by entering **s bytorda** on the command line.
- interpreted by all processing commands which work on raw data.
- Big endian and little endian are terms that describe the order in which a sequence of bytes are stored in a 4-byte integer. Big endian means the most significant byte is stored first, i.e. at the lowest storage address. Little-endian means the least significant byte is stored first. TopSpin only runs on computers with byte order little endian. However, TopSpin's predecessor XWIN-NMR also runs on SGI workstations which are big endian. The byte order of the raw data is determined by the computer which controls the spectrometer and is stored in the acquisition status parameter BYTORDA (type **s bytorda**). This allows raw data to be processed on computers of the same or different storage types. The first processing command interprets BYTORDA, stores the processed data in the byte order of the computer on which it runs and sets the processing status parameter BYTORDP accordingly (type **s bytor dp**). All further processing commands interpret this status parameter and store the data accordingly. As such, the byte order of the computer is handled automatically and is user transparent. 2D and 3D processing commands, however, allow you to store the processed data with a byte order different from the computer on which they run. For example, the commands **xfb big** and **tf3 big** on a Windows or Linux PC store the data in big endian although the computer is little endian. The processing status parameter BYTORDP is set accordingly.

DATE - Date Of Acquisition

- Takes an integer value (# seconds since 1970).
- Shows the date and time of the end of the acquisition specifying:
`month day, year hour:minute:seconds time-zone`
 e.g. November 10, 2004 6:06:19 PM GMT
- The date is stored as an integer number, which expresses the number of seconds since January 1st 1970.



Note that the start of the acquisition is not stored as a parameter but is available in the acquisition audit trail (command **audit acqu**).

DECIM - Decimation Factor Of The Digital Filter

- Takes an integer value.

- Can be viewed with **dpa** or by entering **s decim** on the command line.
- Interpreted by all processing commands which work on raw data.
- Also interpreted by **abs** and **apk**.
- Processing commands account for the group delay of digitally filtered data, by interpreting the following parameters:
 DSPFVS and DECIM (for DSPFVS < 20)
 or
 GRPDLY (for DSPFVS ≥ 20)
- DECIM must be interpreted by third party software which processes digitally filtered Avance data.
- For DSPFVS < 20, the commands **abs** and **apk** check whether DECIM is 1 (no oversampling) or greater than 1 (oversampling) to handle the so called smilies at the spectrum edges (see also the description of DECIM in chapter [Acquisition \(eda\) Parameters](#) [▶ 16]).

DTYPA - Data Type of The Raw Data

- Takes the value int or double.
- Can be viewed with **dpa** or by entering **s dtypa** on the command line.
- Interpreted by all processing commands which work on raw data.
- In TopSpin 2.0 and newer, 1D raw data are, if necessary, stored as double precision (64-bit) data. The spectrometer internal processor stores raw data in 32-bit integer format. If, during acquisition, data overflow would occur, data are transferred to the computer that controls the spectrometer where they are stored in 64-bit double precision format. The acquisition status parameter DTYPA shows whether data are stored as integers (DTYPA = 0) or doubles (DTYPA = 2).



Note that processed data are always stored as integer data.

EXP - Experiment Performed

- Takes a character array value.
- IconNMR sets EXP to the value of the parameter set that was used for the experiment.

FnMODE - Acquisition Mode In The Indirect Directions (2D and 3D)

- Takes one of the values **undefined**, **QF**, **QSEQ**, **TPPI**, **States**, **States-TPPI** or **Echo-Antiecho**. For more information please look up "Introduction to Bruker NMR Pulse Programming User Manual".
- Can be viewed with **dpa** or by entering **s fnmode** (2D).
- Interpreted by 2D and 3D processing commands that access raw data. These are usually **xfb** or **xf2** for 2D data and **tf3** for 3D data.

It is interpreted by processing commands to determine the Fourier transform mode in the indirect direction(s). For historical reasons, MC2 is interpreted when the acquisition status parameter FnMODE has the value **undefined**.

DSPFVS - DSP Firmware Version

- Takes an integer value between 10 and 23.
- Interpreted by processing commands that access raw data.

- Different DSP firmware versions filter the raw data in a different way. It is set according to the acquisition parameter DSPFIRM. Processing commands account for the group delay of digitally filtered data, by interpreting the following parameters:
- DSPFVS and DECIM (for DSPFVS < 20)
or
GRPDLY (for DSPFVS ≥ 20)
- DSPFVS must be interpreted by third party software which processes digitally filtered Avance data.

GRDLY - Group Delay

- Takes a double value ≥ 0.
- Interpreted by processing commands that access raw data
- Processing commands account for the group delay of digitally filtered data, by interpreting the following parameters:
SPFVS and DECIM (for DSPFVS < 20)
or
GRPDLY (for 20 ≤ DSPFVS ≤ 23)
- GRPDLY must be interpreted by third party software which processes digitally filtered Avance data.
- 20 ≤ GRPDLY ≤ 23

LGAIN - Loop Gain; Lock Regulator Gain

- Is set to a value between -80 and 0 dB.
- Can be viewed with **dpa**.
- LGAIN is set at the end of the acquisition to the loop gain value used at that moment, i.e. the value currently set on the BSMS unit. This usually, but not necessarily corresponds to the value of LGain in the **edlock** table. For example, if lock-in was performed with the command **lock**, the loop gain is first read from the **edlock** table and set on the BSMS unit. However, pressing the **Autolock** or **Lock On/Off** key in the BSMS display performs lock-in without first reading the **edlock** table.



Note in this respect that the current value of loop gain can also be changed in the BSMS display or by the command **lgain**.

LOCSHFT - Lock Shift

- Takes one of the values **true** or **false**.
- Can be viewed with **dpa**.
- The value of LOCSHFT indicates whether or not the sample was locked at the time the acquisition of the first scan has been finished.

LTIME - Loop Time; Lock Regulator Time

- Is set to a value between 0.001 and 1.0 seconds.
- Can be viewed with **dpa**.
- LTIME is a lock parameter (**edlock**) rather than an acquisition parameter (see the description of LGAIN above).

LFILTER - Loop Filter; Lock Regulator Cut-Off Frequency Of The Lowpass Filter

- Is set to a value between 1 - 200 Hz.

- Can be viewed with **dpa**.
- LFILTER is a lock parameter (**edlock**) rather than an acquisition parameter (see the description of LGAIN above).

LOCKPOW - Lock Power

- Is set to a value between -60 and 100 dB.
- Can be viewed with **dpa**.
- LOCKPOW is a lock parameter (**edlock**) rather than an acquisition parameter (see the description of LGAIN above).

MASR - MAS Spin Rate

- Takes a float value.
- Can be viewed with **dpa** (submenu **Probe**).
- Set by **masr get**.
- The acquisition status parameters MASR is continuously updated when the MAS monitor is active (can be enabled with the command **set**). MASR is only used in connection with HR-MAS and CP-MAS probes. For high resolution probes the parameter RO becomes relevant.

NC - Normalization Constant

- Takes an integer value.
- Can be viewed with **dpa**.
- Set by acquisition commands and by the processing commands **genfid**, **genser** and **addfid**.
- Interpreted by all processing commands that access raw data.
- Acquisition commands set NC to minus the value of DDR.



Note that for DIGTYP = analog, DDR is 0 and, as such, NC is also 0. The processing commands mentioned above create pseudo raw and NC is set according to the input processed data.

PROBHD - Probe

- Takes a character string value.
- Can be viewed with **dpa**.
- PROBHD is set at the end of an acquisition to the current probe as it was defined with **edprobe** before the acquisition.
- LOCNUC

HOLDER - Sample Changer Holder Position

- Takes an integer value.
- Can be viewed with **dpa**.
- Set by IconNMR

AUTOPOS - Identification Information from BEST-NMR Rack Or Well-Plate

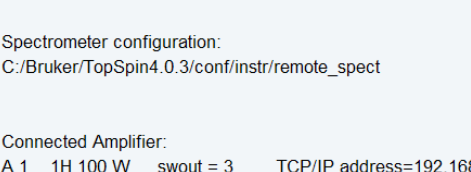
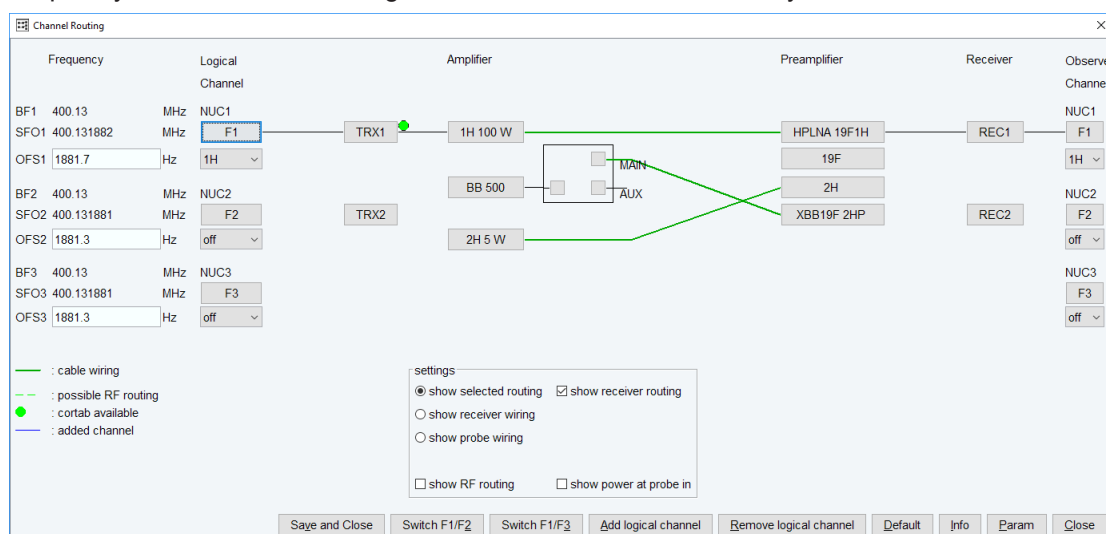
- Takes a character string value (A1-A12, B1-B12, ... , H1-H12).
- Can be viewed with **dpa**.
- Set by IconNMR.

LOCKED - Lock Status During Acquisition

- Takes one of the values TRUE or FALSE.
- Can be viewed with **dpa**.
- The status parameter LOCKED indicates whether or not the magnetic field was permanently locked since the last successful **lock** command. For an nD experiment the parameter LOCKED is updated after the last FID has been acquired and stored to disk.

2.6 Routing (edasp) parameters

The command **edasp** opens the routing table where you can select the nuclei and the spectrometer routing. When you select a nucleus for a certain frequency channel, the basic frequency and the default routing for that channel are automatically set.



The screenshot shows a window titled "edasp" with a standard Windows-style title bar (minimize, maximize, close buttons). The window content is as follows:

Spectrometer configuration:
 C:/Bruker/TopSpin4.0.3/conf/instr/remote_spect

Connected Amplifier:

Below this heading is a list of four items, each preceded by a blue circular icon containing a white lowercase letter 'i'.

- A 1 1H 100 W swout = 3 TCP/IP address=192.168.99.12
- A 2 2H 150 W swout = 4 TCP/IP address=192.168.99.12
- A 3 BB 500 TCP/IP address=192.168.99.12
- A 4 BB 1000 BB 100 W TCP/IP address=192.168.99.13

Below the list, the following text is displayed:

Quadrature Probe Installed = false
 Router mask = 1|2|4|8|
 HPSELECT = yes

In the bottom right corner, there is a button with a blue border and the text "Close".

[illegible]

Parameters Displayed In The Routing Table:

- BF1 - basic frequencies for channel f1.
Same as the **eda** parameter BF1.
- NUC1 - nucleus for channel f1.
Same as the **eda** parameter NUC1.
- SFO1 - irradiation frequency for channel f1.
Same as the **eda** parameter SFO1.
- OFSX1 - irradiation frequency offset for the first X nucleus.
- OFSH1 - irradiation frequency offset for the first 1H.
- OFSF1 - irradiation frequency offset for the first F, 3H or Tl.
- OFSX2 - irradiation frequency offset for the second X nucleus.
- OFSH2 - irradiation frequency offset for the second 1H.
- OFSF2 - irradiation frequency offset for the second F, 3H or Tl.
etc.
When defined for channel f1, these parameters correspond to O1 in **eda**.
When defined for channel f2, these parameters correspond to O2 in **eda**.
etc.



Note that the command **edsp** reads the values for OF* that were stored by the previous **edsp** or **edasp** command. If the latter was performed on different dataset, the OF* values might differ from the corresponding O1, O2 etc. (see the description of **edsp**).

Parameters Which Can Be Viewed By Clicking PARAM

- FCUCHAN - connections between logical frequency channels and FCU's.
- RSEL - connections between FCU's and amplifiers.
- SWIBOX - connections between Switchbox inputs and Switchbox outputs.
- PRECHAN - connections between Switchbox outputs and Preamplifier modules.
- HPMOD - connections between high power amplifiers and Preamplifier modules.

edasp stores its parameters under the current dataset in the file:

`<dir>/data/<user>/nmr/<name>/<expno>/`

acqus - acquisition parameters.

and the dataset independent file:

`<tshome>/conf/instr/<instrum>`

specpar - **edasp** parameters



Note that the routing table can also be opened from the **eda** dialog box, by clicking the NUC1 button.

2.7 Lock (edlock) Parameters

Lock parameters are used for locking the magnetic field and for referencing the spectrum. The lock-in procedure can be performed from the display or with the command **lock** or **lopo**. Referencing the spectrum can be done with the command **sref**.

Lock Parameters Used For Locking The Magnetic Field:

- Lockfreq - lock irradiation frequency.
- Field - Field value (H0).
- BFREQ - Basic frequency.
- Solvent - Sample solvent.
- LPower - Lock power; the power used to irradiate the lock nucleus (-60 to 0 dB).
- LGain - Loop gain; lock regulator gain (-80 to 0 dB).
- LTime - Loop time; lock regulator time constant (0.001 to 1.0 seconds).
- LFilt - Loop filter, lock regulator cut-off frequency of the lowpass filter (1 to 200 Hz).
- LPhase - Lock phase; the phase of the lock signal.
- Nucleus - Observe nucleus.
- Distance - chemical shift of the lock nucleus (irradiation frequency offset).

Lock Parameters Used For Referencing:

- Ref. - chemical shift of the reference signal (default 0).
- Width - width of the region where the reference signal is searched.
- RShift - reference shift for default calibration.

The parameters LPower, LPhase, LGain, LTime and LFilt are probe and solvent dependent. They are stored for each probe and for each solvent separately in:

`<tshome>/conf/instr/<instrum>/prosol/<probeID>/<solvent>/`

bsmspar - probe dependent lock parameters

The other **edlock** parameters are only solvent dependent and are stored in the file:

`<tshome>/conf/instr/`

2Hlock - probe independent lock parameters

3 Spectrometer Configuration Commands

This chapter describes all TopSpin spectrometer configuration commands. These are commands which must be executed once, after installing a new version of the NMR Suite.

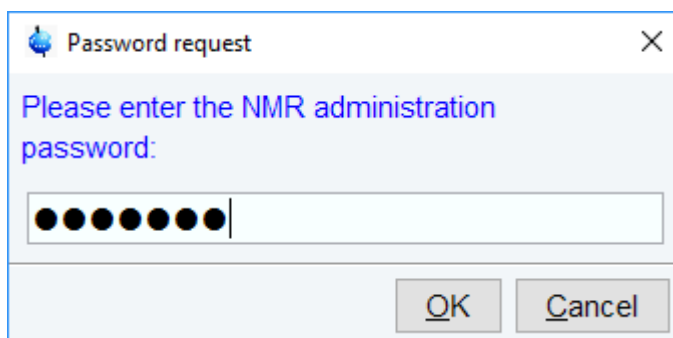
3.1 **cf**

3.1.1 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.



The first cf window is displayed.

Spectrometer Configuration Commands

△ 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

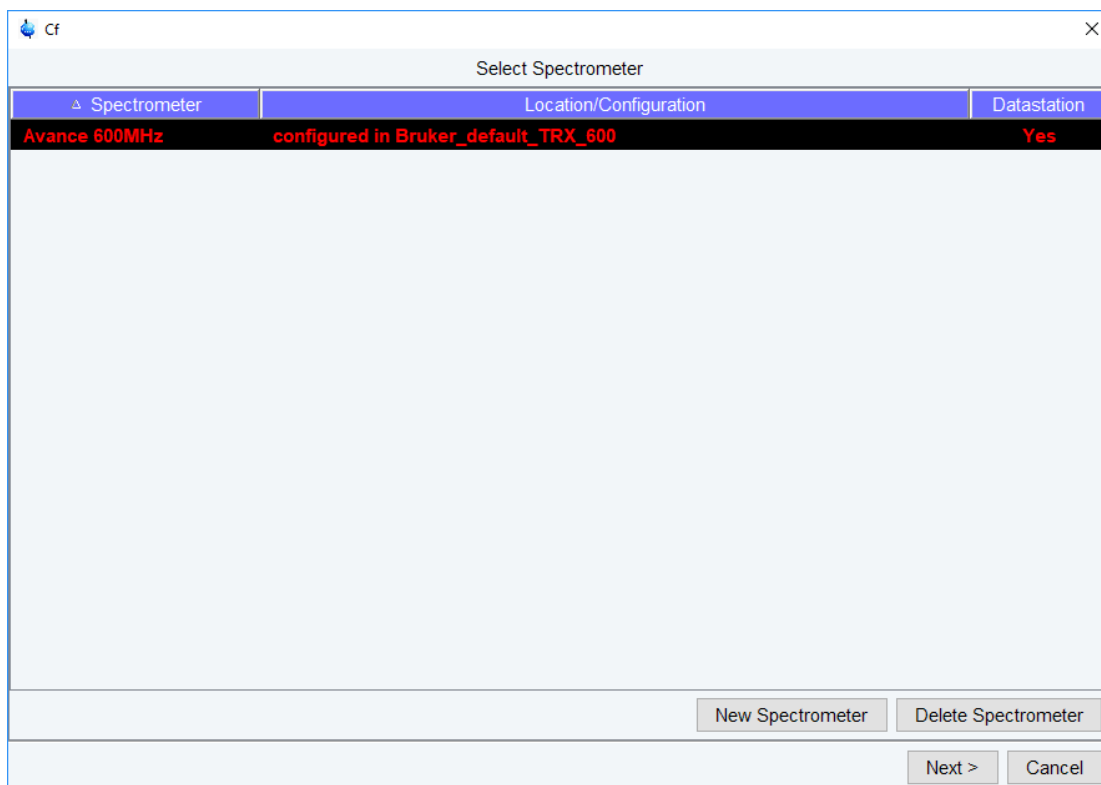
New Spectrometer Delete Spectrometer

Next > Cancel

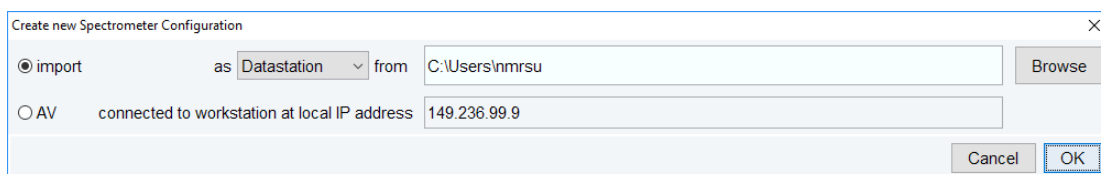
Most likely you will select an existing configuration and click **Next** to confirm this configuration. Click **New Spectrometer** to start a new configuration.

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 doesn't exist.

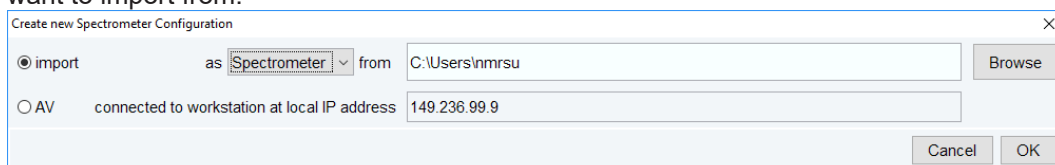


If an older TopSpin version with an appropriate configuration exists, then you can load it by clicking on New Spectrometer. The following window will be displayed.



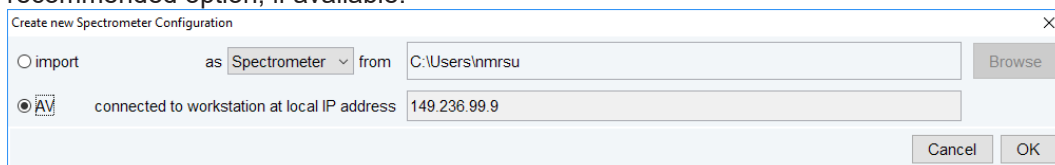
You can choose from one of the following three options.

1. Import a datastation from ... This will be explained in chapter [Configuration of a Processing-Only Workstation Using an Existing Spectrometer Configuration \[▶ 69\]](#) and [Configuration of a Processing-Only Workstation \[▶ 74\]](#) 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.



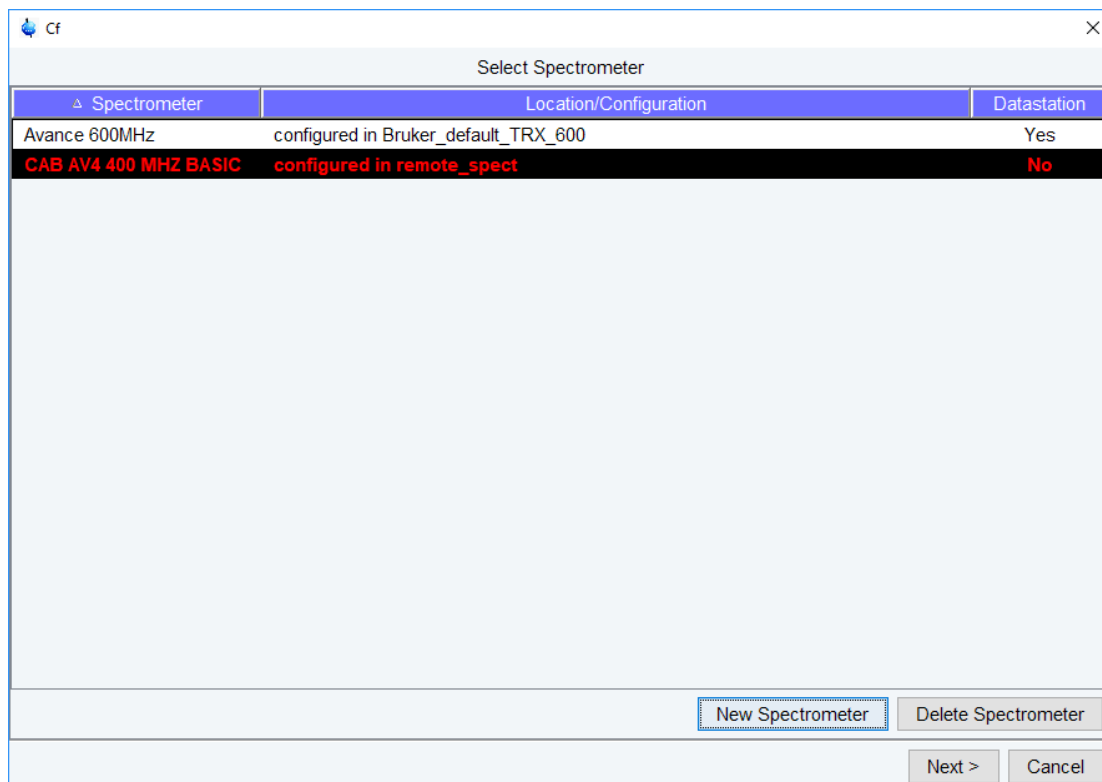
Spectrometer Configuration Commands

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



The dialog box titled "Create new Spectrometer Configuration" has a close button (X) in the top right corner. It contains two radio buttons: "import" (unselected) and "AV" (selected). The "import" option is followed by a dropdown menu set to "Spectrometer" and a text field containing "C:\Users\inmrsu", with a "Browse" button to its right. The "AV" option is followed by the text "connected to workstation at local IP address" and a text field containing "149.236.99.9". At the bottom right are "Cancel" and "OK" buttons.

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



The dialog box titled "Select Spectrometer" has a close button (X) in the top right corner. It features a table with three columns: "Spectrometer", "Location/Configuration", and "Datastation".

△ Spectrometer	Location/Configuration	Datastation
Avance 600MHz	configured in Bruker_default_TRX_600	Yes
CAB AV4 400 MHZ BASIC	configured in remote_spect	No

Below the table is a large empty rectangular area. At the bottom right are buttons for "New Spectrometer", "Delete Spectrometer", "Next >", and "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

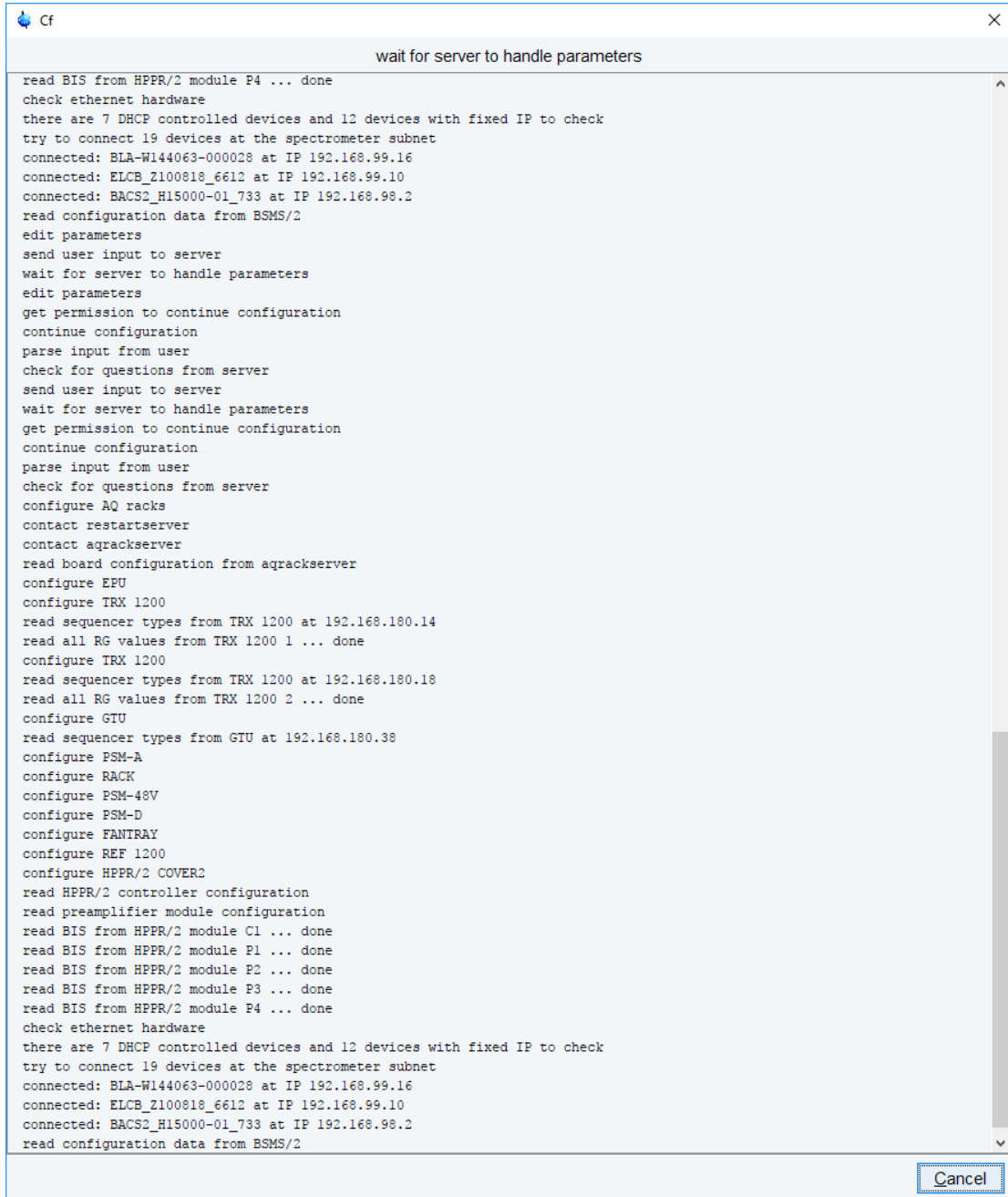
Magnet polarity SN (Bruker) ▼

< Previous Next > Cancel

- 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.

Spectrometer Configuration Commands



```
read BIS from HPFR/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 racks
contact restartserver
contact aqrackserver
read board configuration from aqrackserver
configure EPU
configure TRX 1200
read sequencer types from TRX 1200 at 192.168.180.14
read all RG values from TRX 1200 1 ... done
configure TRX 1200
read sequencer types from TRX 1200 at 192.168.180.18
read all RG values from TRX 1200 2 ... done
configure GTU
read sequencer types from GTU at 192.168.180.38
configure PSM-A
configure RACK
configure PSM-48V
configure PSM-D
configure FANTRAY
configure REF 1200
configure HPFR/2 COVER2
read HPFR/2 controller configuration
read preamplifier module configuration
read BIS from HPFR/2 module C1 ... done
read BIS from HPFR/2 module P1 ... done
read BIS from HPFR/2 module P2 ... done
read BIS from HPFR/2 module P3 ... done
read BIS from HPFR/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.

Edit Configuration 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

< Previous Next > Cancel

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

Summary

CONFIGURATION INFORMATION

Path : /opt/topspin/conf/instr/spect/uxnmr.info
 Date : Wed Jun 28 13:00:10 2017
 Release : TopSpin 4.0.0.b.12
 Installed in : /opt/topspin
 Host : BladeEpu
 OS : CentOS Linux release 7.2.1511 (Core)
 CPU : Intel(R) Core(TM) i7-4700EQ CPU @ 2.40GHz (8 cores at 1703 MHz with Hyperthreading)
 User : root (root)
 System : Avance Neo 400 NMR spectrometer
 1H-frequency : 400.13 MHz
 Description : CAB AV4 400 MHz BASIC
 Bruker Order : 10250092
 Configured in: BladeEpu:/opt/topspin/conf/instr/spect

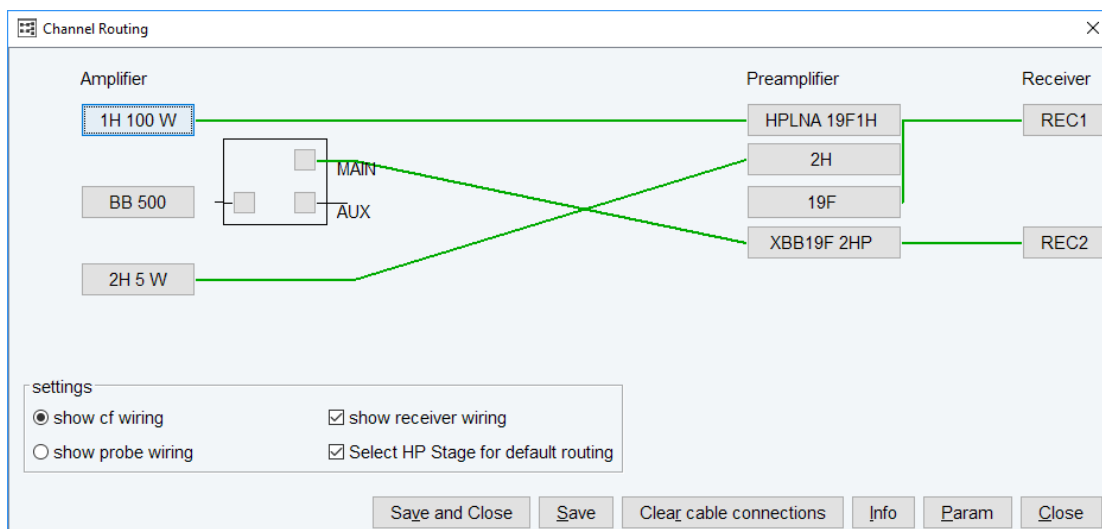
AQ-Rack:
 - EPU: AV4 EPU Embedded Processing Unit H153448/00055 ECL 01.00
 - TRX 1200: AV4 TRANSCEIVER 1200 Z148391/00178 ECL 01.03
 Location: Rack 1 Slot 1
 Connection: at IP 192.168.180.14 via PCIe #3
 Devices: MID at mtd1, DRX at /dev/bbu/drx3.5, RTD at /dev/bbu/rtd3.4
 - FCube1
 - TRX 1200: AV4 TRANSCEIVER 1200 Z148391/00177 ECL 01.03
 Location: Rack 2 Slot 2
 Connection: at IP 192.168.180.18 via PCIe #4
 Devices: MID at mtd4, DRX at /dev/bbu/drx4.5, RTD at /dev/bbu/rtd4.4
 - FCube2
 - GTU: AV4 GT-CONTROLLER UNIT Z148392/00048 ECL 01.00
 Location: Rack 6 Slot 6
 Connection: at IP 192.168.180.38 via PCIe #9
 Devices: MID at mtd7, RTD at /dev/bbu/rtd9.4, GPROC at /dev/bbu/gproc9.7
 Sequencer: GCube, TCube
 - GCube1
 - TCube1
 - PSM-A: AV4 PSM-A Z149510/00066 ECL 01.02
 - RACK: AV4 AQS CHASSIS Z149500/0057 ECL 00.01
 - PSM-48V: AV4 PSM-48V Z149550/0111 ECL 00.00
 - PSM-D: AV4 PSM-D Z149520/0059 ECL 00.01
 - FANTRAY: AV4 AQS FAN TRAY Z149501/0056 ECL 00.00
 - REF 1200: AV4 REFERENCE 1200 Z148270/00066 ECL 01.02
 - HPPR/2 COVER2: HPPR/2 Cover2 Z124567/02083 ECL 00.03
 HPPR2: - HPPR/2 preamplifier connected via AqRack
 Type : HPPR/2
 Controller: Cover/2, with DRU Application firmware = c.
 no LED display for tuning and matching
 Module 1 : HPLNA 19F1H (virtual 50 Ohm reference: 100.0%/0.1deg, reflection meter)
 PN=Z103203, SN=00648 from 20161118
 Module 2 : 2H
 PN=Z003471, SN=00306 from 20161026
 Module 3 : 19F
 PN=Z003493, SN=00213 from 20161017
 Module 4 : XBE19F ZHP
 PN=Z106984, SN=00237 from 20161216

Print Next > Cancel

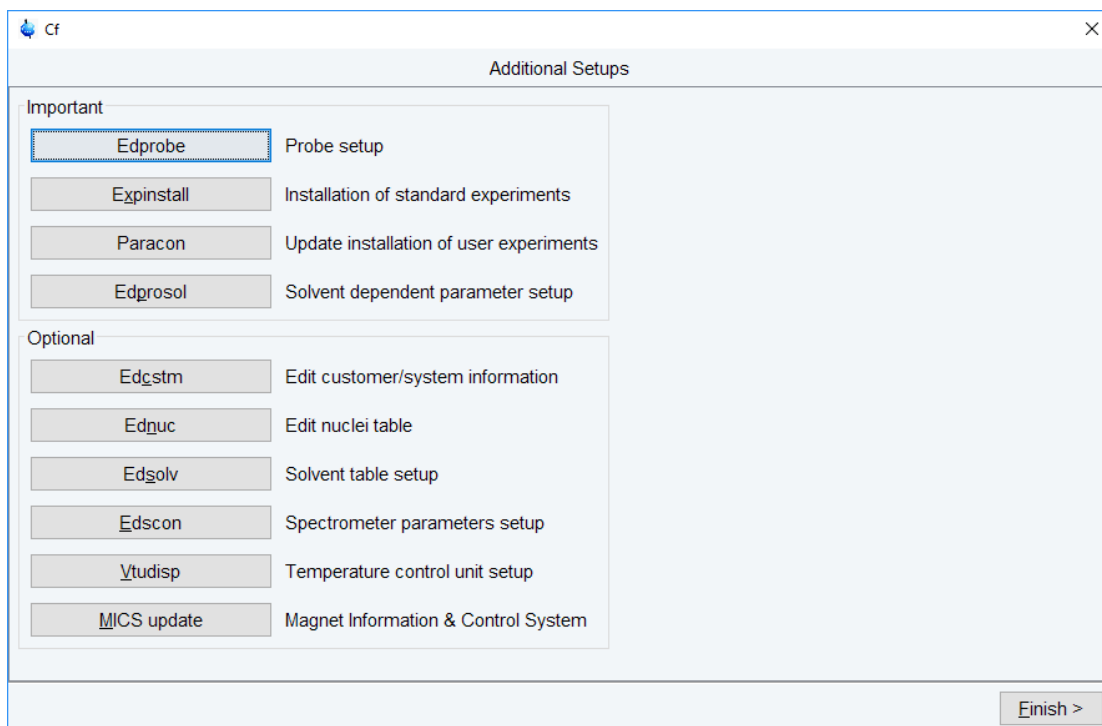
Spectrometer Configuration Commands



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



- Click **Close**. The Additional Setups window will be displayed.

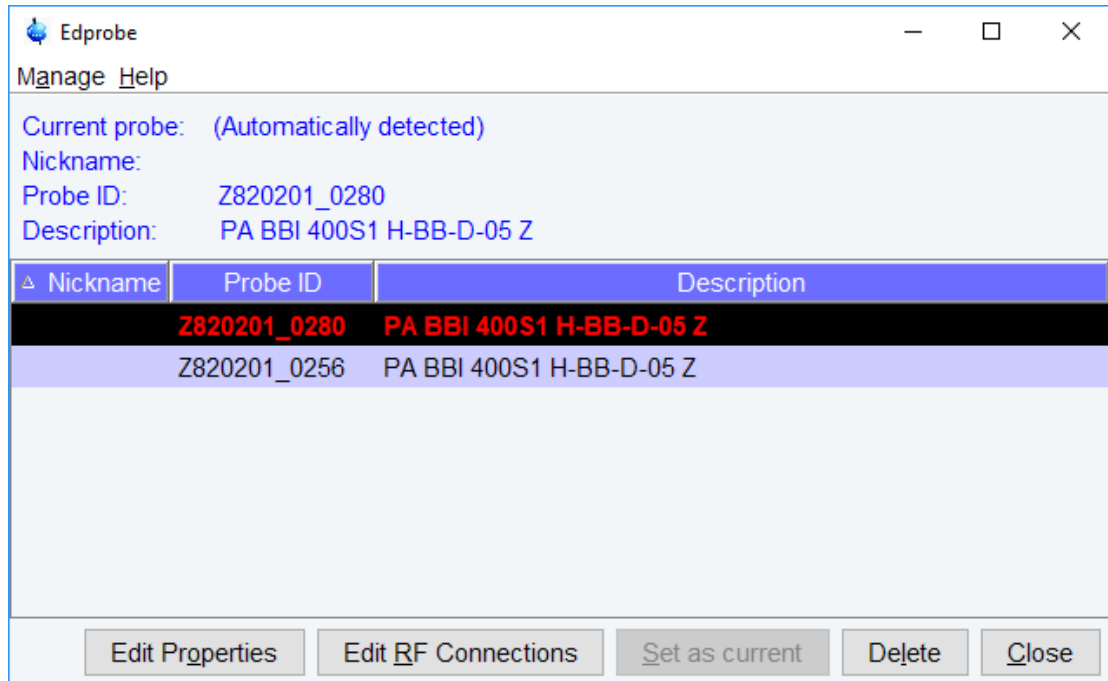


- **Note:** The most important next configuration steps are **Edprobe**, **Expinstall** and **Edprosol**.

Edprobe

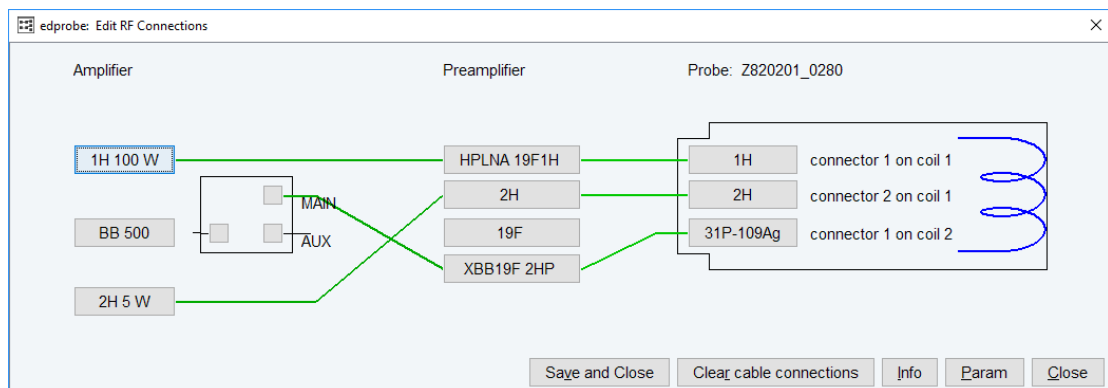
- Click **Edprobe**. The Edprobe window will be displayed.

Spectrometer Configuration Commands



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

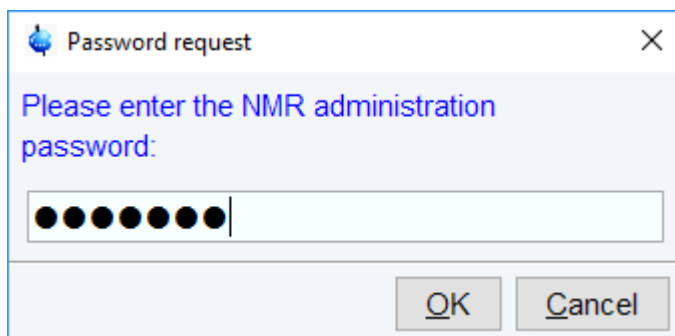
- Click **Edit Properties** to check or set the properties. Click **Close**. The probe RF connections will be displayed.



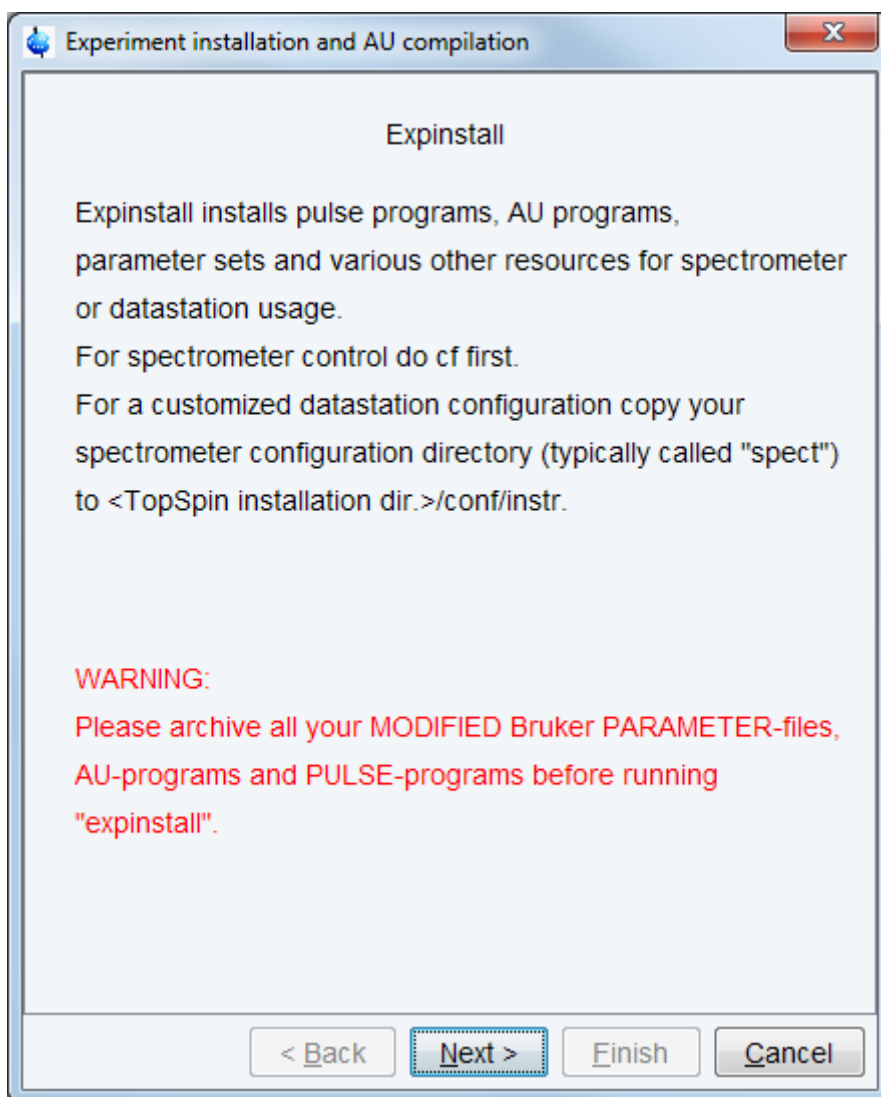
- Check and correct them, if necessary. Click **Save and Close** or **Close**.

Expinstall

- Click **Expinstall**. A Password request window is displayed.



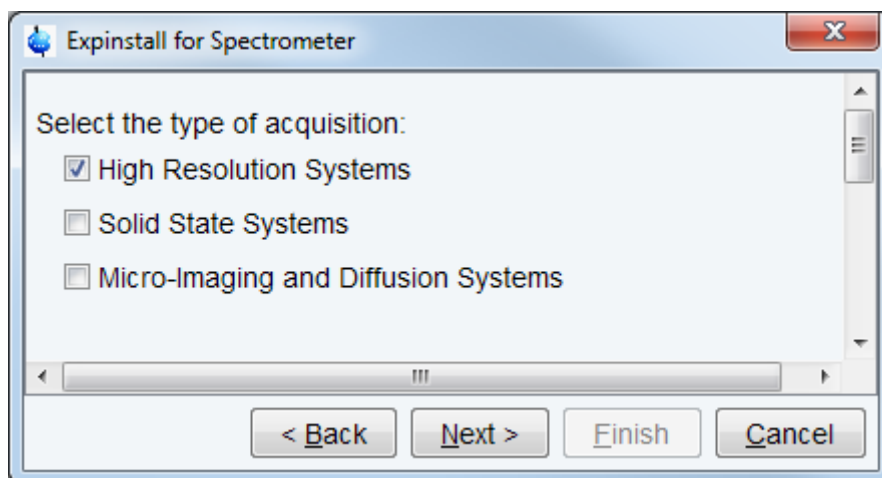
- Enter the NMR administration password to display the first Expinstall window.



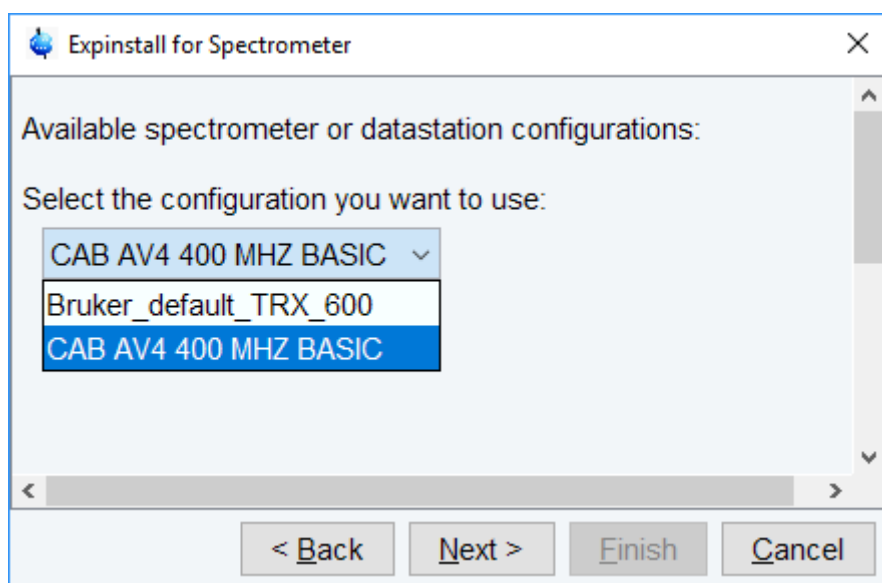
- Click **Next**, if there are no modified Bruker-Parameter files, AU-programs and Pulse-programs or files and programs are archived in a different directory. Individual Parameter files, AU-programs and Pulse-programs with different names to the original Bruker files will not be affected during the installation.

Spectrometer Configuration Commands

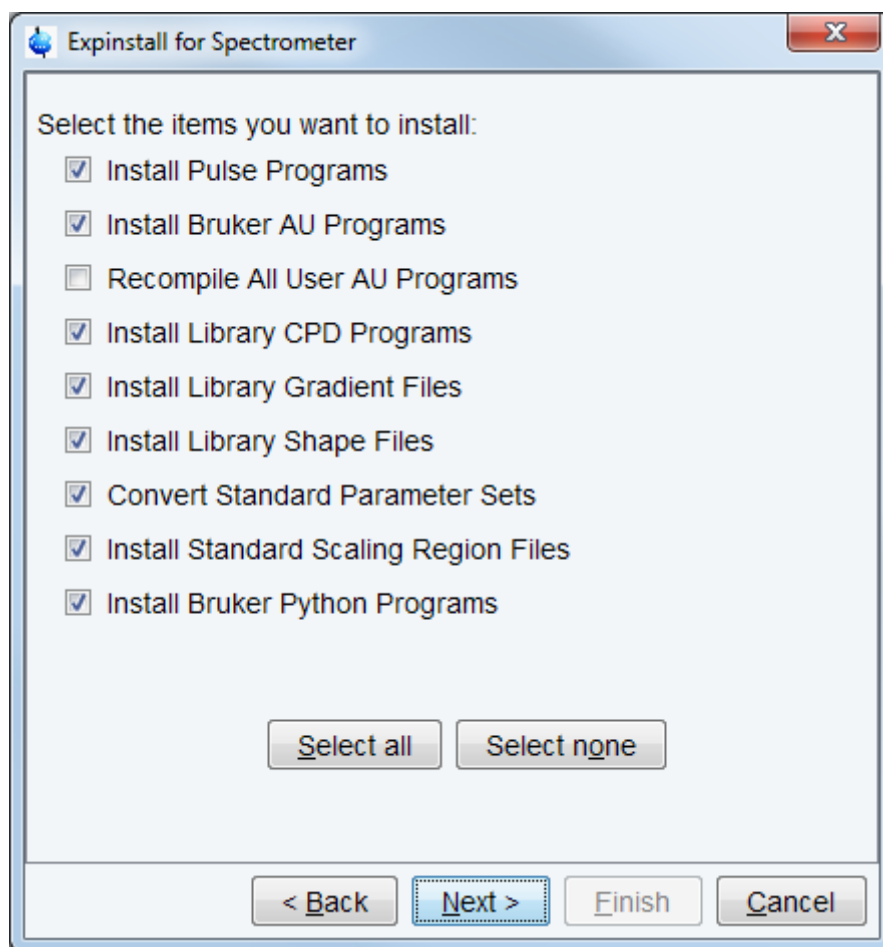
- In the next window select the type of acquisition. In the example a High Resolution System has been checked.



- Click **Next**.

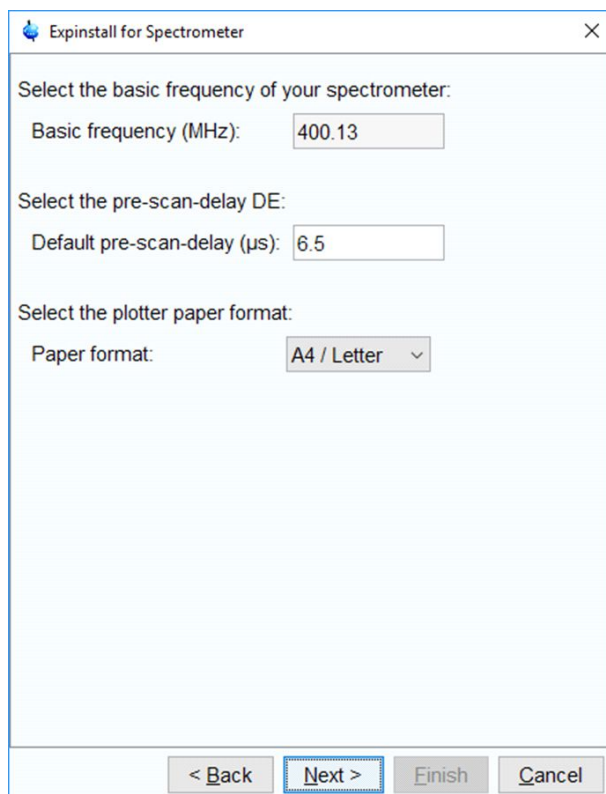


- Select the spectrometer or data station configuration for **expinstall**. Here the **CAB AV4 400 MHZ BASIC** has been selected. If this window is not displayed, then TopSpin has found only one valid configuration, namely the one for the current spectrometer, and immediately continues with the next 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**.



- 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**.

Spectrometer Configuration Commands



Expinstall for Spectrometer

Select the basic frequency of your spectrometer:

Basic frequency (MHz): 400.13

Select the pre-scan-delay DE:

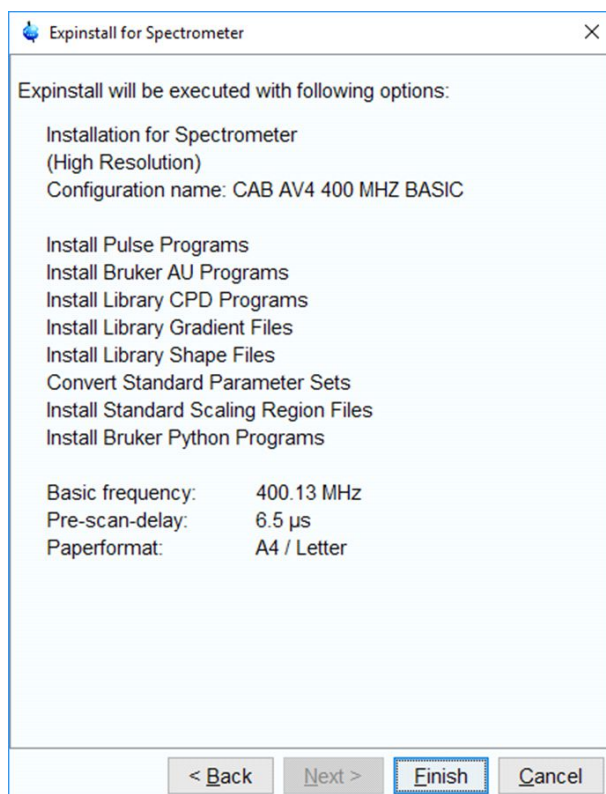
Default pre-scan-delay (μ s): 6.5

Select the plotter paper format:

Paper format: A4 / Letter

< Back Next > Finish Cancel

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



Expinstall for Spectrometer

Expinstall will be executed with following options:

Installation for Spectrometer
(High Resolution)
Configuration name: CAB AV4 400 MHZ BASIC

Install Pulse Programs
Install Bruker 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

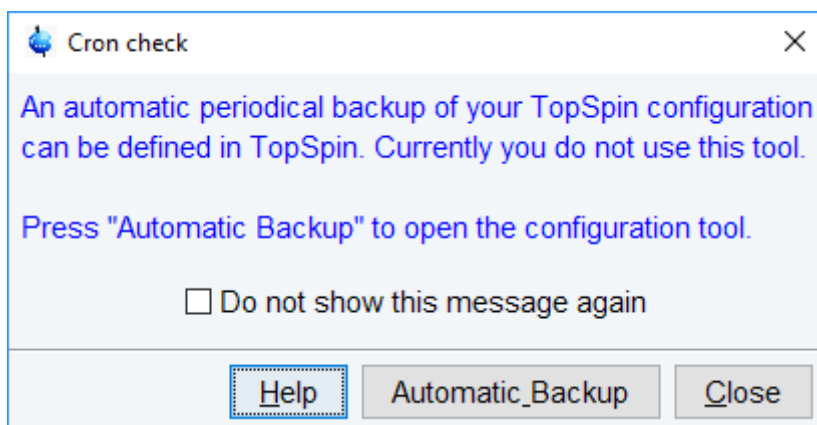
Basic frequency: 400.13 MHz
Pre-scan-delay: 6.5 μ s
Paperformat: A4 / Letter

< Back Next > Finish Cancel

- 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.



- Click **Automatic Backup** to open the NMR Save window.

NMR_Save

Save installation files | Restore installation files | Save user files | Restore user files

Save installation specific files.

Installation specific files are collected and stored into a compressed file. This compressed file can be used 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\TopSpin4.0.0.b.12\nmr_backup Browse

Overwrite existing backup file: ☐

Installation to be saved (TopSpin home): C:\Bruker\TopSpin4.0.0.b.12 Browse

Spectrometer configuration (e.g. spect): Bruker_default_TRX_600

Display default information: ☒

Display additional information: ☐

Execute "Save installation specific files" periodically Automatic Backup

Log:

Save 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 with nmr_save.

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

Note: The command box cannot be edited!

New periodical

Job

Command: `.nmrsave -date -path "C:\Bruker\TopSpin4.0.0.b.12\nmr_backup" -source "C:\B`

Description: `Execute NMR_SAVE`

Execution scope: `TopSpin (requires authentication)`

Options

☒ Off-schedule execution

☒ Direct execution

Rules

Minute of the hour	from: 26	to: --- Ignore ---	+	-
Hour of the day	from: 16	to: --- Ignore ---	+	-
Day of the month	from: 28	to: --- Ignore ---	+	-
Month of the year	from: *	to: --- Ignore ---	+	-
Day of the week	from: *	to: --- Ignore ---	+	-

OK Cancel

- Click **OK** and enter the NMR administration password.
- In the NMR Save window, click **Save**. The compilation of an AU program 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.

Spectrometer Configuration Commands

edprosol

File Edit View Help

Saved Observe and Saved Decouple Prosol Parameter Set for:

Probe: Z820201_0280 PA BBI 400S1 H-BB-D-05 Z Select... Solvent: generic

Observe: 1H Nucleus: 1H

Observe Comment: Default 1H obs 400 Decouple Comment: Default 1H dec 400

90 deg. Pulses HR Square Pulses HR Shape Pulses Others

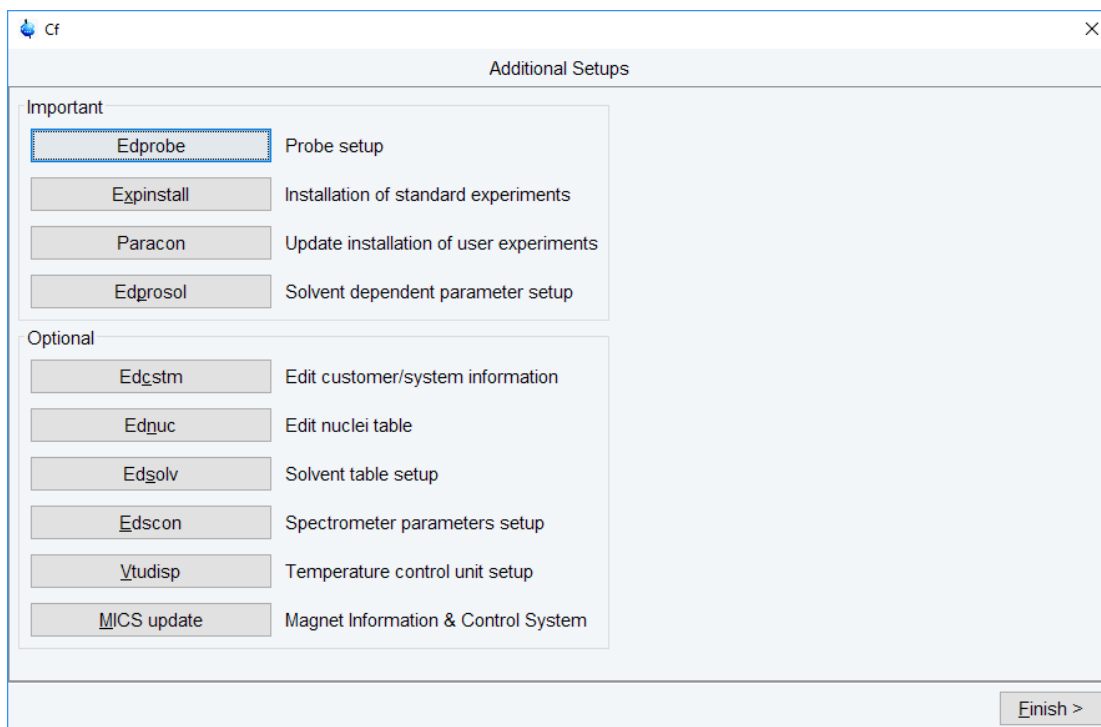
Observe				Decouple			
Nucleus	Pulse Width[μs]	Power[W]	Set	Pulse Width[μs]	Power[W]	Set	Nucleus
1H	10.00	6.3096		10.00	6.3096		1H
2H@1	280.00	2.9992		280.00	2.9992		2H@1
2H@2	0.00	0.0000		0.00	0.0000		2H@2
6Li	0.00	0.0000		0.00	0.0000		6Li
7Li	0.00	0.0000		0.00	0.0000		7Li
9Be	0.00	0.0000		0.00	0.0000		9Be
10B	0.00	0.0000		0.00	0.0000		10B
11B	0.00	0.0000		0.00	0.0000		11B
13C	15.00	80.910		15.00	80.910		13C
14N	0.00	0.0000		0.00	0.0000		14N
15N	30.00	104.95		30.00	104.95		15N
17O	0.00	0.0000		0.00	0.0000		17O
21Ne	0.00	0.0000		0.00	0.0000		21Ne
23Na	0.00	0.0000		0.00	0.0000		23Na
25Mg	0.00	0.0000		0.00	0.0000		25Mg
27Al	0.00	0.0000		0.00	0.0000		27Al
29Si	0.00	0.0000		0.00	0.0000		29Si
31P	0.00	0.0000		0.00	0.0000		31P
33S	0.00	0.0000		0.00	0.0000		33S
35Cl	0.00	0.0000		0.00	0.0000		35Cl

Last Save Print Copy to Solvent Copy to Probe Save

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 of window.



- When done, click **Finish**.

3.1.2 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 with nmr_save)

Spectrometer Configuration Commands

NMR_Save

Save installation files | Restore installation files | Save user files | Restore user files

Save installation specific files.

Installation specific files are collected and stored into a compressed file. This compressed file can be used 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\TopSpin4.0.0.b.20\nmr_backup Browse

Overwrite existing backup file: ☐

Installation to be saved (TopSpin home): C:\Bruker\TopSpin4.0.0.b.20 Browse

Spectrometer configuration (e.g. spect): remote_spect v

Display default information: ☐

Display additional information: ☒

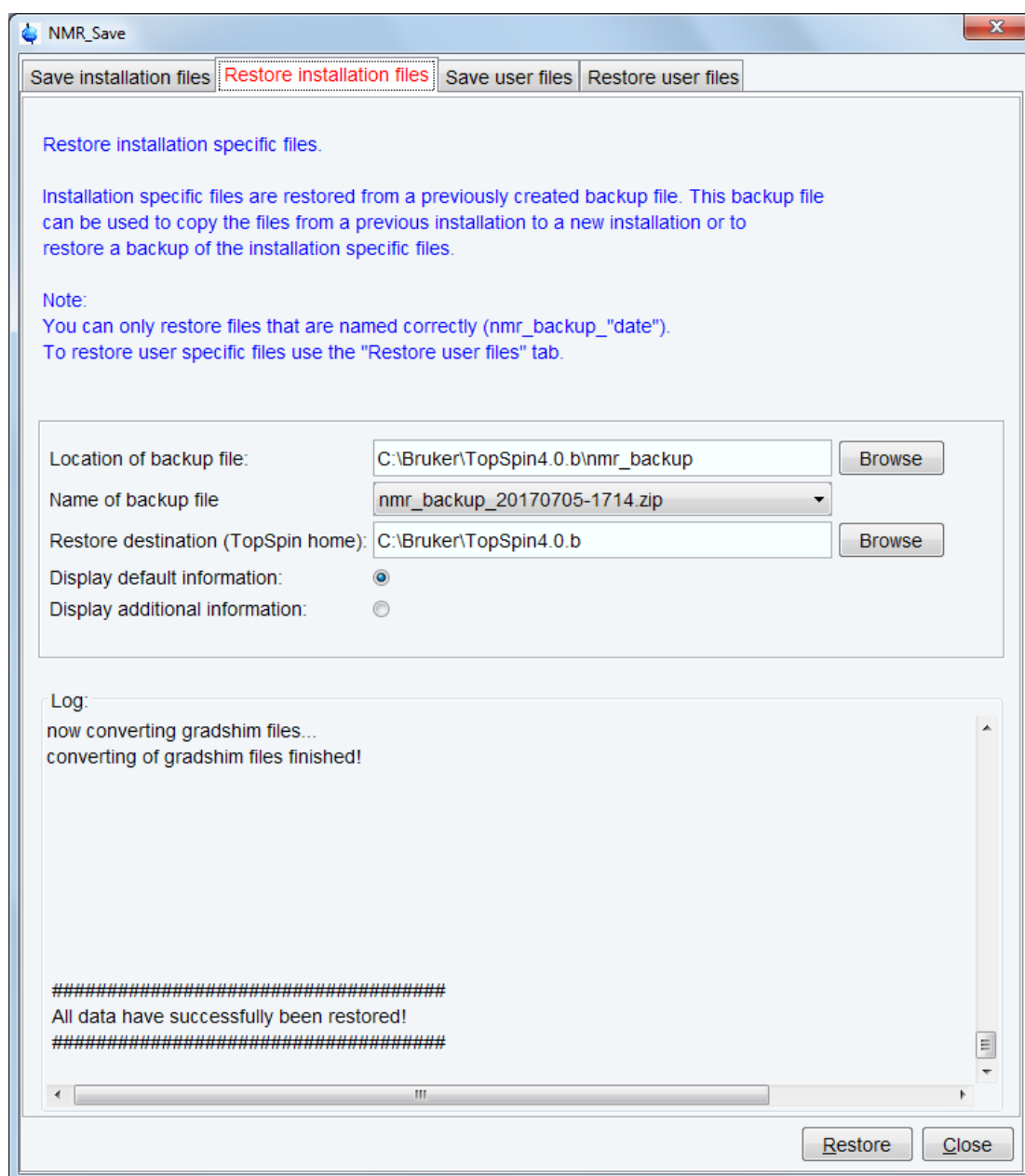
Execute "Save installation specific files" periodically Automatic Backup

Log:

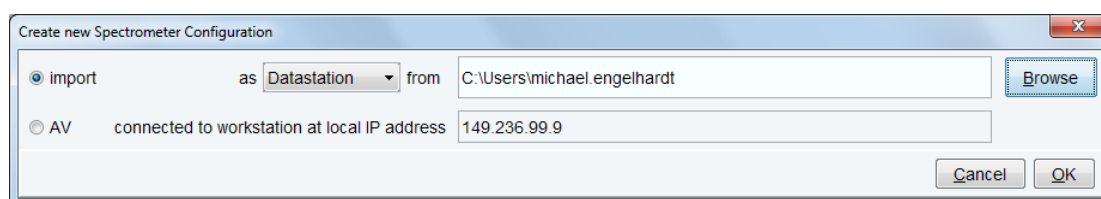
```
#####  
Backing up of NMR data was successful!  
The backup file  
  
C:\Bruker\TopSpin4.0.0.b.20\nmr_backup\nmr_backup_20170705-1714.zip  
  
has been generated!  
#####
```

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 with nmr_save)

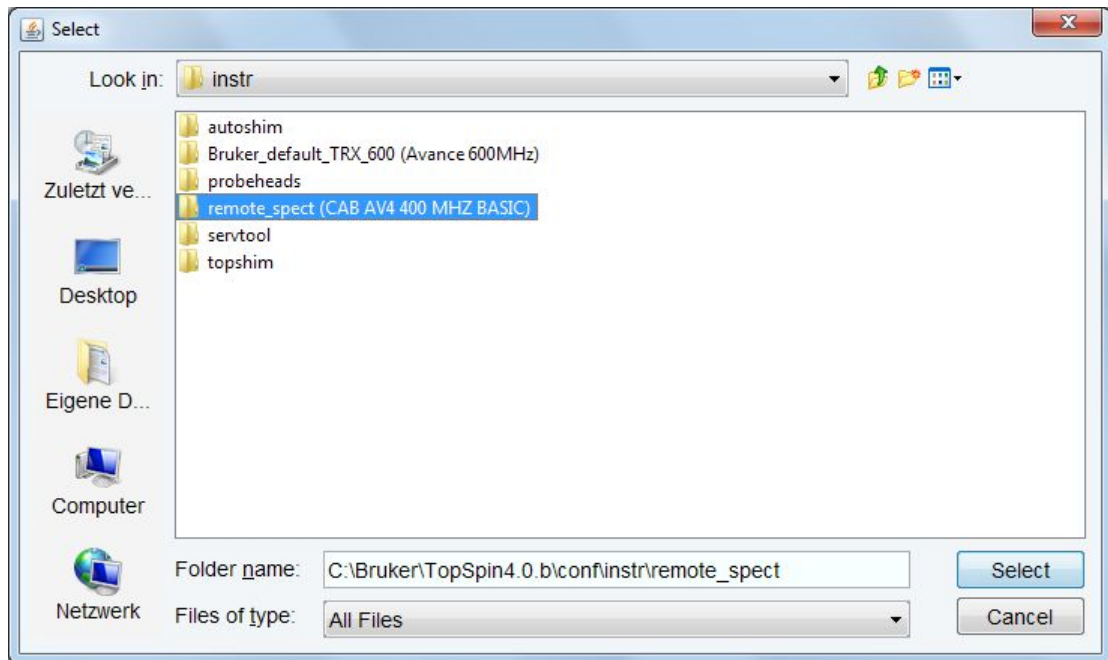


- The spectrometer configuration is now available. It will appear in the expinstall window and can be used to configure the Processing-only system.
- Click **cf** in the Configuration check window or type **cf** in the command line of the **TopSpin** main window. Enter the NMR administration password 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.

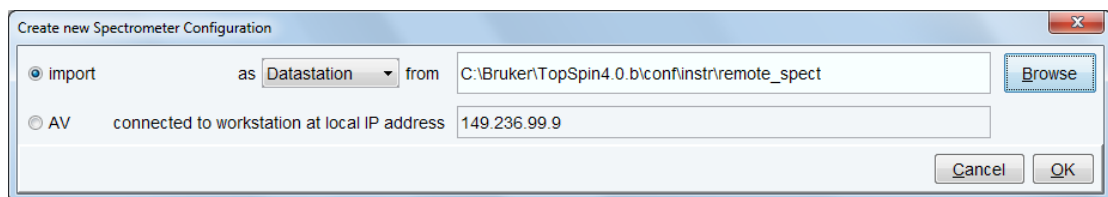


Spectrometer Configuration Commands

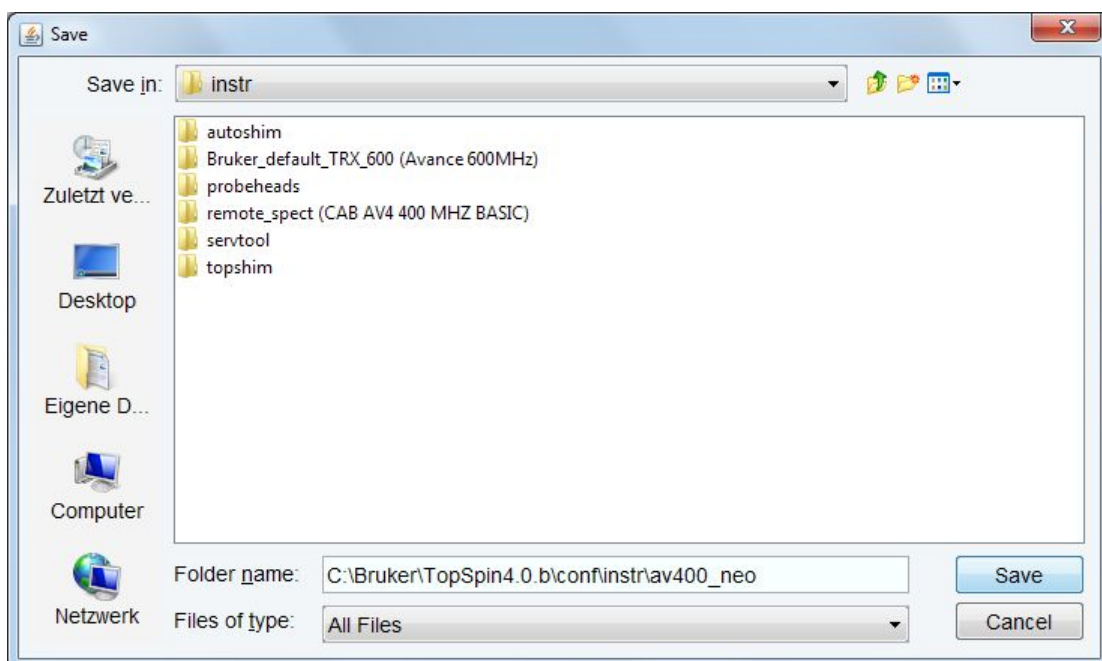
Here the configuration stored as remote_spect has been selected:



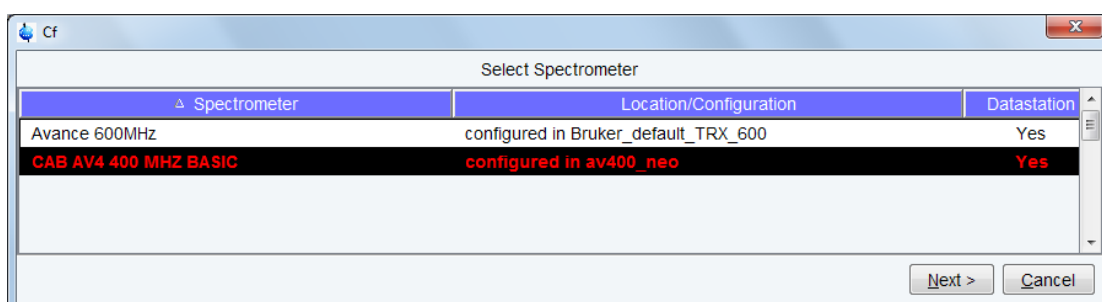
- Click **Select**, the name will be entered in the “from” field:



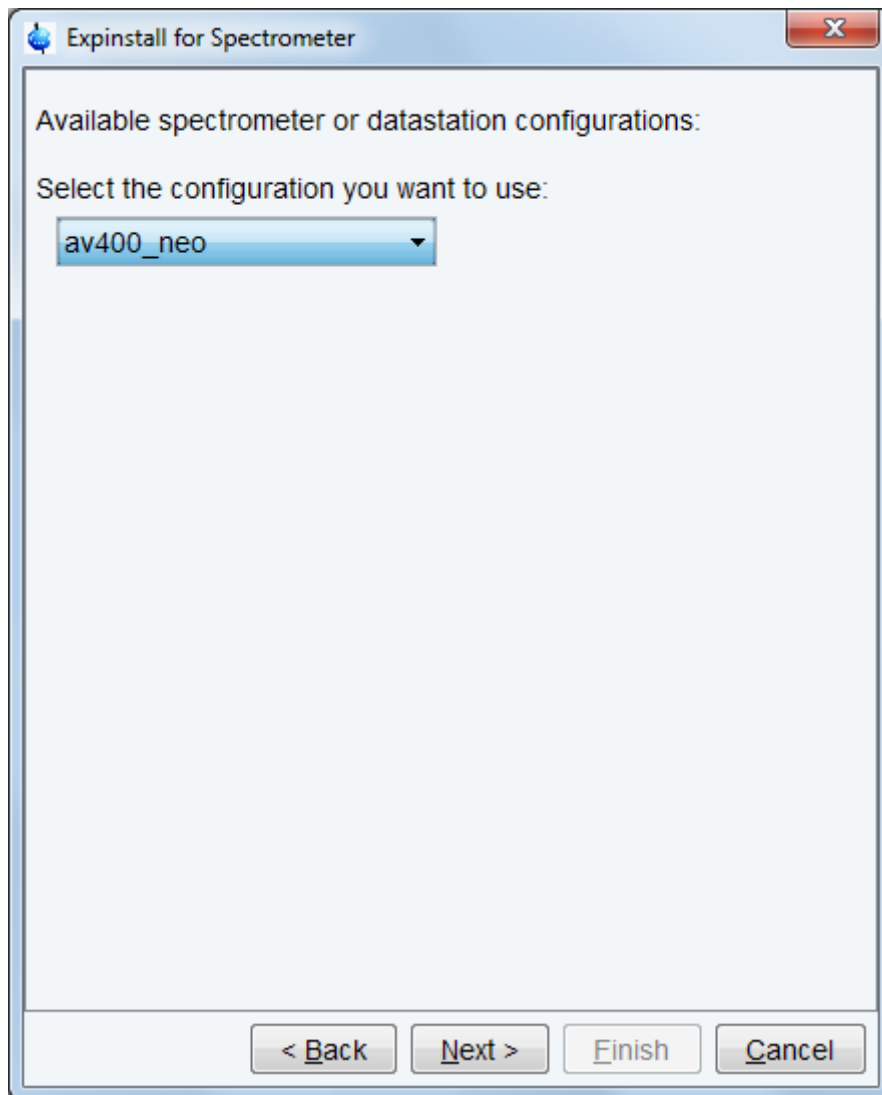
- Click **OK** and enter a suitable name for the spectrometer configuration to describe it in a meaningful way, e.g. av400_neo:



- Click **Save**.



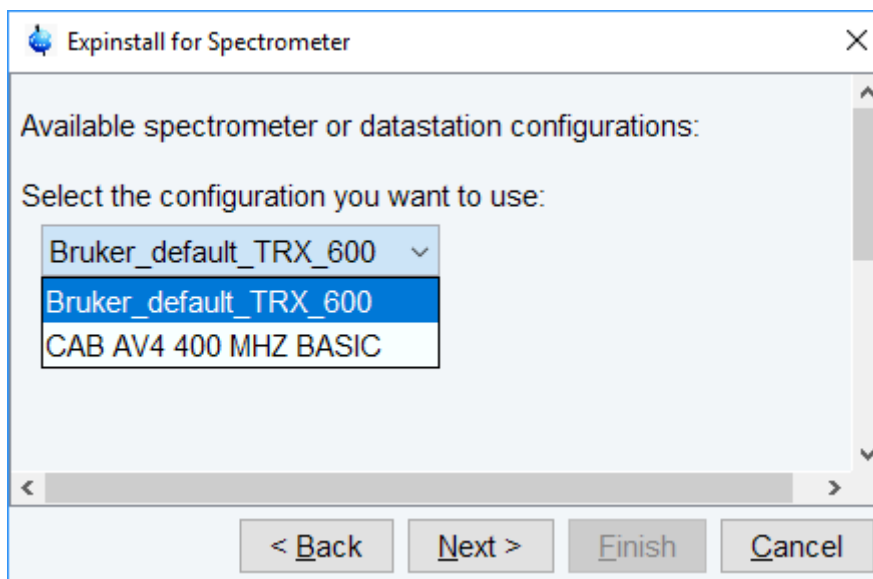
The **cf** window will be displayed. Click **Cancel** and continue with **edprobe** and **expinstall**.



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

3.1.3 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.



3.2 cortab

NAME

cortab - Setup acquisition correction table

DESCRIPTION

The command **cortab** opens a window from which amplifier and receiver correction tables for acquisition can be created (see the next figure).

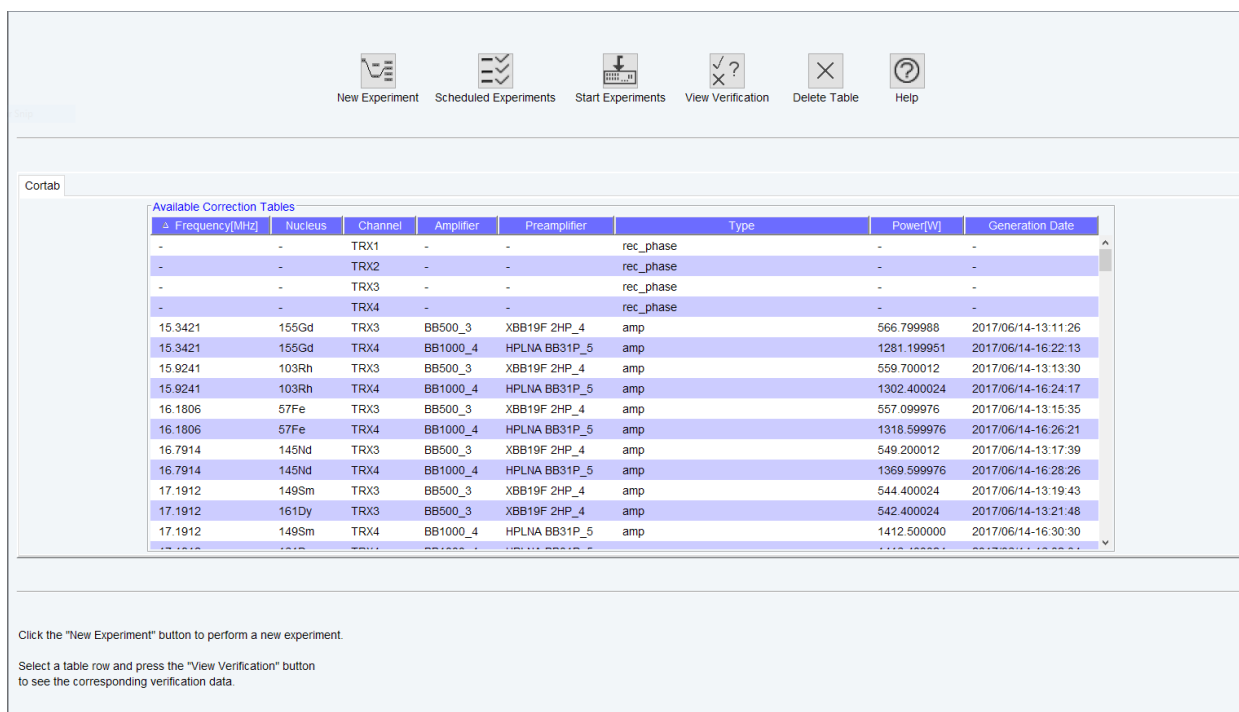


Figure 3.1: Cortab Main Window

Before this window is opened, you are prompted for the NMR Administration password. The correction tables are used to correct the non-linearity of the pulse power level versus the pulse length, and also to cancel out the influence of the receiver gain on the phase of the

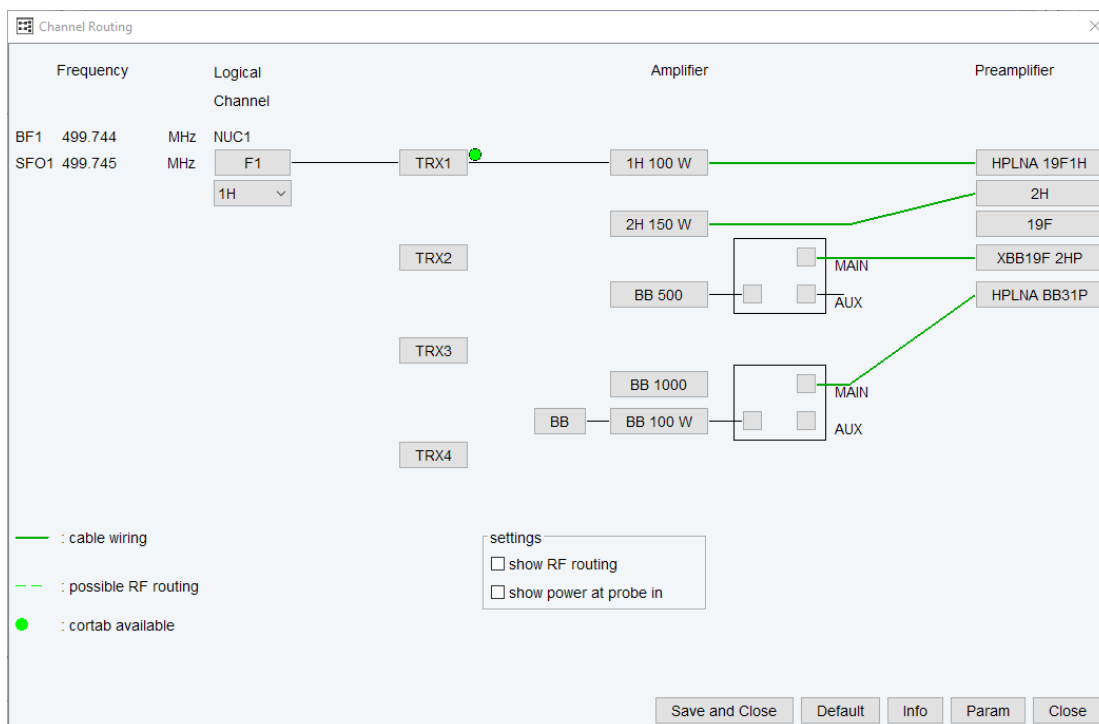
resulting spectrum. The amplifier linearization is performed in a range from -6 to above 75 dB and involves both amplitude linearization and phase correction, whereas the receiver phase correction is performed in a receiver gain range from 0.25 to above 1000. For the amplifier linearization, it is required that the amplifier output is connected to an external attenuator (the Cortab Box) which, in turn, is connected to the receiver input. The Cortab program will inform you how to connect the cables. The result of an amplifier linearization is a correction table which is a list of correction values for the pulse amplitudes and phase values. It also contains a check sum which makes it possible to detect whether the file has been changed in any way other than by Cortab.

An example of a correction table is shown in the next table.

AMP_POWER	
# power	in dB correction in %
-6.000	0.000
-5.000	-32.644
-4.000	-38.510
-3.000	-37.361
-2.000	-35.032
-1.000	-31.672
0.000	-29.128
1.000	-24.939
2.000	-22.977
.. ..	
72.000	-0.008
AMP_PHASE	
# power in dB	correction in degree
-6.000	0.000
-5.000	-0.636
-4.000	0.622
.. ..	
72.000	4.323
# real probe input power in [W] (at -6dB)	
AMP_VALUE	
60.000000	0.00
# NAME_OF_TABLE:	amp2_1H_2
# DATE_OF_ORIGIN:	2010/01/05-14:23:22.356
##END	
# hash MD5: 99 A6 79 CA 61 B1 75 1D 2E D1 6C 79 84 FD 08 2F	

Table 3.1: Correction Table

Once a correction table exists for a specific nucleus and routing, it is automatically used by acquisition commands like **zg** (this can be verified in the **edasp** window of the acquisition data set by a green dot, shown in the next figure.



If you want to check the accuracy of the amplifier linearization, Cortab allows you to do that by running a so called verification test. This test is always performed after the linearization procedure but can also be done in a separate experiment.

The receiver phase linearization ("REC Phase Linearization") is independent and may be performed even if other correction tables already exist. It creates an additional table where theoretical and experimentally determined receiver gain values are listed (rec<x>_calibration.txt).

Amplifier linearization can be performed in two possible ways:

For the linearization the amplifier output is connected to the HPPR preamplifier (as in an NMR experiment) and the preamplifier output is connected to the Cortab Box.

The signal path including the preamplifier is used for the linearization procedure because it is a better simulation of the NMR experiment.

The Cortab window allows you to set up the linearization experiments for various nuclei, perform these experiments and view the results. Correction tables that already exist are displayed in a list ('Available Correction Tables'). The list also contains a key word ('amp', 'pow' or 'rec') for each correction table, indicating whether the respective table belongs to an amplifier (amp) or a Receiver (rec). In case of an amplifier table the respective maximum amplifier output power (measured at the input of the probe) is also displayed. The 'pow' key does not represent a correction table but indicates that merely a maximum output power value is defined for a certain routing without the existence of a correction table. If an amplifier table is generated for the respective routing, 'pow' will be replaced by 'amp'. In the reverse case, if an amplifier table is deleted, 'amp' will be replaced by 'pow' provided that the amplifier table contains a valid output power value.

A regular Cortab session involves the steps listed below. Each step is specified by the corresponding button in the main Cortab window.

New Experiment

To start a new experiment the Power Check (POWCHCK) must be deactivated. Clicking this button opens a dialog box where you can define one or more Cortab experiments. Cortab experiments should be defined for each nucleus and routing that you intend to use in your

NMR measurements, an exception being the Receiver Phase Linearization which is frequency independent and needs to be performed only for one single (arbitrarily chosen) nucleus.

The following functions are available:

- BLA Power Definition without measurement (this generates an 'pow'table)
- BLA Verification
- REC Phase Linearization + Verification (this generates a 'rec' table)
- REC Phase Verification

In case a Cortab box is installed some further experiments are possible (see description of Cortab box features below).

BLA and REC experiments must be executed in two separate series because they require different hardware connections. First you must set up one series for the REC functions and execute this series (see **Start Experiments** below). Then you can set up and execute a second series for the amplifier linearization.



Please note that the Cortab correction is mainly determined by the BLA linearization (see the [Table 3.1 \[76\]](#)). This improves the quality of the resulting correction tables. The verification procedure is optional. It allows you to check the quality of the respective linearization results. It simply repeats the linearization but does not create a correction table. Instead, the existing correction table is used and the resulting amplitude and phase values are stored together with the calculated 'ideal' values in the verification files (see **View Verification** below). Thus, the verification files are directly correlated with the quality of the correction tables used.

Note that you can also run a verification procedure without doing a linearization first. This can be useful to compare the corrected with the uncorrected amplifier characteristics.

• New Experiment => Select

Opens the routing table (like **edasp**) where you can determine the appropriate hardware routing for the chosen experiment. In case of a REC phase correction, however, the complete routing is determined by the software and no user interaction is necessary. After clicking the **SAVE** button, the selected experiment (function) is added to the scheduled series. Instructions are displayed regarding the required hardware connections. Carefully follow the outlined instructions (e.g. to find the preamplifier which must not be used) to prevent damaging the hardware units of the spectrometer. In one Cortab series, you can add:

- experiments for various nuclei
- one nucleus with various routings
- linearization and verification

You cannot, however, set an REC correction and a BLA linearization in one series because they require different hardware connections. After having scheduled the experiment, you are prompted for the maximum amplifier output power. This value corresponds to the power (in Watts) measured at the output of the respective HPPR preamplifier module (i.e. at the input of the probe) when you are pulsing with maximum power and using the routing you have already specified. If this power is already known by the system, it will be displayed, otherwise zero is shown. A valid output value is crucial for any kind of output power limitation (e.g. to reduce the possibility of probe damage) of the acquisition software.

However, if the respective power value is not known, you can either use zero (ignoring the power limitation possibilities of the acquisition software) or measure it with a wattmeter. In the following dialog window (Quick Experiment Setup) you will be able to (optionally) select a variable number of additional nuclei (together with their amplifier output power, as mentioned above) that are to be linearized with the same routing as the

experiment you have already determined. This saves time because you only need to set up the routing table once, even if you want to generate a linearization table for multiple nuclei. The nuclei are selected by applying a user defined search pattern using the tokens ',' (separator) and '-' (nucleus range); for example, the search pattern "1H, 31P-29Si" would select both 1H and all the nuclei in the frequency range between 31P and 29Si. The system automatically stores the last ten search patterns so that they can be reused for further setups (e.g. with a different routing). It is also possible to edit the search patterns by editing the respective file *quick_exp_setup.txt* in the *cortab/etc* directory.

- **New Experiment => Finish**

Closes the dialog box and returns to the main Cortab window

Start Experiments

Clicking this button executes all experiments in the currently scheduled series. They are performed in the order in which they appear in the list. If a correction table already exists for the current experiment, it is renamed by appending the current date to its name. Its file will be overwritten if a further experiment with the identical setting is started at the same date. Please note that you must, temporarily, switch off the peak power limitation in order to run Cortab. To do that, run **cf** deactivating POWCHK. After Cortab has finished, run **cf** again activating POWCHK. At the beginning of the linearization, you may be prompted for the total external attenuation used. Cortab uses this value to generate scaled correction tables.

Each linearization experiment involves the following steps:

- A receiver gain test

This determines the optimum receiver gain for the current experiment. If this is successful, the experiment continues with the next step. If this is not successful, the experiment aborts and an information window will appear telling what to do. Just follow the instructions.

- The actual Cortab experiment, for example the BLA amplifier linearization.

In principle, you are ready now. The correction table has been created and it will automatically be used by the acquisition. If, however, you want to check the Cortab result, you can do that with the **View Verification** button (or - for a quick preview - by simply moving the mouse over the respective table entry in the Cortab Main Window), or simply double-click on an entry of the 'Available Correction Tables' list as described below.

View Verification

This button is only active when an entry is selected in the Available Correction Tables list of the Cortab window. Clicking this button (or double-clicking a list element) will then open a window where the results of the selected experiment are shown. The window consists of the following fields:

- Date of the experiments
- A list of dates at which Cortab experiments were performed.
- Name of the experiments

When a date is selected, a list of result filenames created at that date is displayed. The respective file extensions denote the creation time of each test. For example:

Amp_Power_res<1048>

Amp_Phase_res<1048>

When you click an entry, the contents of the corresponding file are shown. Note that files like Amp_Power_res do not contain the actual correction values but rather the theoretical "perfect" values and the experimental values acquired on the base of the existing correction table. The smaller the difference between theoretical and experimental values, the better is the corresponding correction table. Therefore, the result files contain two simple statistical

key values which make it easier to estimate the overall quality of the correction file (average deviation and standard deviation from the theoretical values). The smaller these values are, the better is the correction table used for the verification.



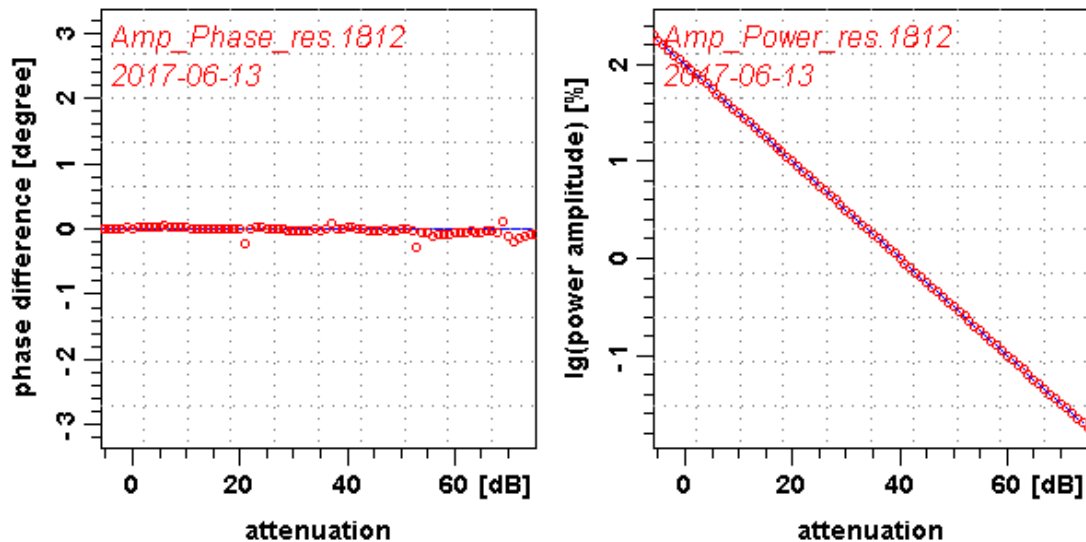
Please note that verification files can be deleted to save disk space without affecting the correction tables they correspond to.

- A data field where the contents of the selected file are displayed.

Furthermore, the following push buttons are available:

- **View Graph**

Opens a window with graphical and printable representation of the Cortab result.



- **OK**

Closes the **View Graph** window and returns to the main Cortab window.

Scheduled Experiments

Clicking this button opens a dialog box where the currently scheduled experiments are shown. The dialog box contains the following buttons:

- **Remove All** : removes all experiments from the scheduled list.
- **Remove** : removes the selected experiment from the list.
- **OK** : exits the dialog box and returns to the main Cortab window.

Cortab experiments use two spectrometer channels simultaneously:

- The pulse channel: selected by the user in the Cortab New Experiment, i.e. the channel that is routed to the amplifier) that is being corrected.
- The observe channel: automatically selected by the Cortab program. If the pulse channel is f1, the observe channel is f2. Otherwise the observe channel is f1.

USING A CORTAB BOX

If a Cortab box is installed some further experiments are available:

- **BLA Linearization + Verification + Power Scaling** (generates the 'amp' table and measures the maximum output power of the amplifier).

- BLA Power Measurement (measures the maximum output power of the amplifier).

Additionally, in the Cortab box Routing Scheme in the New Experiment Window (see the next figure), it has to be determined which amplifier is connected to which input of the Cortab box. After that it is possible to set up and schedule experiments for all amplifiers selected in the Cortab box Routing Scheme since the Cortab box will switch the amplifier outputs automatically for each experiment.

New Experiment

Cortab

Experiment Choice

Experiment	Type
BLA Linearization + Verification + Power Scaling	CORTAB
BLA Power Definition Without Measurement	CORTAB
BLA Power Measurement (removes cortab table)	CORTAB
BLA Verification	CORTAB
REC Phase Linearization + Verification	CORTAB
REC Phase Verification	CORTAB

CortabBox Routing Scheme

Amplifier: 1H100 (BLNK 1) is connected to input 1 (optionally via Hppr)

Amplifier: BB500 MAIN (BLNK 3) is connected to input 2 (optionally via Hppr)

Amplifier: 2H150 (BLNK 2) is connected to input 3 (optionally via Hppr)

Amplifier: BB1000/100 MAIN (BLNK 4) is connected to input 4 (optionally via Hppr)

Use CortabBox: ☒

Cable Loss Correction

Use cable loss correction table: ☐

Please select an experiment and click the 'Select' button.
Click 'Finish' to return to the main window.

If you wish to use the CortabBox please activate the 'Use CortabBox' button and assign the desired amplifier outputs to the respective inputs of the CortabBox according to the actual wiring. The software will then allow you to schedule all experiments that can be performed using the CortabBox.

Select **Finish**

Figure 3.2: Cortab - New Experiment

SEE ALSO

[zg \[► 195\]](#)

3.3 edcstm

NAME

edcstm – edit customer / system setup

DESCRIPTION

The command **edcstm** opens a window where customer / system information can be edited. This window can also be opened from **Manage | Spectrometer | Experiment / Parameters | Edit customer / system information (edcstm)**.

The information entered here is used in preparation of the spectrometer and / or accessory acceptance protocols. All general information provided in these reports is taken from **edcstm** window.

Customer Info	
Customer Name*	John Doe
Operator Name	Johanna Doe
Company*	Example Company
Address	My street 99
Postal Code	12345
City*	Big Town
Country*	Gondwana
Phone Contact Customer*	+123456789
Mobile	
Fax	
E-Mail*	John.Doe@example.company.com
Bruker Info	
Engineer*	Bruker Engineer
Office*	Rheinstetten
Central Hotline Phone*	+497215166155
Central Hotline E-Mail*	helpdesk.bbto.de@bruker.com
System Info	
Order No.*	10264764
Contract Service No.	if applicable
System Type	CAB AV4 500 MHZ EXT
Console Part and Serial No.	H03128T2/0665
Coil	BZH0185070E03
Dewar	D315-54-6856
Shim System Offset*	792
Shim System Angle	n/a
CryoProbe Order No.	if applicable
Location	Room XYZ
Register No.	internal customer number
* Required Fields	
<input type="button" value="Save"/> <input type="button" value="Cancel"/> <input type="button" value="Close"/>	

It contains three sections of information:

1. Customer Info

Customer Name*, Operator Name, Company*, Address, Postal Code, City*, Country, Phone Contact Customer*, Mobile, Fax and E-Mail*

2. Bruker Info

Engineer*, Office*, Central Hotline Phone*, Central Hotline E-Mail*

3. System Info

Order No. *, Contact Service No., System Type, Console Part and Serial No., Coil, Dewar, Shim System Offset*, Shim System Angle, CryoProbe Order No., Location, Register No.

It is advisable to enter the information as precisely as possible. The content will be used in spectrometer acceptance protocols, accessory installation protocols, repair and maintenance protocols etc. The file is also copied into the **savelogs** archive to provide help desk functions with system and contact information.



Please note that the fields marked with * are required fields. Some information will automatically be taken from the installation procedure (command [cf \[51\]](#)).

To edit this information the NMR administration password is required.

OUTPUT FILES

- <tshome>/conf/global/edcstm.info

3.4 ednuc

NAME

ednuc - Edit nuclei table

DESCRIPTION

The command **ednuc** opens the nuclei table showing a list of nuclei with their names, receptivity, spin and basic frequency (see the next figure).

Nucleus	Name	Receptivity (rel. 13C)	Spin	Frequency (rel. 1H)
1H	Hydrogen	5680.0	1/2	400.13
2H	Deuterium	0.00821	1	61.422391232
3H	Tritium	1.0E-9	1/2	426.794559166
3He	Helium	0.00326	1/2	304.816781268
6Li	Lithium	3.58	1	58.883474912
7Li	Lithium	1540.0	3/2	155.505710936
9Be	Beryllium	78.8	3/2	56.225519357
10B	Boron	22.1	3	42.988598755
11B	Boron	754.0	3/2	128.377605166
13C	Carbon	1.0	1/2	100.612768526
14N	Nitrogen	5.69	1	28.90493105
15N	Nitrogen	0.0219	1/2	40.544820786
17O	Oxygen	0.0611	5/2	54.243451394
19F	Fluorine	4730.0	1/2	376.498366214
21Ne	Neon	0.0359	3/2	31.587446585
23Na	Sodium	525.0	3/2	105.84198747
25Mn	Manganese	1.54	5/2	24.494498125

Figure 3.3: ednuc - Nuclei table

The buttons of the nuclei table have the following functions:

- **Add/Edit**
Edit a table entry or add a new one. A dialog is opened (see the next figure) where you can enter or change values. If you enter a new **Nucleus**, an entry is added to the list, otherwise the current entry is edited.
- **Delete**
Delete the selected entry/entries.
- **Restore**
Restore the original nuclei table. All changes you made will be undone. This must be done once, if you have changed the basic frequency with **cf**.
- **Save**
Save any changes the nuclei table. You will be prompted for the NMR administration password.
- **Close**
Close the nuclei table.

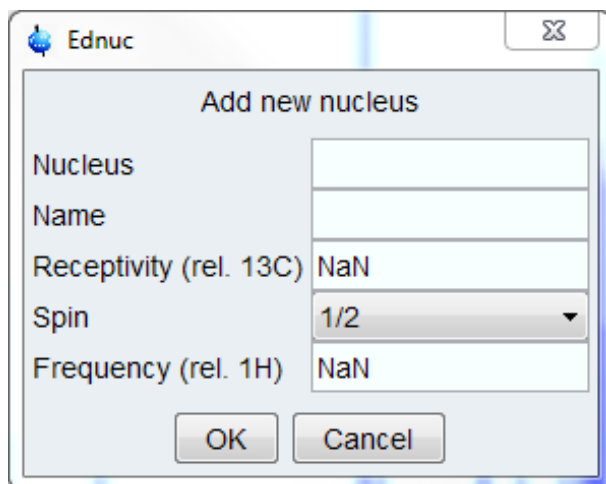


Figure 3.4: ednuc - Add new nucleus



Note that double-clicking a table entry also opens the dialog you see in the figure above but only allows you to change the frequency.

INPUT FILES

- <tshome>/conf/instr/<instrum>/
 - *nuclei* - nuclei table
- <tshome>/exp/stan/nmr/lists/
 - *nuclei.all* - complete nuclei table (input and **Restore**)

OUTPUT FILES

- <tshome>/conf/instr/<instrum>/
 - *nuclei* - nuclei table

SEE ALSO

[edsolv](#) [▸ 91], [e](#) [▸ 144][dprobe](#) [▸ 144], [edlock](#) [▸ 109], [edprosol](#) [▸ 84]

3.5 edprosol

NAME

edprosol - Edit probe and solvent dependent parameters

DESCRIPTION

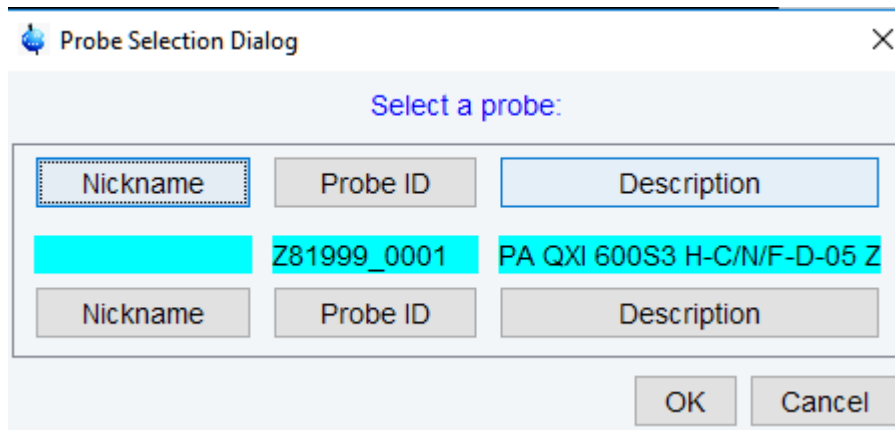
The command **edprosol** opens a dialog box in which you can set the probe and solvent dependent (Prosol) parameters (see the next figure).

This is typically done during the installation of your spectrometer for all probes and solvents you want to use. However, you can also run **edprosol** again at a later time to set the Prosol parameters for additional probes and/or solvents.

Setting the Prosol parameters involves the following steps:

- Select the probe, solvent(s) and nucleus by clicking:
 - **Probe**
By default, the current probe (as defined with [edprobe](#) [▸ 144]) is selected. Prosol parameters must be defined for each probe separately.

To select a probe click on the **Select ...** field: a list of all available probes will be shown.



– **Solvent**

The default value is **generic**. If you keep that value, the same prosol values will be stored for all solvents. If, however, you select a specific solvent, the prosol parameters will be specifically stored for that solvent. If **getprosol** is executed and prosol parameters exist for the solvent in the dataset then these values are read, otherwise the generic values are read.

– **Observe / Decouple**

The combination of the Observe and Decouple nuclei is read from the current dataset. If one wants to set prosol values for a certain nucleus then the nucleus can be selected through the Observe / Decouple drop-down list or by directly clicking on the corresponding nucleus line.

– **Observe Comment / Decouple Comment**

This step is optional. You can enter two comment lines; for example the conditions under which the pulses/power levels have been determined (filters etc.).

–

edprosol

File Edit View Help

Saved Observe and Saved Decouple Prosol Parameter Set for:

Probe: Z859801_0005 PA QXI 500S2 H/P-C/N-D-05 Z BTO Select ... Solvent: generic

Observe: 1H Nucleus: 1H

Observe Comment: Default 1H obs 500 Decouple Comment: Default 1H dec 500

90 deg. Pulses HR Square Pulses HR Shape Pulses Others

Observe				Decouple			
Nucleus	Pulse Width[μs]	Power[W]	Set	Pulse Width[μs]	Power[W]	Set	Nucleus
1H	10.00	7.7257		10.00	7.7257		1H
2H	200.00	8.8973		200.00	8.8973		2H
13C	15.00	102.19		15.00	102.19		13C
15N	45.00	87.395		45.00	87.395		15N

Last Save Print Copy to Solvent Copy to Probe Save

Figure 3.5: Edit prosol parameters (Base View)

The above figure shows the default layout of the **edprosol** window (Base View).

The **edprosol** menu bar offers the following functions:

- **File:** contains functions for file handling
- **Edit:** contains two primary functions (amongst others):
Set Default Pulse Widths: resets pulses to the default values.
Set Default Descriptions: resets the descriptions to the default values.
- **View:** allows to toggle between two display modes: **Base View** and **Full View**. Compared to the **Base View** option the **Full View** option shows additionally the relations between the prosol parameters and the pulses used in the pulse program. The relations are stored in the assignment file that can be selected in the Pulse Assign File line.

edprosol

File Edit View Help

Saved Observe and Saved Decouple Prosol Parameter Set for:

Probe: Z859801_0005 PA QXI 500S2 H/P-C/N-D-05 Z BTO Solvent: generic

Pulse Assign File:

Observe: 1H Nucleus: 1H

Observe: 1H Decouple: 1H

Observe Comment: Default 1H obs 500 Decouple Comment: Default 1H dec 500

90 deg. Pulses: HR Square Pulses HR Shape Pulses Others

Observe					Decouple				
Nucleus	Pulse Width[μs]	Power[W]	rel	Set	Pulse Width[μs]	Power[W]	rel	Set	Nucleus
1H	10.00	7.7257	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	10.00	7.7257	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	1H
2H	200.00	8.8973	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	200.00	8.8973	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	2H
13C	15.00	102.19	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	15.00	102.19	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	13C
15N	45.00	87.395	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	45.00	87.395	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	15N
Nucleus	Pulse Width[μs]	Power[W]	rel	Set	Pulse Width[μs]	Power[W]	rel	Set	Nucleus

Figure 3.6: Edit prosol parameters (Full View, no pulse assign file selected).

edprosol

File Edit View Help

Saved Observe and Saved Decouple Prosol Parameter Set for:

Probe: Z859801_0005 PA QXI 500S2 H/P-C/N-D-05 Z BTO Solvent: generic

Pulse Assign File: /bruker/TopSpin4.0.4.b.15/exp/stan/nmr/lists/prosol/pulseassign/default

Observe: 1H Nucleus: 1H



Observe: 1H Decouple: 1H


Observe Comment: Default 1H obs 500 Decouple Comment: Default 1H dec 500

90 deg. Pulses: HR Square Pulses HR Shape Pulses Others

Observe					Decouple				
Nucleus	Pulse Width[μs]	Power[W]	rel	Set	Pulse Width[μs]	Power[W]	rel	Set	Nucleus
1H	10.00	7.7257	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	10.00	7.7257	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	1H
2H	200.00	8.8973	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	200.00	8.8973	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	2H
13C	15.00	102.19	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	15.00	102.19	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	13C
15N	45.00	87.395	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	45.00	87.395	<input type="button" value="⏏"/>	<input type="button" value="⏏"/>	15N
Nucleus	Pulse Width[μs]	Power[W]	rel	Set	Pulse Width[μs]	Power[W]	rel	Set	Nucleus

Figure 3.7: Edit prosol parameters (Full View, pulse assign file selected).

In Full View mode once a pulse assign file has been selected, the icon  allows to view the relations between the prosol parameters and the pulses used in the pulse program (column rel). If no pulse assign file has been selected, the icon  appears in this column.

In both view modes the icon  allows to calculate all power levels of all pulses that correspond to the respective observe or decouple pulse. A dialogue window opens and the user can choose to calculate all pulses of the set or only the calculated pulses:

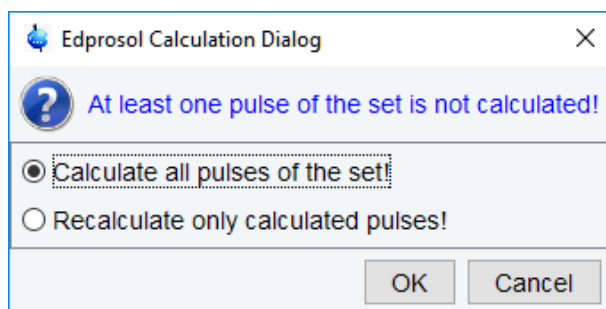


Figure 3.8: Prosol: Calculating dialog window



Calculating all pulses of the set will include also individually calibrated pulses.

View Mode for Power toggles the power levels between Watt and dB.

- **Help:** provides access to the prosol-related help files.

There are four different tabs to enter the pulses and power levels used in Bruker pulse programs:

- **90 deg. Pulses**
Shows the list of 90 deg. observe and decouple pulses.
- **HR Square Pulses**
Shows the list of square pulses (e.g. cpd pulses and roesy and tocsy spinlock pulses).
- **HR Shaped Pulses**
Shows the list of shaped pulses (e.g. selective excitation pulses, selective refocusing pulses, bandselective excitation pulses).
- **Others**
Shows some general pulses and delays that are not nucleus dependent, like the pre-scan delay DE, FILCOR etc.
FILCOR is a correction to the acqt0 value which is used by the baseopt filter. It takes into account that the excitation signals as well as the FID need some time to propagate through the cables and the transmitter or receiver, respectively. This propagation time creates an inevitable delay between the excitation and the receiving of the FID. In contrast to the value acqt0 which depends solely on the pulse program, FILCOR is a hardware correction value. Typical values are in the order of 1 µsec or less.
- The buttons on the bottom of the **edprosol** window provide functionality to save, print and copy the prosol parameters.
- To the left of the **Save** button, you will find the following buttons:
 - **Last Save**
Resets the prosol parameters to the last backup.
 - **Print**

Print the currently selected prosol parameters.

– **Copy to Probe**

Open a list of all probes. You can select the probe(s) for which you want to store the prosol parameters.

– **Copy to Solvent**

Open a list of all solvents. You can select the solvent(s) for which you want to store the prosol parameters and then click **Save** to store it.

The **edprosol** window allows you to set up a probe dependent tune file. You can do that by clicking **Edit | Edit tune file**. Probe dependent tune files are read by the command **tune .sx**.

The prosol parameters are interpreted by the **getprosol** command that copies them to the corresponding acquisition parameters. The relations between prosol and the pulses used in the pulse program are listed in the relation files (pulse assign files). If the pulse program refers to a specific relations file (pulse assign file) it will be interpreted. If no relations file is specified in the pulse program the default relations file will be interpreted.



Note that **getprosol** is automatically performed as part of the IconNMR automation.

Note that the probe and solvent dependent lock parameters are set with **edlock**.

INPUT FILES

- <tshome>/exp/stan/nmr/lists/group/
example - example tune file (input for first **File | Edit tune file**)
- <tshome>/prog/tcl/xwish3_scripts
edprosol - Tcl/Tk script that is started by **edprosol**
- <tshome>/prog/tcl/libtix/prosol/lib/lists
routing - default spectrometer routing

INPUT AND OUTPUT FILES

If you select Solvent(s) **All**:

- <tshome>/conf/instr/<instrum>/prosol/<probeID>/
 - *nucleus.channel.amplifier* - standard prosol parameters
 - *params* - global (channel independent) prosol parameters
 - *tune file* - probe dependent tune file (input for **File | Edit tune file**)

If you select a specific solvent:

- <tshome>/conf/instr/<instrum>/prosol/<probeID>/<solvent>
 - *nucleus.channel.amplifier* - standard prosol parameters
 - *params* - global (channel independent) prosol parameters
 - *tune file* - probe dependent tune file (input for **File | Edit tune file**)
 -

SEE ALSO

[getprosol](#) [► 164], [edlock](#) [► 109]

3.6 edscon

NAME

edscon - Edit spectrometer constants

DESCRIPTION

The command **edscon** opens a dialog window, where you can set certain spectrometer parameters (constants) (see the next figure).

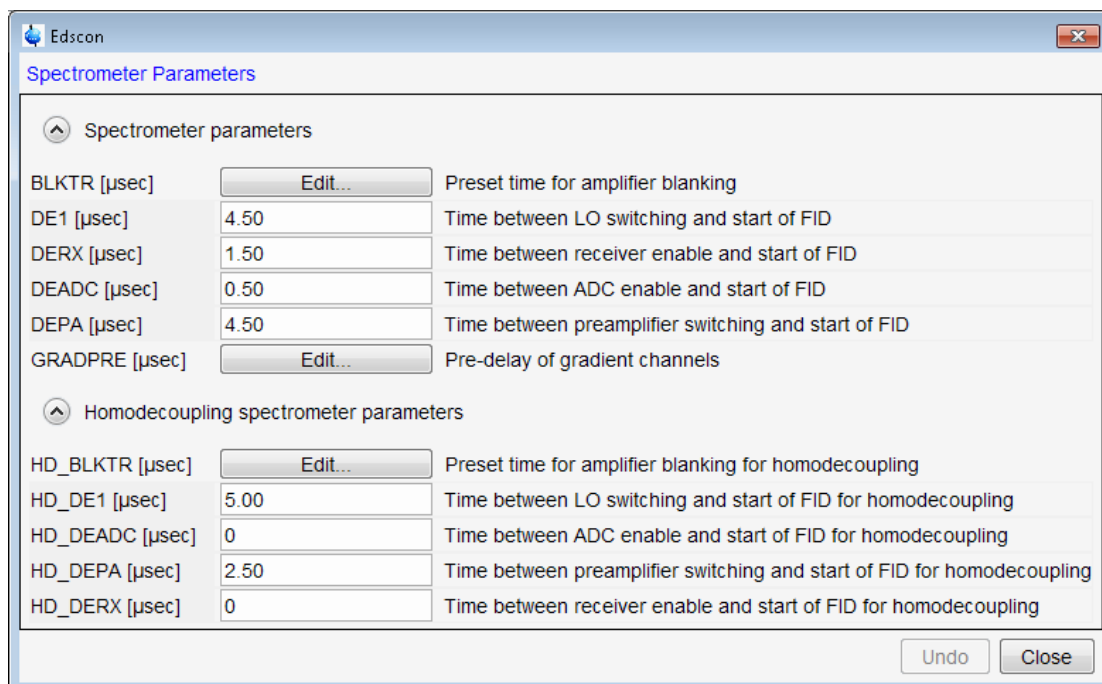


Figure 3.9: Edscon

The term constant refers to the fact that these parameters count for all datasets. **edscon** must be executed once as part of the spectrometer configuration.

Changes in the **edscon** parameters can be stored by clicking **OK**. You will be prompted for the NMR Administrator password.

BLKTR is an array of amplifier blanking preset times. This means they only allow RF signals to pass during the time they are blanked. Because of the finite switching time, blanking is triggered before the start of the RF pulse. The amplifier is blanked BLKTR µsec before the pulse. It is unblanked (allows no further RF passing) at the end of the pulse.

The use of the **edscon** preset parameter BLKTR can be switched off by inserting the statement

```
preset off
```

at the beginning of a pulse program. This has the same effect as setting all elements of BLKTR to zero. In this case, the blanking steps described above occur at the beginning of the RF pulse. Nevertheless, you can enable the preset blanking for each individual channel, e.g.:

```
2µ gatepulse 1 ;enable blanking for channel f1
```

```
2µ gatepulse 1|2 ;enable blanking for channel f1 and f2
```

In this example, the blanking of the transmitter and preamplifier is triggered 2 µsec before the RF pulse.

The **edscon** dialog box also shows the so called pre-scan subdelays. These are all part of the pre-scan delay DE. This is a hidden delay (it is not specified in the pulse program) that is automatically introduced by the `go` statement.

DE consists of 5 pre-scan delays DE1, DERX, DEADC, DEPA and DE itself. The sub-delays DE1, DERX, DEPA and DEADC are global parameters which depend on the properties of the respective spectrometer hardware. DE is also set globally but can be changed temporarily by

defining a value in the pulse program. DE mostly depends on the dead-time of the probe. It starts with the "go = .." instruction of the pulse program. All delays end simultaneously at the beginning of the data sampling. They act as pre-delays to the data sampling. At the beginning of each subdelay a certain action is performed:

- DE1: the intermediate frequency (if required) is added to the frequency of the observe channel. This corresponds to the execution of the syrec statement (default 4.5 µsec).
- DERX: the receiver gate is opened (default 1.5 µsec).
- DEADC: the digitizer is enabled (default 0.5 µsec).
- DEPA: the preamplifier is switched from transmit to observe mode (default 4.5 µsec).

For example, a DERX value of 3 µsec would mean that the receiver gate is opened 3µsec before the data sampling starts.

Please note that there is also a mandatory order required for those predelays in order to start the data sampling correctly, i.e. DE1 >= DEPA >= DERX >= DEADC.

Normally, the default values, which have been set during the installation of your spectrometer, can be used. Each subdelay has a maximum of DE - 1 µsec.

In most pulse programs, data sampling is performed by the `go` statement, which automatically triggers the actions mentioned above after the corresponding pre-scan subdelay. If, however, data sampling is performed by the `adc` statement, these actions must explicitly be specified in the pulse program. Each action can be performed by a statement with the same name, in lower case letters, as the corresponding pre-scan subdelay. For example, the receiver gate can be opened with the `derx` statement. You can type **edpul zgadc** to look at an example of a pulse program using the `adc` statement. For more information on this topic click:

Help | Manuals | Programming Manuals | Pulse Programming

The prescan subdelays only play a role for digitally filtered data (DIGMOD = digital or digital homodecoupling). For DIGMOD = analog, the parameter DE has a different purpose. It is used to achieve a near zero first order phase correction of the spectrum. In this case, it does not consist of subdelays.

INPUT AND OUTPUT FILES

- <tshome>/conf/instr/<instrum>/
 - *scon* - spectrometer constants

SEE ALSO

[cf \[51\]](#)

3.7 edsolv

NAME

edsolv - Edit solvent table

DESCRIPTION

The command **edsolv** opens the solvent table (see the next figure).

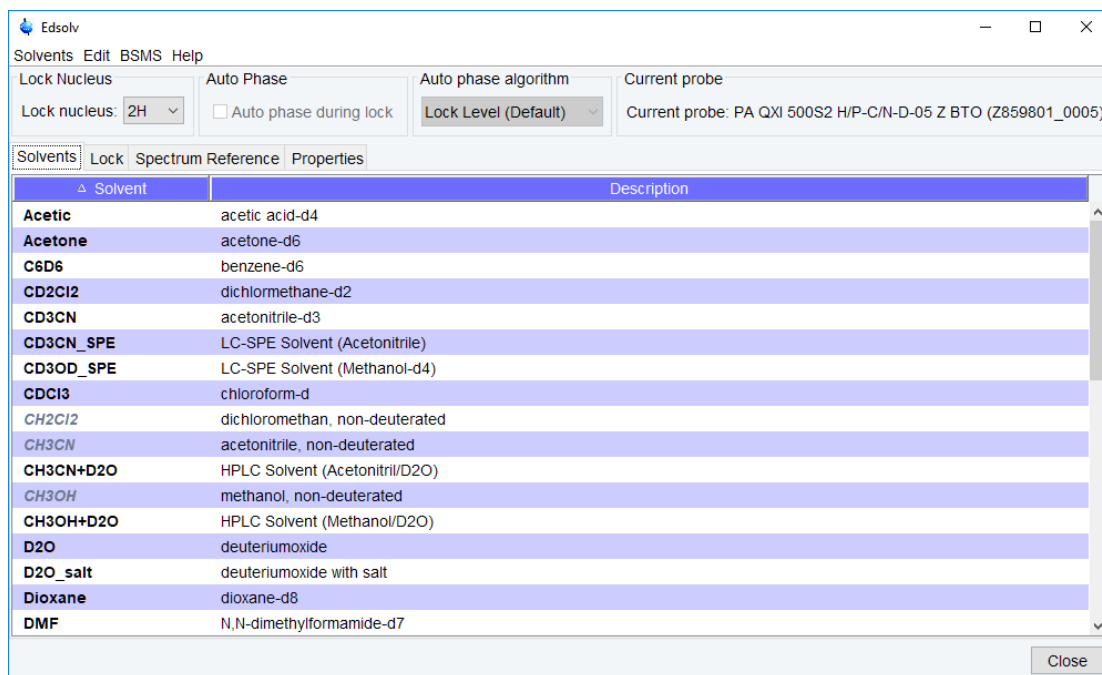
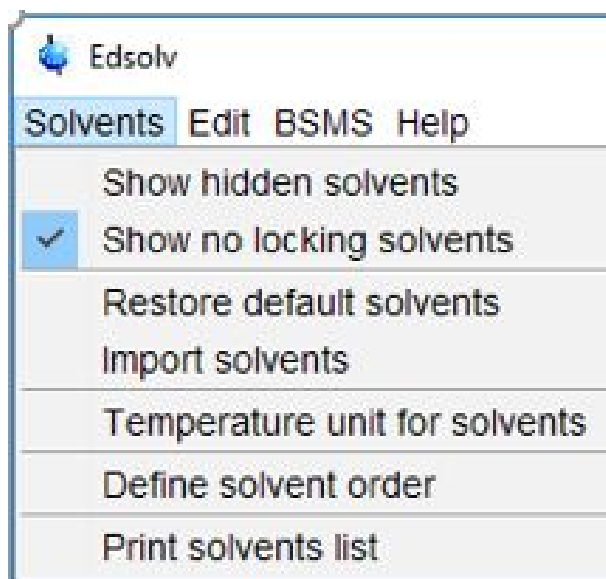


Figure 3.10: edsolv

This table contains one line for each solvent and shows the solvent name and a short description. For **edsolv**, the Solvents tab is automatically selected and highlighted. Please note that the same table is also opened with the **edlock** command. Then, the Lock tab is automatically selected and highlighted.

The **Solvents** tab offers the following functionalities:



The **Edit** tab offers the following functions:

- **Add new solvent**

The easiest way to add a new solvent is to right click on an existing solvent with properties close to your new solvent. Select **Copy and paste** solvent to copy from this existing solvent to the new solvent. Enter the name of the new solvent and its description.

Example: For a new solvent CD₂Cl₂ right click on CDCl₃, which has similar properties. Enter the name of the new solvent CD₂Cl₂ and in the description field, enter dichloromethane-d₂. For the CD₂Cl₂ example, enter 176K for the melting point and 312K for the boiling point. These two values are just reference for now but might be used in future. You can define the solvent as hidden, specify if this solvent is used as lock solvent and activate the Auto Phase mode.

Change to the Lock Parameters by clicking the **Lock tab**, select the new solvent and right click to select **Edit Lock parameters**. You'll find all parameters of the solvent used for copy and paste in the first step.

- In the Signals part, change the shift in ppm according to the signal used for locking in your new solvent. For the CD₂Cl₂ example, change the shift of the dichloromethane resonance to 5.33 ppm.
- You might want to optimize further lock parameters as described in Optimizing Lock Parameters (see [edlock](#) [▶ 109])

Select the **spectrum reference tab**, right click the new solvent to select **Edit spectrum reference parameters**. Adjust the reference shift and search width according to your needs. For the most commonly used reference standard TMS just leave the reference shift at 0 ppm and the search width at 0.5 ppm. In this case the search range is +/- 0.25 ppm around 0 ppm, which is suitable for TMS.

Please note, all solvents not marked as lock solvents will only appear in the list if the **Show no locking solvents** is active in the Solvents pull down menu (see above). These solvents cannot be used with the lock command.

- **Edit solvent**

The parameters entered here are shown when you click on the **Properties** tab. Double-clicking on a solvent line in the **Properties** table opens the **Edit Solvent** dialog.

- Delete solvent
- Copy and paste solvent
- Copy the selected probe to all solvent
- Copy probe to all solvents
- Delete probe from all solvents
- Search solvent

You can also right-click in the table to add, edit, delete, copy and paste or hide a solvent.

Before you start an experiment, you must set the parameter SOLVENT to an entry from the solvent table. If you do this from **eda**, you can click the arrow button to the right of this parameter and select an entry from the solvent list.

SEE ALSO

[ednuc](#) [83], [edprobe](#) [144], [edlock](#) [109], [edprosol](#) [84]

3.8 edsp

NAME

edsp/edasp - Set up nuclei and spectrometer routing

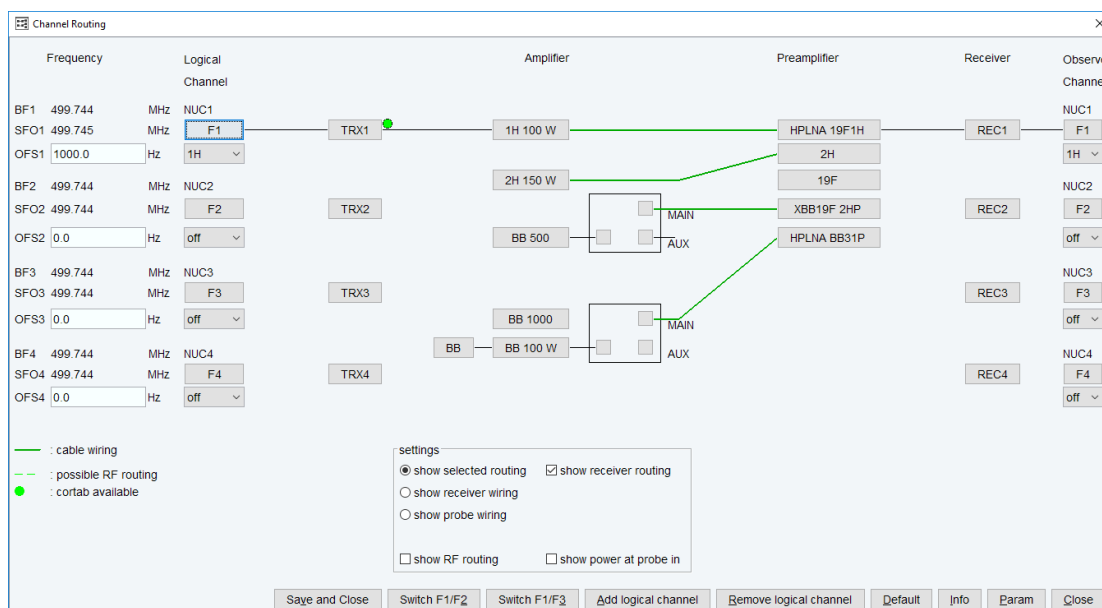
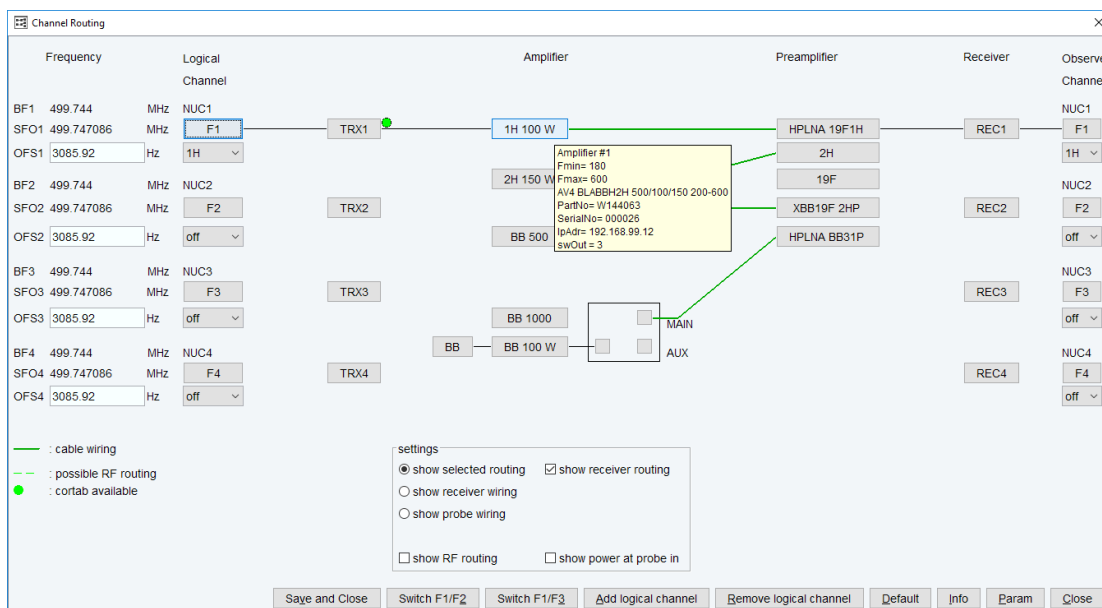


Figure 3.11: **edsp** nuclei and spectrometer routing

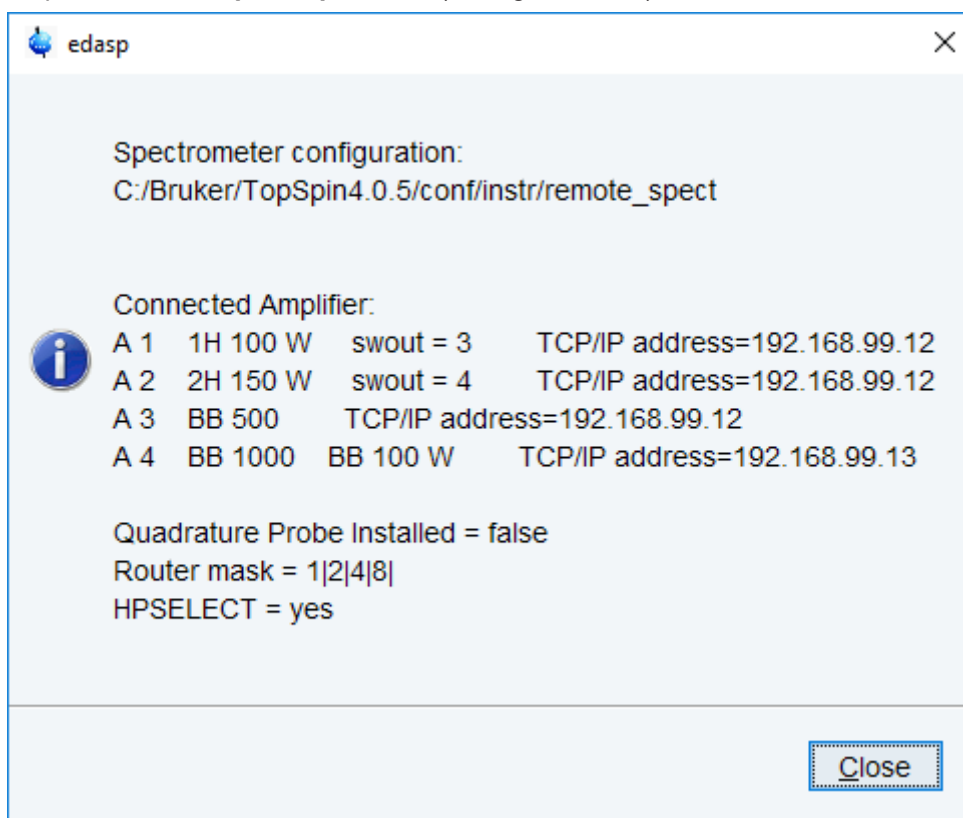
DESCRIPTION

The command **edsp** allows you to set up the nuclei and the spectrometer routing for the current experiment. **edsp** is equivalent to **edasp** except for the following:

edasp reads the irradiation frequencies offsets OFS1, OFS2, OFS3 etc. from the current dataset. **edsp** reads the irradiation frequencies that were last saved.

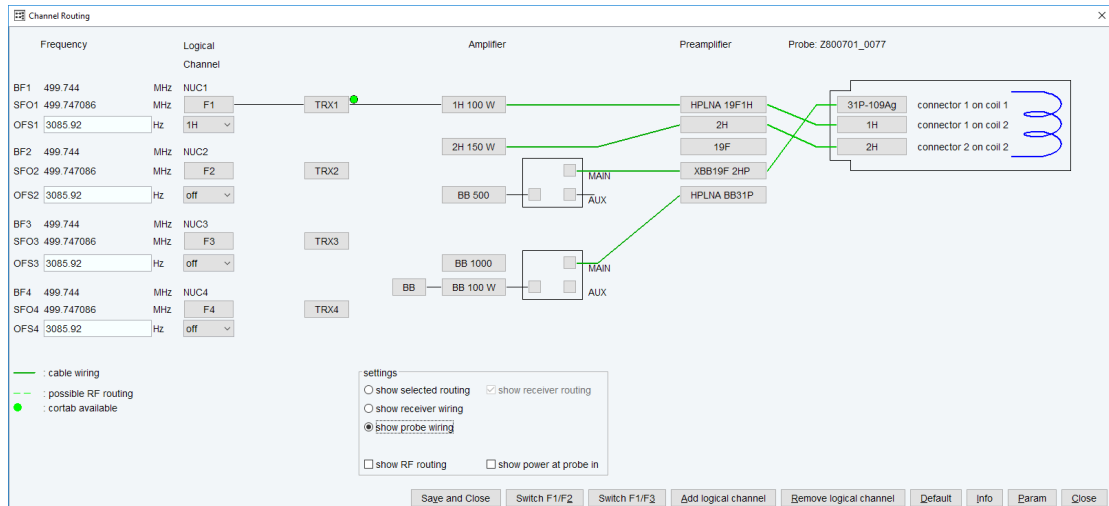


Information about the amplifiers can be easily obtained by dragging the mouse on the amplifier in the **edsp/edasp** window (see figure above).



Probe wiring can also be inspected:

Spectrometer Configuration Commands



The following figures will present several features (tabs) that can be obtained through the main **edsp/edasp** window:

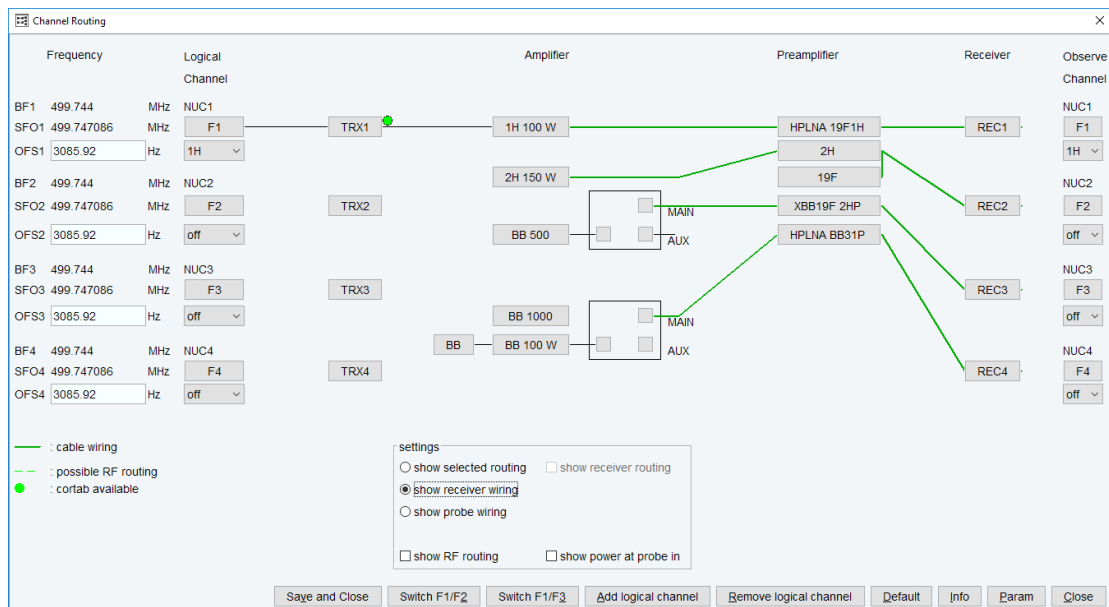


Figure 3.12: **edsp/edasp**: show receiver wiring

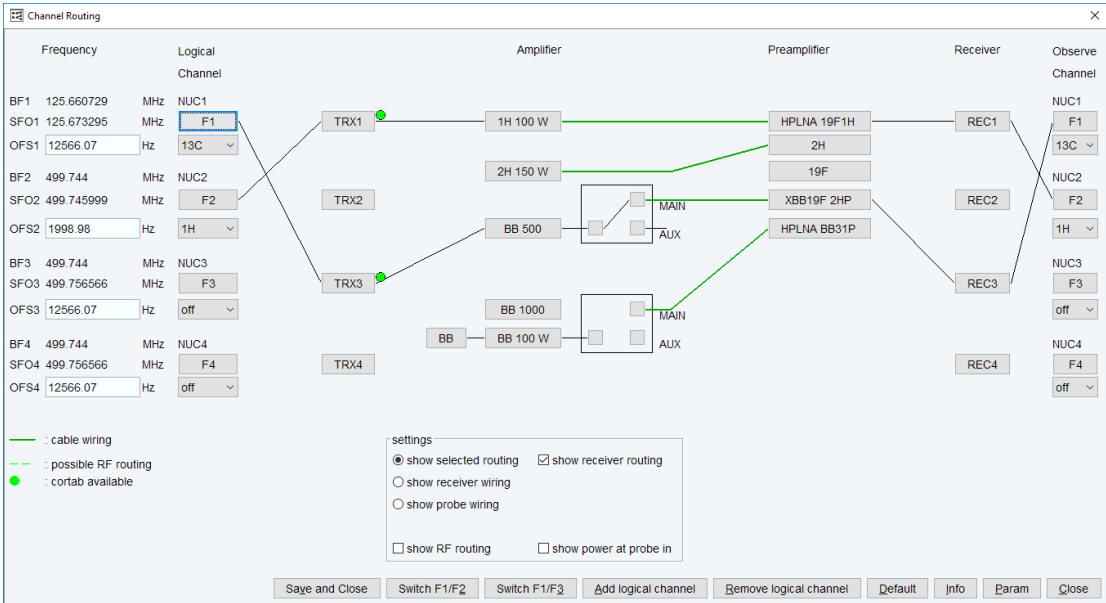


Figure 3.13: **edsp/edasp** after *rpar* C13CPD all

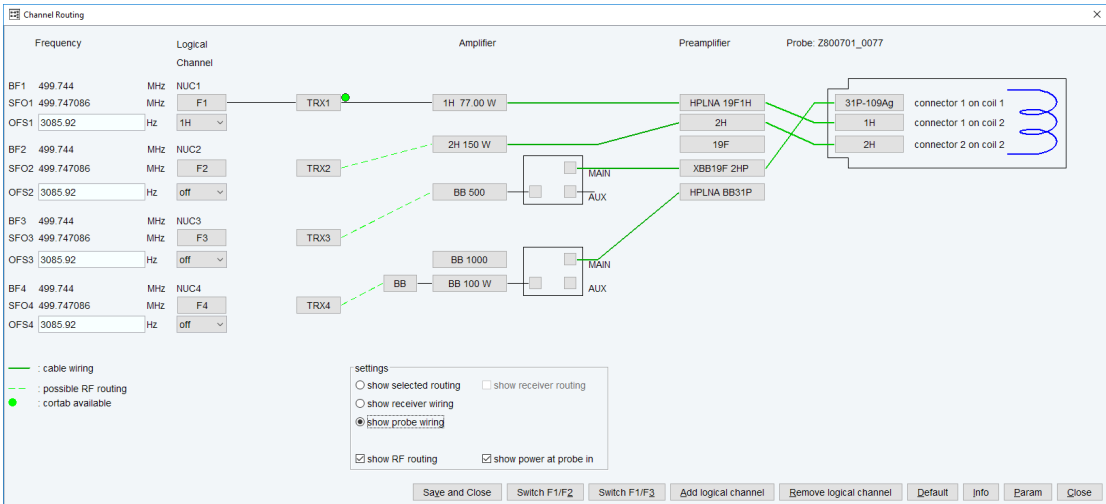


Figure 3.14: **edsp/edasp**: *tab* shows probe wiring and probe power at probe in

[illegible]

Figure 3.15: **edsp/edasp** "param"

edsp reads the irradiation frequencies offsets OFS1, OFS2, OFS3 etc. that were stored by the previous **edsp** or **edasp**.

As such, **edsp/edasp** allows you to transfer the frequency offset for a certain nucleus from one dataset to another. For example:

DATASET 1

rpar PROTON all

edasp or edsp =>

BF1 500.130 MHz NUC1

SFO1 500.135 Mhz F1

OFS1 **5000.00** Hz 1H

SAVE

DATASET 2

rpar C13CPD all

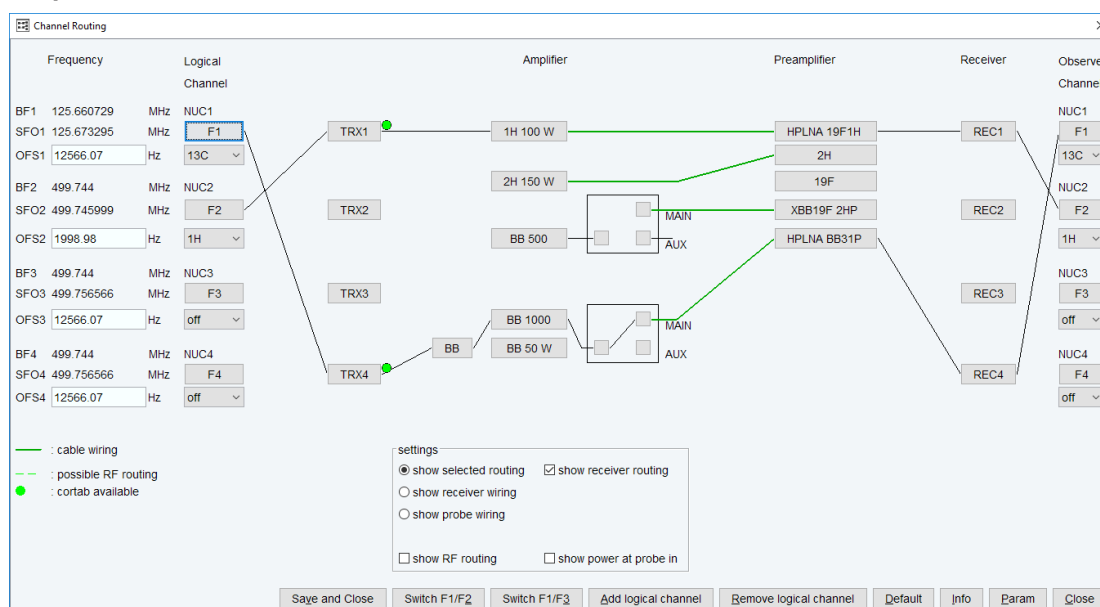


Figure 3.16: **edsp/edasp: rpar 13CPD all**

edsp =>

BF1 125.757 MHz NUC1

SFO1 125.758 Mhz F1

OFS1 1000.00 Hz 13C

BF2 500.130 MHz NUC2

SFO2 500.135 Mhz F2

OFS2 **5000.00** Hz 1H

The irradiation frequencies SFO1, SFO2 etc. are automatically adjusted to the corresponding frequency offsets.

The command **edsp** will be executed as part of the spectrometer configuration (command **cf**) and must be executed before **expinstall** which installs the standard parameter sets.

INPUT AND OUTPUT PARAMETERS

see **edasp**

INPUT AND OUTPUT FILES

see **edasp**

SEE ALSO

[cf](#) [51], [edasp](#) [162], [expinstall](#) [99]

3.9 expinstall

NAME

expinstall - Install pulse programs, AU programs, parameter sets etc.

DESCRIPTION

The command **expinstall** installs pulse programs, AU programs, parameter sets and various other resources for spectrometer usage. On a spectrometer, it must be performed once, after the installation of TopSpin and after **cf** has been done. On a datastation, **cf** is not needed and you can run **expinstall** immediately after the installation of TopSpin.

Configure a Spectrometer

- Click **Manage | Spectrometer | Experiments/Parameters | expinstall** or enter **expinstall** on the command line. A password request window is displayed.

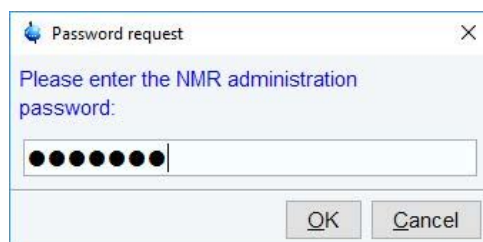


Figure 3.17: NMR Super-User Password Request

- Enter NMR administrator password to display the first Expinstall window.

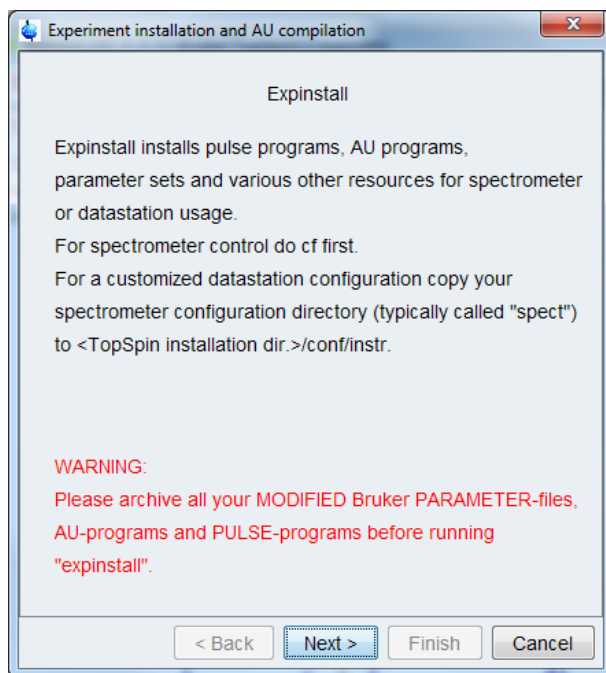
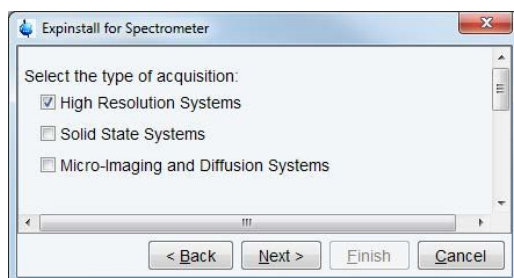
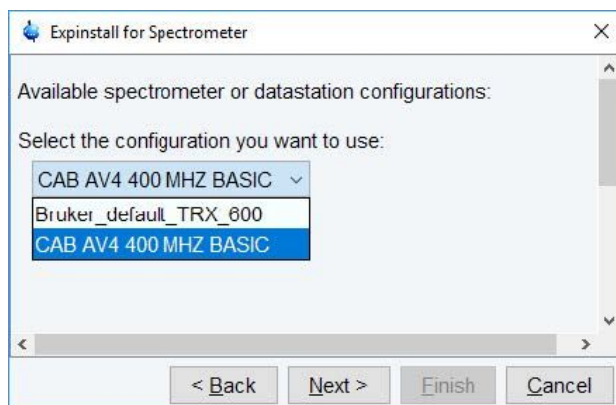


Figure 3.18: **expinstall**: AU programs installation and compilation window

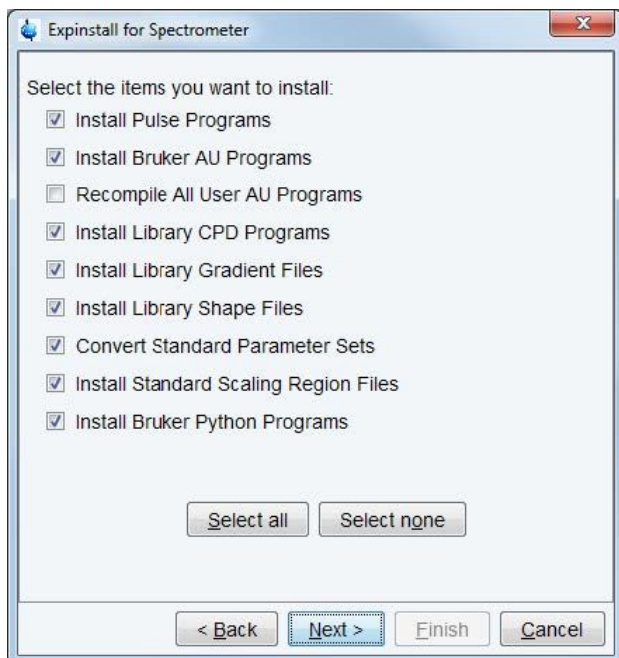
- Click **Next**. Bruker supplies Parameter files, AU-programs, Pulseprograms and other files in particular folders. **Expinstall** moves these folders to <TopSpin installation dir.>/exp/ stan/nmr/_expinstall_automatic_backup and installs new copies.
- Individual Parameter files, AU-programs, Pulseprograms and other files that reside in user-specific folders are not affected by expinstall.
- In the next window select the type of acquisition. In the example a High Resolution System has been checked.



- Click **Next**

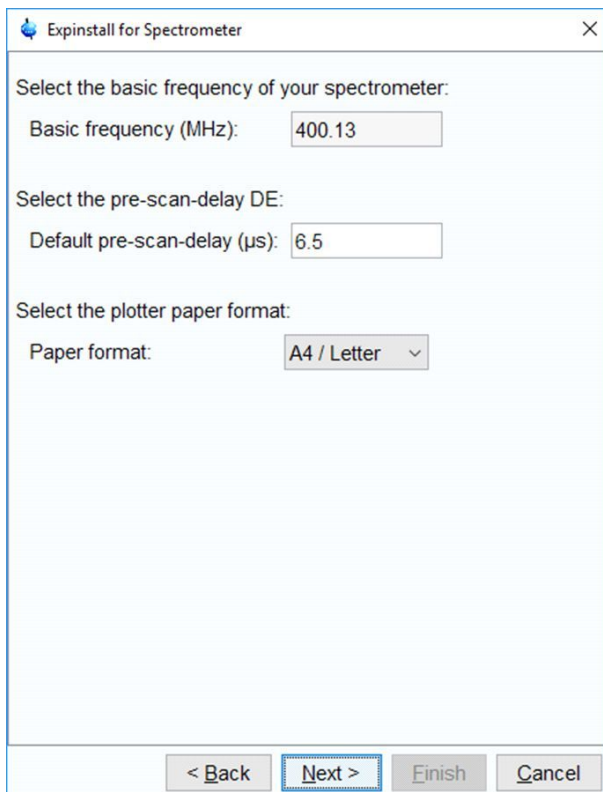


- Select the spectrometer or data station configuration for **expinstall**. Here the **CAB AV4 400 MHZ BASIC** has been selected. If this window is not displayed, then TopSpin has found only one valid configuration, namely the one for the current spectrometer, and immediately continues with the next 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**.



- 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**.

Spectrometer Configuration Commands



Expinstall for Spectrometer

Select the basic frequency of your spectrometer:

Basic frequency (MHz):

Select the pre-scan-delay DE:

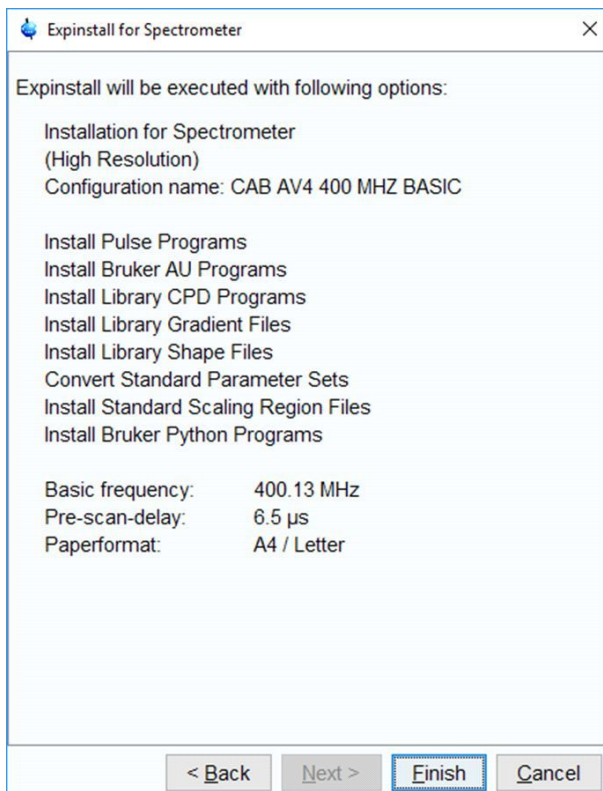
Default pre-scan-delay (μ s):

Select the plotter paper format:

Paper format:

< Back Next > Finish Cancel

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



Expinstall for Spectrometer

Expinstall will be executed with following options:

Installation for Spectrometer
(High Resolution)
Configuration name: CAB AV4 400 MHZ BASIC

Install Pulse Programs
Install Bruker 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

Basic frequency: 400.13 MHz
Pre-scan-delay: 6.5 μ s
Paperformat: A4 / Letter

< Back Next > Finish Cancel

- 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.

Configure a Datastation like a Spectrometer

If you want to configure your datastation like your spectrometer, you must first copy the configuration directory:

<tshome>/conf/instr/<instrum>

From that spectrometer to the data station. Here:

- <tshome> is TopSpin home, the directory where TopSpin is installed.



Note that this can be different on the spectrometer than on the datastation.

- <instrum> is the configuration name.

See also the description of the command **nmr_save**.

After copying the configuration directory, execute **expinstall** as described above for the spectrometer.

INPUT PARAMETERS

If the task **Convert standard parameter sets** is selected, **expinstall** uses the following input parameters:

From the parameter sets as delivered with TopSpin:

- BF1 – BF8 - basic frequencies for channel f1 to f8.
- SFO1- SFO8 - irradiation (carrier) frequencies for channels f1 to f8.
- IN0 - increment for delay D0 (2D and 3D parameter sets only).
- IN10 - increment for delay D10 (3D parameter sets only).
- SW - spectral width in ppm.
- SPOFFS[0-63] - shaped pulse frequency offset.

OUTPUT PARAMETERS

If the task **Convert standard parameter sets** is selected, **expinstall** stores the following parameters in the parameter sets:

- BF1 – BF8 - basic frequencies for channel f1 to f8.
- SFO1- SFO8 - irradiation (carrier) frequencies for channels f1 to f8.
- SF - spectral reference frequency.
- IN0 - increment for delay D0 (2D and 3D parameter sets only).
- IN10 - increment for delay D10 (3D parameter sets only).
- SW - spectral width in ppm.
- SPOFFS[0-63] - shaped pulse frequency offset.
- DIGTYP - digitizer type.
- DR - digital resolution.
- DIGMOD - digitizer mode.
- DECIM - decimation factor of the digital filter.
- DE - prescan delay.

- All routing parameters as defined with the commands **edsp** / **edasp**.

SEE ALSO

[cf \[51\]](#), (cplbruk, cpluser, compileall, rpar, wpar)

3.10 ha

NAME

ha - Show hardware Ethernet addresses.

DESCRIPTION

The command **ha** opens the dialog window showing the addresses of the Ethernet accessible hardware devices. For each device, the Ethernet address is displayed and an **Open** button is available. Clicking this button opens the default web browser showing the respective hardware configuration. Here, you can set various configuration settings.

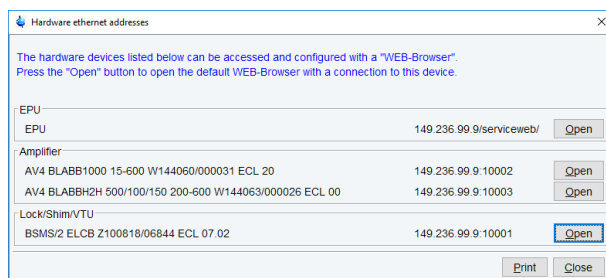


Figure 3.19: **ha**

The command **ha** can also be started from the TopSpin menu:

Click **Spectrometer => Setup => Ethernet addresses of hardware**

or

Click **Options => Spectrometer Tools => Ethernet addresses of hardware**

SEE ALSO

[cf \[51\]](#)

3.11 nmr_save, nmr_restore, user_save, user_restore

NAME

nmr_save - Save installation specific files

nmr_restore - Restore installation specific files

user_save - Save user specific files

user_restore - Restore user specific files

DESCRIPTION

The commands **nmr_save** and **user_save** save installation/user specific files in a backup TAR-file.

The commands **nmr_restore** and **user_restore** extract a backup TAR-file to the same or to a different installation.

All these commands open the dialog window shown in the next figure, the individual commands being available as tabs.

NMR_Save

Save installation files | Restore installation files | Save user files | Restore user files

Save installation specific files.

Installation specific files are collected and stored into a compressed file. This compressed file can be used 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\TopSpin4.0\nmr_backup Browse

Overwrite existing backup file: ☐

Installation to be saved (TopSpin home): C:\Bruker\TopSpin4.0 Browse

Spectrometer configuration (e.g. spect): ▼

Display default information: ☒

Display additional information: ☐

Execute "Save installation specific files" periodically Automatic Backup

Log:

Save Close

Figure 3.20: *nmr_save*

Here you can specify:

- **Location of the backup file:** the storage directory of the backup file.
- **Installation to be saved :** The TopSpin home directory.
- **Spectrometer configuration:** as enter during **cf**.

Furthermore, you can select

- **Display default information:** the path of the created backup file.
- **Display additional information:** the path of the created backup file, information about directories being saved and converting/renaming information.

The button **Define cron job** opens the cron dialog where you can define a periodic save of Bruker or user files (see also command **cron**).

Here 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**)
- IconNMR user information (**iconnmr**)
- Program Licenses (TopSpin, NMRSim, NMR Guide)
- Various lists like **scl**, **f1**, **ds** (**edlist**, **zg**, **gs**)
- TopSpin macros (**edmac**)
- Probe and solvent dependant parameters (**edprosol**)
- Lock parameters (**edlock**)
- Probe information (**edprobe**)
- Nucleus information (**ednuc**)
- RF Shapes and gradients

etc.

Furthermore the files *prog/logfiles/heliumlog*,

prog/logfiles/heliumloig.err and *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 beginning with TopSpin 3.0 the whole directory *<diskless>/crco_data/cryotool_log/* will be saved.

For more details about the commands *nmr_save*, *nmr_restore*, *user-save* and *user-restore* please refer to the respective Bruker TopSpin Installation Guides for Windows XP, Windows Vista or Linux.

INPUT AND OUTPUT FILES

- *<tshome> /nmr_backup*
 - *nmr_backup_<date>-<time>.tar* (**nmr_save**)
 - *nmr_backup_<username>-<date>-<time>.tar* (**user_save**)
- *<tshome>/exp/stan/nmr/au/src/*
 - *nmr_save* - AU program executed by **nmr_save**

INPUT AND OUTPUT DIRECTORIES

nmr_save stores various subdirectories/files of:

- *<tshome>/exp/stan/nmr/py/*
- *<tshome>/exp/stan/nmr/lists*
- *<tshome>/exp/stan/nmr/par/*
- *<tshome>/exp/stan/nmr/au/src/*
- *<tshome>/plot/layouts/*
- *<tshome>/conf/instr/*

- <tshome>/prog/tcl/xwish3_scripts/
- <tshome>/exp/stan/nmr/parx/preemp/
- <tshome>/QTP/
- <tshome>/data/final/nmr/protocolfiles/
- <tshome>/conf/global
- <tshome>/prog/server/export.conf

user_save stores various subdirectories/files of:

- <userhome>/.topspin-<hostname>
- <tshome>/exp/stan/nmr/py/
- <tshome>/exp/stan/nmr/lists
- <tshome>/exp/stan/nmr/par/
- <tshome>/exp/stan/nmr/au/src/

INPUT AND OUTPUT DIRECTORIES

SEE ALSO

[cf \[51\]](#), [expinstall \[99\]](#), (cron)

3.12 paracon

NAME

paracon - Change the basic frequency in parameter sets

DESCRIPTION

The command **paracon** changes the basic frequency in parameter sets. This allows you to use parameter sets that were created on a spectrometer with a different frequency. It opens dialog box shown in the next figure.

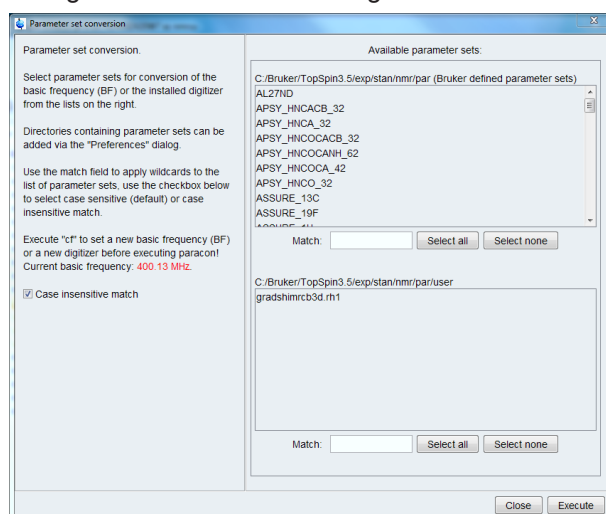


Figure 3.21: **paracon**

Here you can setup a list of available parameter sets. You can select Bruker and/or User defined parameter sets and uses a match string. The matching parameter sets appear in the right part of the dialog box. To start the conversion, select one or more parameter sets and click **OK**.

INPUT AND OUTPUT PARAMETERS

Acquisition parameters:

- BF1 - BF8 - basic frequency for frequency channel f1 to f8.
- SFO1 - SFO8 - irradiation (carrier) frequencies for channels f1 to f8.
- O1 - O8 - irradiation frequency offset for frequency channel f1 - f8 in Hz.
- SW - spectral width in ppm.

Processing parameters:

- SF - spectral reference frequency.

INPUT AND OUTPUT FILES

- <tshome>/exp/stan/nmr/par/*/
 - acqu - acquisition parameters
 - proc - processing parameters

SEE ALSO

[expinstall](#) [► 99]

3.13 Miscellaneous

3.13.1 Using two different gradient systems

In some special configurations your spectrometer can be equipped with two different kinds of gradient amplifiers:

- The internal GAB in the BSMS common to most spectrometers
- An additional imaging gradient system (BGA, GREAT)

In most of such cases, there are also two different probes available, one which should be used together with the GAB and another one which should be used together with the imaging system.

Once the assignment of a specific probe to a certain type of gradient amplifier system and the preemphasis settings for that probe have been saved, the acquisition (and in particular also **topshim**) will always take those saved settings and choose the gradient system according to the currently installed probe, as specified in **edprobe**.

Choosing a different gradient system for a specific probe can be accomplished as follows (applies also for the rare case of using the same probe with two different gradient systems):

- If you need your current preemphasis settings for future work, make a backup before: enter **setpre** and click on **write to epu** and close the **setpre** window
- Enter **setpre -select** and choose the desired system by clicking on it
- Then the usual **setpre** window pops up
- Perform all relevant settings there
- Click on **save as default**, otherwise these changes will have no effect
- Remember that this overrides all your previous settings for the default configuration

The respective parameters formerly used in **edscon** (GRADCHAN, GRADPRE) have no effect anymore.

4 Lock Commands

This chapter describes the commands that are involved in locking the magnetic field. Avance spectrometers use a digital lock which is provided by the BSMS unit. Locking the magnetic field is done by measuring the signal of a lock nucleus and adjusting the magnetic field whenever its frequency shifts. Common lock nuclei are 2H and 19F.



Please note that the Fourier 80 Lock procedures are described in the Fourier 80 User Manual.

4.1 edlock

NAME

edlock - Edit the lock table

DESCRIPTION

The command **edlock** opens the lock table; a dialog box in which the lock parameters can be set (see the next figure). For **edlock**, the **Lock** tab is automatically selected and highlighted. Please note that the same table is also opened with the **edsolv** command. Then, the **Solvent** tab is automatically selected and highlighted.

Δ Solvent	Probe	Lock Power	Lock Power Instep	Loop Gain	Loop Time	Loop Filter	Shift [ppm]
Acetic	Generic	-38	10	-10	0.1	100	2.03
Acetone	Generic	-38	10	-2	0.1	200	2.04
C6D6	Generic	-26	10	-0	0.2	300	7.16
CD2Cl2	Generic	-38	10	-2	0.1	200	5.32
CD3CN	Generic	-38	10	-2	0.1	200	1.93
CD3CN_SPE	Generic	-38	10	-10	0.1	100	1.93
CD3OD_SPE	Generic	-35	10	-5	0.1	100	3.3
CDCl3	Generic	-30	10	-12	0.4	100	7.24
CH3CN+D2O	Generic	-18	10	-10	0.3	100	4.7
CH3OH+D2O	Generic	-18	10	-10	0.3	100	4.7
D2O	Generic	-18	10	5	0.25	500	4.7
D2O_salt	Generic	-18	10	5	0.25	500	4.7
Dioxane	Generic	-38	10	-2	0.1	200	3.53
DMF	Generic	-38	10	-2	0.1	200	2.91
DMSO	Generic	-20	10	5	0.25	500	2.49
EtOD	Generic	-30	10	-15	0.2	100	1.11
H2O+D2O	Generic	-18	10	-5	0.35	100	4.7
H2O+D2O_salt	Generic	-18	10	-5	0.35	100	4.7
HDMSO	Generic	-25	10	-9.4	0.464	50	2.49
Juice	Generic	-18	10	-5	0.35	100	4.7
MeOD	Generic	-35	10	-5	0.1	100	3.3
Plasma	Generic	-18	10	-5	0.35	100	4.7
Pyr	Generic	-38	10	-2	0.1	200	8.71
T_H2O+D2O+Me4NCl	Generic	-18	10	-5	0.35	100	4.7
T_H2O+D2O+NaAc	Generic	-18	10	-5	0.35	100	4.7

Figure 4.1: edlock

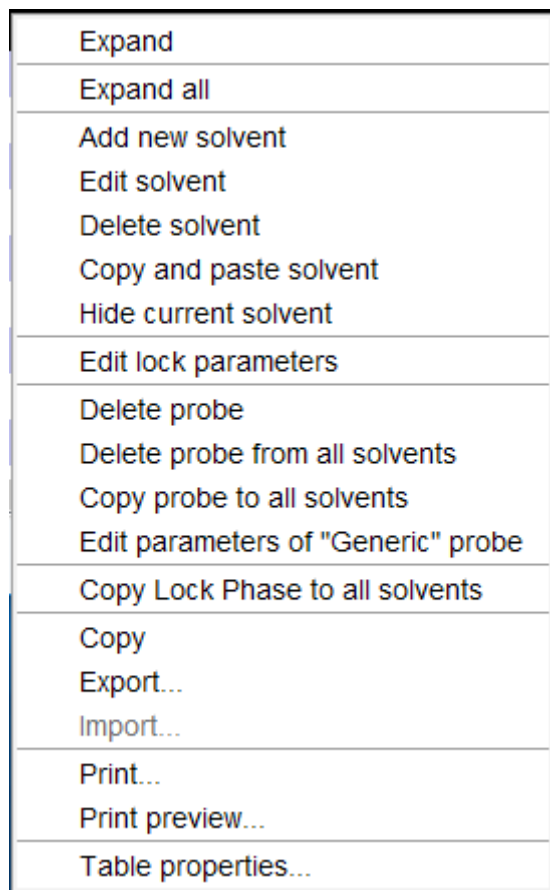
edlock must be executed once for each probe and each lock nucleus. The lock parameters can be determined from the BSMS display (command **bsmsdisp**).

Before you run **edlock**, you must have defined the current probe with the command **edprobe**. Furthermore, you must have defined the lock nucleus by setting the parameter **LOCNUC**. This can be done with **eda** or by entering **locnuc** on the command line. In most experiments, the lock nucleus is deuterium. As such, **LOCNUC** is set to 2H in most Bruker standard parameter sets (see **rpar**).

When **edlock** is executed for the first time on a certain probe, a default lock table, which is delivered with TopSpin, is opened.

The main part of the lock table shows a list of solvents and, for each solvent, the lock parameters. Most lock parameters are used for locking the magnetic field during the acquisition. Others, however, are used for referencing the spectrum after the acquisition has finished.

With a right-click on a solvent line several commands and options become available (see screenshot below).



Lock Parameters Used To Lock The Magnetic Field:

- Lock Power - power used to irradiate the lock nucleus (-60 to 0 dB)
- Lock Power Instep - displays the Initial Step for the Lock Power.

This value is used for the Initial Lock Step, to be added to the Lock Power. Example: For CDCl₃, the Lock Power is -28, the InStep is +10, so the Initial Lock Power Step will be done with -18 dB.

- Loop Gain - lock regulator gain (-80 to 0 dB).

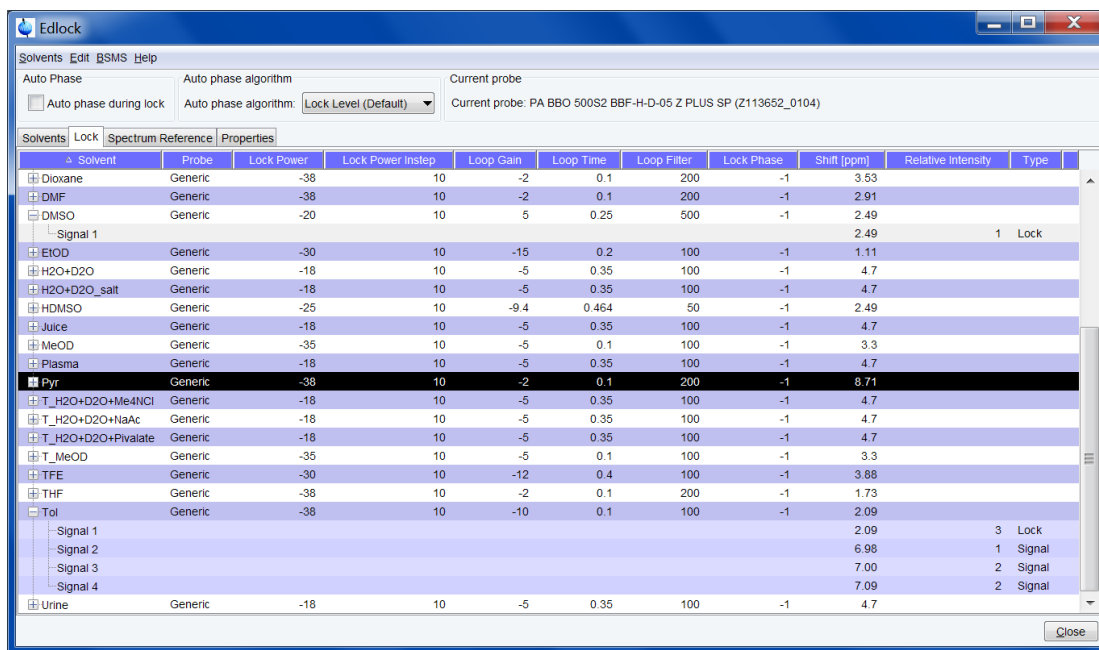
It is set at the end of the acquisition to the loop gain currently set on the BSMS unit. This usually, but not necessarily corresponds to the value of the Loop Gain in the table. If lock-in was performed with the command **lock**, the loop gain is first read from the table and set on the BSMS unit. However, using **autolock** or **Lock on/off** in bsmsdisp performs lock-in without first reading the table.

- Loop Time - lock regulator time constant (0.001 - 1.0 seconds).
- Loop Filter - lock regulator cut-off frequency of the lowpass filter (1 - 200 Hz).
- Lock Phase - the phase of the lock signal.

- Shift [ppm] - Chemical shift of the lock nucleus (irradiation frequency offset).
- Relative intensity - provides the relative intensity where a solvent has several signals.
- Type - if a solvent has several signals, then Type defines which signal is used for locking. This is either the sharpest or the best separated one. Typically, the most intense signal is used (see relative intensity).

Relative intensity and type are only shown when a solvent has been selected.

The lock parameters are interpreted by the commands **lock** and **lopo**.



The screenshot shows the Edlock software window with a menu bar (Solvents, Edit, BSMS, Help) and a toolbar. Below the toolbar is a section for 'Auto Phase' with a checkbox 'Auto phase during lock' and a dropdown 'Auto phase algorithm' set to 'Lock Level (Default)'. To the right, it says 'Current probe: PA BBO 500S2 BBF-H-D-05 Z PLUS SP (Z113652_0104)'. The main area is a table with columns: Solvent, Probe, Lock Power, Lock Power Instep, Loop Gain, Loop Time, Loop Filter, Lock Phase, Shift [ppm], Relative Intensity, and Type. The table lists various solvents like Dioxane, DMF, DMSO, EtOD, H2O+D2O, H2O+D2O_salt, HDMSO, Juice, MeOD, Plasma, Pyr, T_H2O+D2O+Me4NCl, T_H2O+D2O+NaAc, T_H2O+D2O+Pivalate, T_MeOD, TFE, THF, and Urine. Some solvents have multiple signals listed below them, each with its own relative intensity and type (Lock, Signal).

Solvent	Probe	Lock Power	Lock Power Instep	Loop Gain	Loop Time	Loop Filter	Lock Phase	Shift [ppm]	Relative Intensity	Type
Dioxane	Generic	-38	10	-2	0.1	200	-1	3.53		
DMF	Generic	-38	10	-2	0.1	200	-1	2.91		
DMSO	Generic	-20	10	5	0.25	500	-1	2.49		
Signal 1									2.49	1 Lock
EtOD	Generic	-30	10	-15	0.2	100	-1	1.11		
H2O+D2O	Generic	-18	10	-5	0.35	100	-1	4.7		
H2O+D2O_salt	Generic	-18	10	-5	0.35	100	-1	4.7		
HDMSO	Generic	-25	10	-9.4	0.464	50	-1	2.49		
Juice	Generic	-18	10	-5	0.35	100	-1	4.7		
MeOD	Generic	-35	10	-5	0.1	100	-1	3.3		
Plasma	Generic	-18	10	-5	0.35	100	-1	4.7		
Pyr	Generic	-38	10	-2	0.1	200	-1	8.71		
T_H2O+D2O+Me4NCl	Generic	-18	10	-5	0.35	100	-1	4.7		
T_H2O+D2O+NaAc	Generic	-18	10	-5	0.35	100	-1	4.7		
T_H2O+D2O+Pivalate	Generic	-18	10	-5	0.35	100	-1	4.7		
T_MeOD	Generic	-35	10	-5	0.1	100	-1	3.3		
TFE	Generic	-30	10	-12	0.4	100	-1	3.88		
THF	Generic	-38	10	-2	0.1	200	-1	1.73		
Tol	Generic	-38	10	-10	0.1	100	-1	2.09		
Signal 1									2.09	3 Lock
Signal 2									6.98	1 Signal
Signal 3									7.00	2 Signal
Signal 4									7.09	2 Signal
Urine	Generic	-18	10	-5	0.35	100	-1	4.7		

The loop gain, loop time and loop filter can also be set with the TopSpin commands **lgain**, **ltime** and **lfilter**, respectively. Furthermore, they can also be set from the BSMS keyboard menu.



Note the difference between loop gain which can be set in **edlock** or with **lgain** and lock gain which can be set in the BSMS display. The AU program **loopadj** automatically optimizes the lock phase, lock gain, loop gain, loop filter and loop time.

Note that **loopadj** optimizes these parameters for best long-term stability, but not for best lineshape, resolution or homogeneity (for more information type **edau loopadj** and look at the header of the AU program).

Optimizing Lock Parameters

Lock Power

After the sample has been locked and shimmed, start the auto-power routine from the **bsmsdisp** command. For lock solvents with long T1 relaxation times (e.g. CDCl3), auto-power might take an unacceptably long time. In this case a manual optimization of the lock power is recommended. Increase the lock power until the lock signals begins to oscillate (until saturation), and then reduce the power level slightly (approximately 3 - 6 dB). Do not reduce too much, as this will affect the field stability. Alternatively, you might use a gradient experiment (e.g. Parameter set COSYGPSW, or the pulse program **preempp2**) to observe the gradients on the lock. In case of optimum lock power, the lock signal will return to normal level after the gradient. An overshoot before returning to the normal level is caused by saturation, so reduce the lock power until this overshoot is no longer visible.

Lock Phase

Use the auto-phase feature in **bsmsdisp** to optimize the Lock Phase.

Lock Gain

Use the auto-gain feature in **bsmsdisp** to optimize the Lock Gain.

Loop Gain, Loop Time and Loop Filter

Generally, these parameters should be already suitable in the default Bruker Solvent list, so there should be no need to change them. However, the AU program loopadj can be used to automatically optimize loop gain, loop time and loop filter for optimal long-term stability.

Alternatively, the following procedure might be used:

Note the Lock Gain value after the auto-gain routine has optimized it. Using this value, select the appropriate values for the loop filter, loop gain and loop time as shown in the following table:

Lock RX Gain (after auto gain) [dB]	Loop Filter [Hz]	Loop Gain [dB]	Loop Time [sec]
120	20	-17.9	0.681
	30	-14.3	0.589
110	50	-9.4	0.464
	70	-6.6	0.384
100	100	-3.7	0.306
	160	0.3	0.220
	250	3.9	0.158
	400	7.1	0.111
90	600	9.9	0.083
	1000	13.2	0.059
	1500	15.2	0.047
	2000	16.8	0.041

Example:

Auto-gain determines a lock gain of 100 dB. From the table, the user should set the loop filter to 160 Hz, the loop gain to 0.3 dB and the loop time to 0.220 sec.

This procedure is recommended to use with shielded magnets. For non-shielded magnets a general procedure cannot be given, so the relation between the three parameters should be determined individually. If in doubt, it is recommended to leave the Bruker default parameters unchanged.

Optimizing Lock Phase

At the top of the **edlock** table, the auto phasing of the lock signal can be turned on or off. When auto phase is turned on, the algorithm can be selected from the dropdown list. Autophase and lock are treated differently. The behavior of the lock command with respect to Autophase handling can be controlled independently with a checkbox in the **edlock** window. When turned on, the FFA algorithm (Spectrum) is used. The default behavior is no Autophase during lock and **lock level default** for the algorithm. In this state the table will contain the lock phase column. With Autophase turned on, the lock phase column is not needed and therefore unavailable.

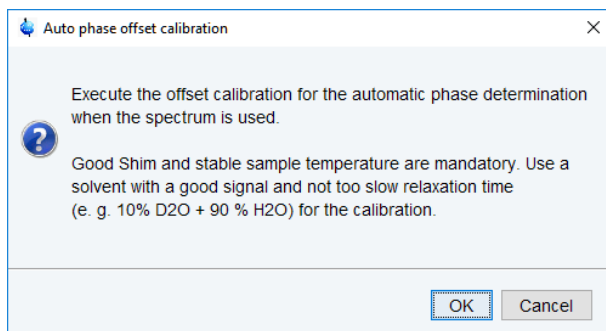
There are three selections for the Autophase algorithm:

- **Lock level default:** This uses the old algorithm, optimization via lock level.

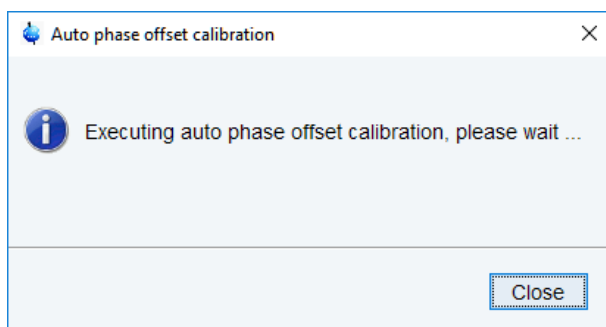
- **Enhanced lock level:** This also uses the old algorithm, but with wider range. It will therefore need more time.
- **Spectrum:** This is the new algorithm (FFA). It will also take longer, but not that much, because a spectrum is measured anyway during locking. This is the recommended selection if Autophase is activated for the L-TRX and execution time is not critical, e.g. in case of high throughput samples.

Calibration of the Autophase offset

This calibration is mandatory if **Autophase** is selected and spectrum selected for the algorithm. It can be selected via the pull down menu entry **BSMS | Calibrate Autophase offset**. This control can also be added to the BSMS Display (**bsmsdisp**) if needed. The following window will be displayed:



Please follow the instructions, insert the recommended sample and click **OK** when finished.



Please wait until the offset calibration is ready (approximately 1½-2 minutes). The result can be checked on the ELCB Webpage. Click **LOCK | LOCK Configuration | Autolock Configuration** and check **Phase offset FFA to Lock**.

BSMS Service Web

Auto Lock Configuration

Auto Lock (FFA)	
Auto Lock Mode	Field correction (default) ▾
Auto Lock Behaviour	Auto Lock with automatic Phase Adjustment ▾
FFA Size	8192 (default)
Recovery Deviation	1.000 dB
H0 Calibration Factor (Frequency <-> Field)	1.00000
Auto Phase	
Auto Phase Algorithm	Evaluate from FFA ▾
Mute Time before FFA Auto Phase	5.0 s
Phase Offset FFA to Lock	203.6 °
<input type="button" value="Set"/> <input type="button" value="Refresh"/>	

The ELCB Webpage can also be used to activate the Phase offset calibration. Use the BSMS Service Page and choose **Calibration | Auto Lock Phase Calibration**. Again, use a suitable sample as outlined in the Auto Phase Calibration Info field.

BSMS Service Web

LOCK Parameter & Commands

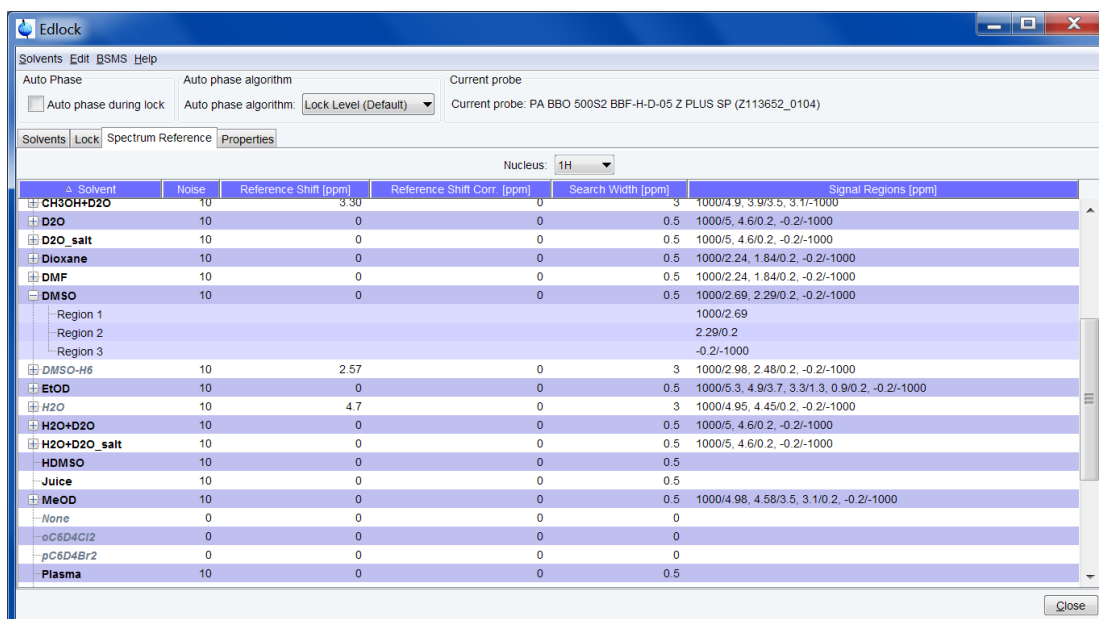
LOCK Parameters				
Field	Field [FJ]	1445.85	Drift [FJ/d]	0.00
	Sweep Amplitude	5.0	Sweep Rate [Hz]	0.20
Acquisition	Shift [ppm]	4.800	Power [dBm]	-35.0
	Phase [°]	27.1	Gain [dB]	119.5
Display	Display Mode	Absorption ▾	DC [%]	-75.0
Controller	Gain [dB]	-5.0	Time [s]	0.100
	Filter [Hz]	100.0		
<input type="button" value="Set"/> <input type="button" value="Refresh"/>				
LOCK Commands				
Auto	<input type="button" value="Auto Lock"/> <input type="button" value="Auto Gain"/> <input type="button" value="Auto Power"/> <input type="button" value="Auto Phase"/> <input type="button" value="Auto Phase Calibration"/>			
	<input type="button" value="Auto OFF"/>		State: Auto Lock Idle	
Manual	<input type="button" value="Lock ON"/> <input type="button" value="Lock OFF"/> <input type="button" value="Mute RF"/>		<input type="button" value="Lock On"/> <input type="button" value="Sweep ON"/> <input type="button" value="Sweep OFF"/> <input type="button" value="Sweep Off"/>	
Auto Phase Calibration	A good Shim and a stable sample temperature are mandatory. Use solvents with a good signal and not too long relaxation, e. g. 10% D2O + 90% H2O.			
H0 Calibration	<input type="button" value="Start H0 Calibration"/> <input type="button" value="Stop / Abort"/>			



Important: The phase offset calibration should be repeated if the 2H Preamplifier is exchanged.

Lock Parameters Used To Reference The Spectrum:

Clicking the **Spectrum reference** tab opens the default list of spectrum reference parameters for the default solvents.



- Noise – Signal to Noise value for reference signal detection (initially 10)
- Reference Shift [ppm]- chemical shift of the reference signal (default 0).
- Reference Shift Corr. [ppm] – additional chemical shift correction value. This value is added after the referencing signal has been detected and referenced.
- Search Width [ppm] - This specifies the search width window for the reference signals, e.g. a value of 0.5 ppm will search from -0.25 to 0.25 ppm from the specified reference shift.
- Signal Regions – relative intensity scaling of spectrum peaks is performed on the listed regions. The gaps between the regions are excluded.

These parameters are interpreted by the command **sref**.

The **BSMS Tab** offers the following functionalities:

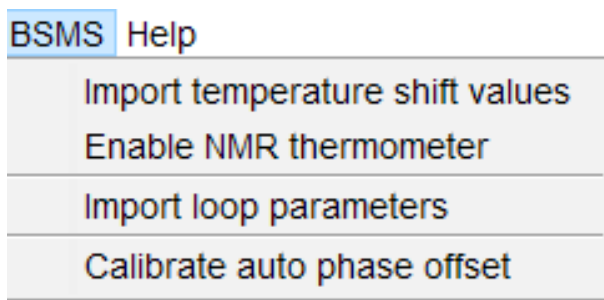


Figure 4.2: **BSMS** Tab Help menu

In IconNMR automation, the lock parameters are read from the lock table and used as they are. For more information, refer to the spectrometer hardware documentation which is available on the BASH CDROM.

INPUT AND OUTPUT PARAMETERS

See DESCRIPTION above

SEE ALSO

[lock](#) [▸ 117], [lopo](#) [▸ 123], [edprobe](#) [▸ 144], [lockdisp](#) [▸ 119], [lgain](#), [ltime](#), [lfilter](#) [▸ 116]

4.2 lgain, ltime, lfilter

NAME

lgain - Set the lock regulator loop gain.

ltime - Set the lock regulator loop time.

lfilter - Set the lock regulator loop filter.

SYNTAX

lgain [<gain>]

ltime [<time>]

lfilter [<filter>]

DESCRIPTION

The command **lgain** allows you to set the loop gain, a lock regulator parameter. It takes one argument; a loop gain value between -80 and 0 dB. This value is only used when the lock-in process is done by pressing **Lock On/Off** or **Autolock**. When lock-in is done with the TopSpin command **lock**, the loop gain is set to the **edlock** parameter **LGain**.

ltime and **lfilter** work like **lgain**, except that they set the regulator parameters loop time and loop filter, respectively.

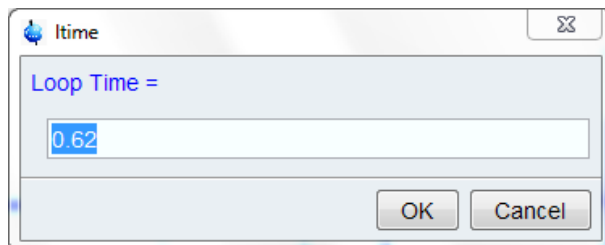


Figure 4.3: ltime

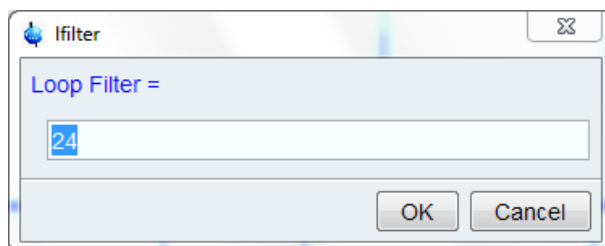


Figure 4.4: lfilter

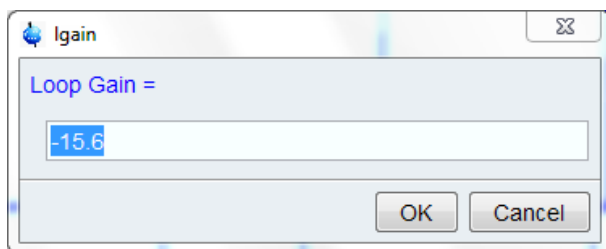


Figure 4.5: lgain

The AU program **loopadj** automatically optimizes lock gain, lock phase, loop time, loop gain and loop filter.

The regulator (loop) parameters can also be set in the BSMS display.

For information on how to determine the lock parameters click **Help | Manuals**

| **Acquisition User Guides | Basic 1D and 2D Experiments.**

Furthermore, you can refer to the spectrometer hardware documentation which is available on the BASH CDROM.

USAGE IN AU PROGRAMS

LTIME(value)

LGAIN(value)

LFILTER(value)

SEE ALSO

[lock \[117\]](#), [lopo \[123\]](#), [edlock \[109\]](#)

4.3 lock

NAME

lock - Lock the magnetic field

SYNTAX

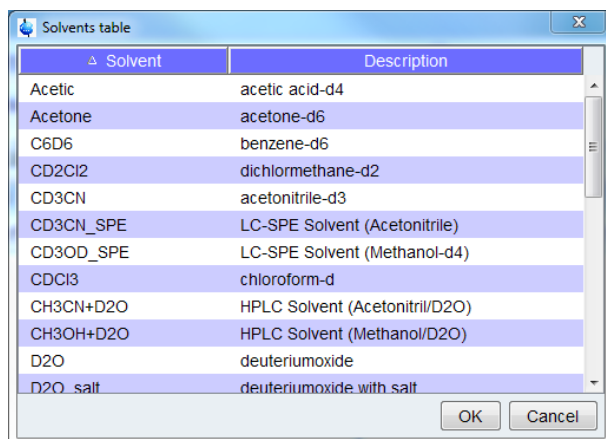
`lock [<solvent> | -acqu | -noauto]`

DESCRIPTION

The command **lock** performs the lock-in procedure. It takes one argument and can be used in the following ways:

- **lock**

Opens a dialog box with a list of solvents (see the next figure).



Solvent	Description
Acetic	acetic acid-d4
Acetone	acetone-d6
C6D6	benzene-d6
CD2Cl2	dichloromethane-d2
CD3CN	acetonitrile-d3
CD3CN_SPE	LC-SPE Solvent (Acetonitrile)
CD3OD_SPE	LC-SPE Solvent (Methanol-d4)
CDCl3	chloroform-d
CH3CN+D2O	HPLC Solvent (Acetonitrile/D2O)
CH3OH+D2O	HPLC Solvent (Methanol/D2O)
D2O	deuteriumoxide
D2O_salt	deuteriumoxide with salt

Figure 4.6: lock

When you select a solvent and click **OK**, it reads the lock parameters for that solvent from the lock table which has been set up with the command **edlock** and performs an **autolock**. The **autolock** procedure is also suitable for solvents with multiple lock signals. For each solvent with multiple signals only one lock signal is defined in the **edlock** table.

Right-click in the table to copy or export the selected entry or to modify the table properties.



Note that **lock** only shows the Solvents for the current lock nucleus (parameter LOCNUC), in this case 2H.

- **lock <solvent>**

Reads the lock parameters for the specified solvent and performs an **autolock** accordingly.

- **lock -acqu**

Reads the lock parameters for the solvent defined by the acquisition parameter SOLVENT and performs an **autolock**.



Note that IconNMR executes **lock -acqu**.

- **lock -noauto**

Reads the lock parameters for the solvent defined by the acquisition parameter SOLVENT and performs a **lock**. It does not adjust the field (capture range 10 units).

The **autolock** procedure involves the following steps:

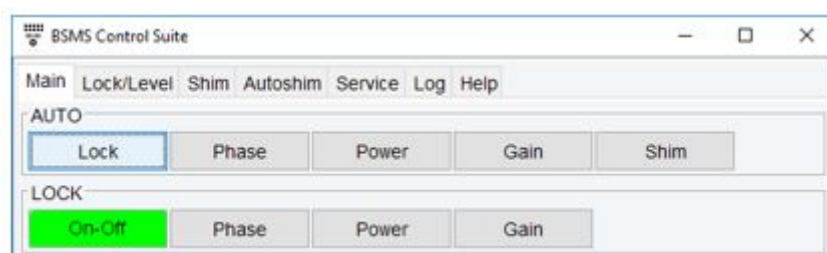
- Irradiation of the lock nucleus with frequency **Lock Freq + Reference Shift**.
- Acquisition of the lock nucleus FID.
- Fourier transform and magnitude calculation of the acquired FID.
- Determination of the position of the lock signal in the spectrum.
- Adjusting the Field such that the lock signal is exactly on resonance.
- Optimization the lock power and lock gain.



Note that the lock irradiation frequency (**Lockfreq + Reference Shift**) is solvent dependent. The value of **Reference Shift** is the chemical shift of the lock nucleus in the current solvent. As such, the irradiation frequency is approximately on resonance and **lock** needs to make only minimum field adjustments (capture range 1000 units). The advantage of this procedure is that the signal of the reference substance (e.g. TMS) appears at approximately the same position for each solvent.

The lock signal can be viewed in the lock display window which can be opened with the command **lockdisp** (see the description of this command).

The lock-in procedure can also be performed through the **bsmsdisp** command by pressing the **Auto Lock** or **Lock On/Off** key.



In that case the lock parameter values that are currently stored on the BSMS unit are used. These can be modified in the BSMS display.

INPUT PARAMETERS

- Set by the user with **eda** or by typing **solvent** etc.:
 - SOLVENT - sample solvent (input for **lock -acqu** and **lock -auto**)
 - LOCNUC - lock nucleus
- Set by the user with **edlock**:
 - See also [edlock](#) [109].

USAGE IN AU PROGRAMS

- LOCK
Executes the command **lock -acqu**.

SEE ALSO

[edlock](#) [109], [lopo](#) [123], [lockdisp](#) [119], [lgain](#), [ltime](#), [lfilter](#) [116]

4.4 lockdisp

NAME

lockdisp - Open the lock display window.

DESCRIPTION

The command **lockdisp** opens the lock display window in which the lock signal is shown (see the next figure).

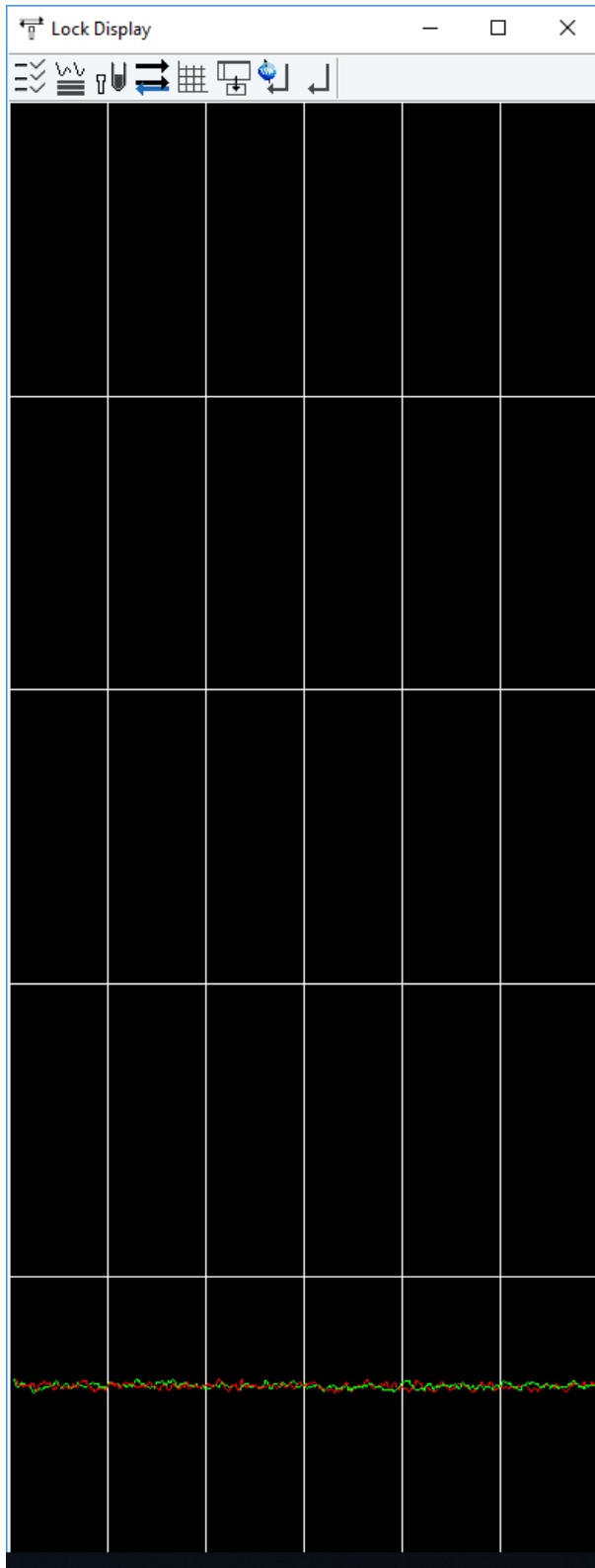


Figure 4.7: Lock Display with locking signal

At the top of the lock window the following buttons are available:



Open the User Preferences window [**set**] (see next figure).

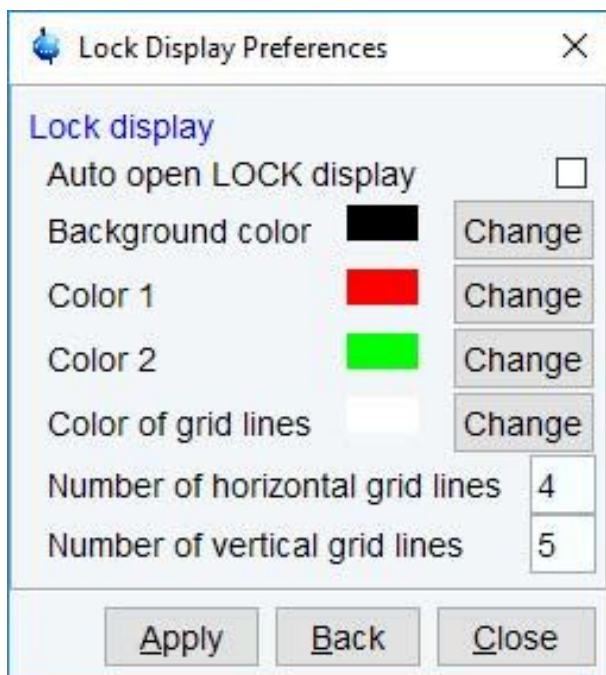


Figure 4.8: **lockdisp**: Lock Display Preferences



Toggle lock monitor mode.



Lock current sample.



Toggle lock display mode between **single** and **dual** color.



Toggle grid: both, vertical, horizontal, off single.



Detach lock window from main TopSpin window.



Select TopSpin main window.



Close the lock display window.

The lock signal is the NMR signal of the lock nucleus, typically ^2H or ^{19}F .

The lock display can be used in two different ways:

- When the field is unlocked.

In this case the lock frequency is swept and lock signal shows a pattern of wiggles with a maximum intensity at the resonance frequency. This pattern can be used to set the field value and lock phase. The field value can be adjusted from the BSMS display (**bsmsdisp**) until the maximum lock signal lies at the center of the lock display window. The lock phase can be adjusted until the intensity is about the same on both sides of the center.

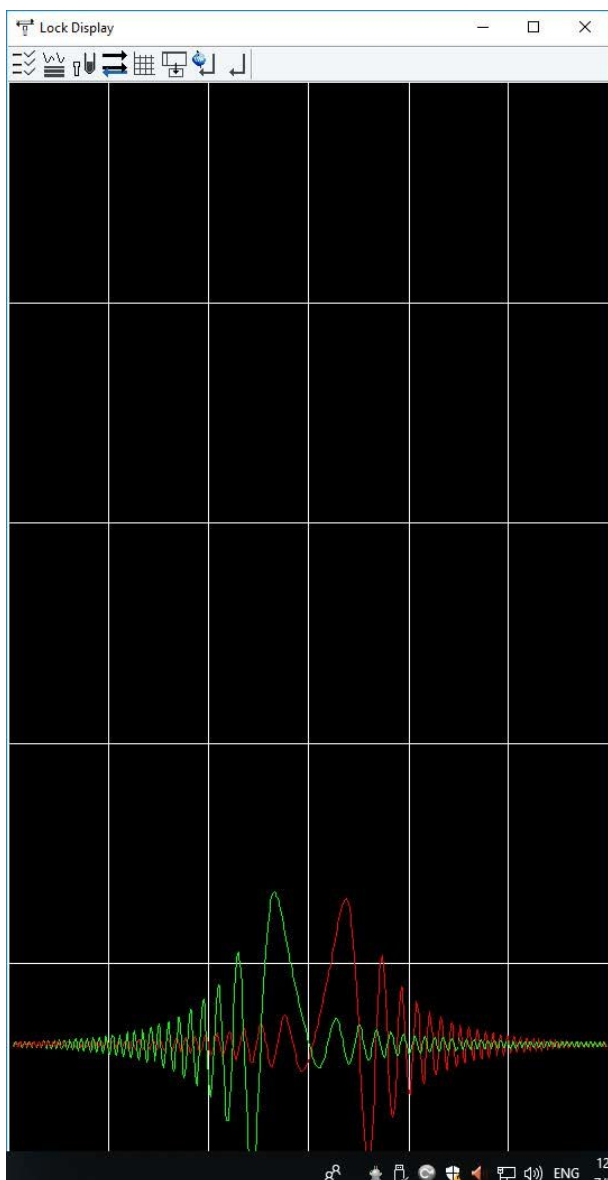


Figure 4.9: **lockdisp**: lockdisplay before locking. The wiggles here represent the ^2H signal observed in CW mode

- When the field is locked.

In this case the lock frequency is kept at the resonance position of the lock nucleus and is only adjusted in response to changes in the magnetic field. The lock signal is a horizontal line in the upper part of the lock display window. Furthermore, the position of this line can be used for shimming the magnet. When the homogeneity of the field improves, the lock signal increases, i.e. the line moves upward.

SEE ALSO

[lock](#) [► 117], [edlock](#) [► 109]

4.5 lopo

NAME

lopo - Set the lock parameters.

DESCRIPTION

The command **lopo** shows a list of available solvents (see the next figure).

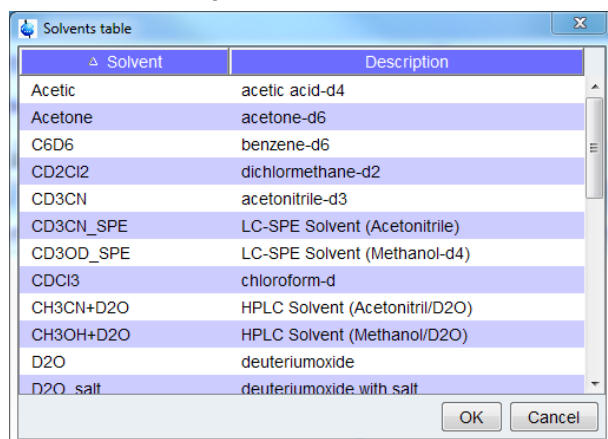


Figure 4.10: **lopo**

When you select a solvent and click **OK**, it sets the lock parameters according to the **edlock** table. As such, the lock power, loop gain, loop time, loop filter, lock phase and frequency shift are set to the lock table values of Lockpower, LoopGain, LoopTime, LoopFilt, LockPhase and Distance, respectively. These values are set on the BSMS unit without performing lock-in.

Right-click in the table to copy or export the selected entry or to modify the table properties.

The command **lopo** is useful if you want to observe the lock signal first. The lock-in procedure can then be performed by pressing the **Lock On/Off** or **Autolock** key in the BSMS display.



Note that:

lopo => **Autolock** is equivalent to **lock -acqu**

lopo => **Lock On/Off** is equivalent to **lock -noauto**

INPUT PARAMETERS

- Set by the user with **eda** or by typing **solvent** etc.:
 - SOLVENT - sample solvent
 - LOCNUC - lock nucleus
- Set by the user with **edlock** :
 - See also [edlock](#) [109]

INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
 - **acqu** - acquisition parameters
- <tshome>/conf/instr/
 - **probe** - current probe as defined by **edprobe**
- <tshome>/conf/instr/<instrum>/

- 2Hlock - lock table for nucleus 2H
 - 19Flock - lock table for nucleus 19F
- <tshome>/conf/instr/<instrum>/prosol/<probeID>/<solvent>/
bsmspar - solvent and probe dependent lock parameters

USAGE IN AU PROGRAMS

- LOPO

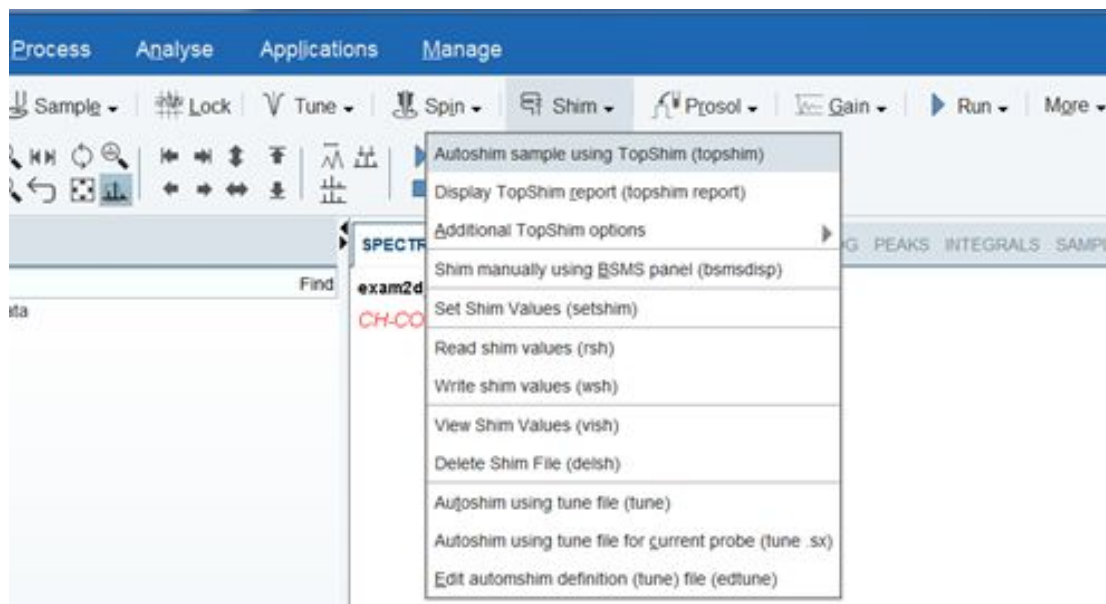
SEE ALSO

[lock](#) [► 117], [edlock](#) [► 109], [lockdisp](#) [► 119], [lgain](#), [ltime](#), [lfilter](#) [► 116]

5 Shim Commands

This chapter describes the commands which are involved in shimming the magnet. Shimming can be started with reading an appropriate shim set for the current sample and then optimizing the shim through the BSMS display (**bsmsdisp**). In automation, the optimization is performed by an automatic shimming procedure. Furthermore, if you are using a gradient probe, you can perform gradient shimming.

All shim commands can be reached through the Shim tab.



Please note that the Fourier 80 Shim procedures are described in the Fourier 80 User Manual.

5.1 autoshim

NAME

autoshim - Autoshim switching

DESCRIPTION

The command **autoshim** controls the autoshim function of the BSMS unit. It takes one argument and can be used as follows:

autoshim on

turn autoshimming on

autoshim off

turn autoshimming off

Entering **autoshim** on the command line has the same effect as pressing the AUTOSHIM key through the BSMS display. The shims for which the step size is set to a value greater than 0 are optimized. It is typically used in automation.

USAGE IN AU PROGRAMS

- AUTOSHIM_ON
- AUTOSHIM_OFF

SEE ALSO

[tune](#) [135], [ed tune](#) [132], [rsh](#), [wsh](#), [vish](#) [133], [del par](#), [del gp](#), [del sh](#) [220]

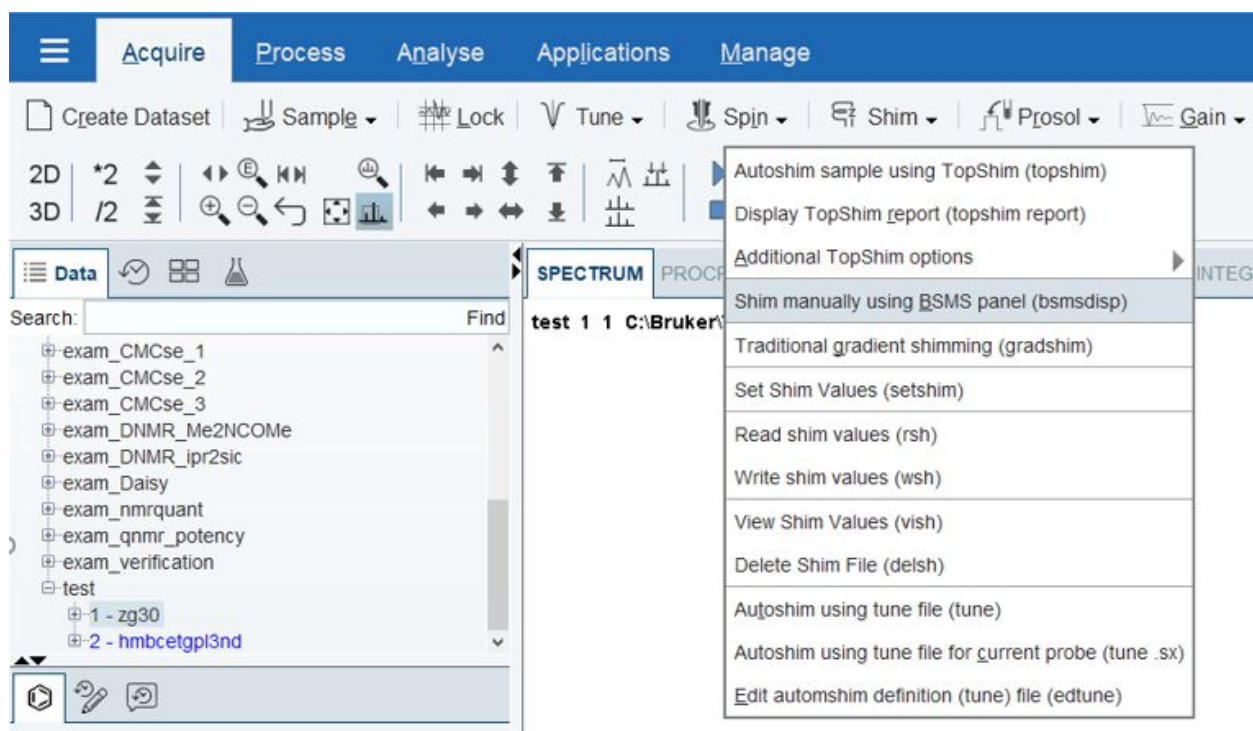
5.2 bsmsdisp

NAME

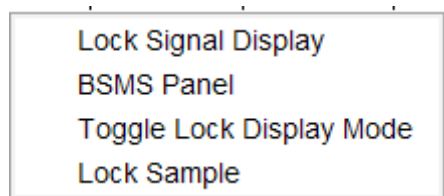
bsmsdisp – Opens the BSMS (Bruker Smart Magnet control System) control panel.

The BSMS provides an overview of the most important features and states of the shim system and magnet. It can be opened in four different ways:

- from the TopSpin menu clicking **Acquire | Shim | Shim manually using BSMS (bsmsdisp)**:



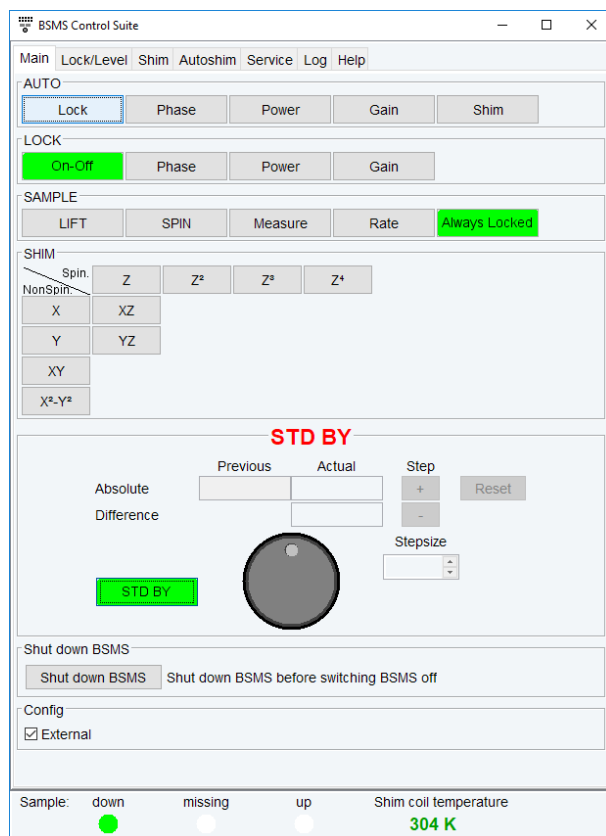
- with right click in the Lock display in the Acquisition Status Bar | **BSMS panel**:






- clicking the BSMS icon in the TopSpin menu bar
- or by typing **bsmsdisp** in the command line.

The BSMS Control Suite main window is opened:



The BSMS Main window tab offers the most prominent functions to control the magnet and the shim system:

- AUTO – Automatic lock, phase, power, gain and shim procedure
- LOCK – Switch lock on / off, lock phase, lock power, lock gain
- SAMPLE – LIFT or SPIN the sample on/off, Measure (show the actual spin rate in Hz), Rate (show/set the intended spin rate), Always locked shown green (is shown if the lock is on), Lock lost shown red (shows if the lock is lost)
- SHIM – displays a subset of currently available shim gradients
- The control window offers the possibility to change the respective values using the control knob, in steps using the stepsize or entering absolute values manually.
- The STD BY button  offers the possibility to deselect the settings.
- Shut down BSMS – is recommended before hardware turn-off
- Config. – offers the possibility to show the BSMS window in TopSpin or in an external window.
- The status bar at the bottom of the BSMS window shows the status of the current sample (down, missing or up) and the current shim coil temperature.

The tab **Lock/Level** offers the possibility to change advanced lock parameters (e.g., AUTO, LOCK, LOOP, SWEEP, HELIUM LEVEL, SHIM COIL TEMPERATURE).

The screenshot shows the 'BSMS Control Suite' window with the 'Lock/Level' tab selected. The interface is organized into several sections, each with a set of buttons:

- AUTO**: Phase (highlighted in green), Power, Gain, Lock, Shim.
- LOCK**: On-Off (highlighted in green), Field, Drift, DC, Phase, Power, Gain, Shift.
- LOOP**: Gain, Time, Filter.
- SWEEP**: On-Off, Ampl, Rate.
- HELIUM LEVEL**: Last read, Read, Measure.
- SHIM COIL TEMPERATURE**: Coil temp.

Below these sections is a large control area titled 'STD BY' in red. It contains:

- Radio buttons for 'Absolute' and 'Difference'.
- Input fields for 'Previous' and 'Actual' values.
- 'Step' controls: '+' and '-' buttons, and a 'Reset' button.
- A 'Stepsize' input field with up/down arrows.
- A large circular knob.
- A green button labeled 'STD BY'.

At the bottom, a status bar shows:

- Sample: down (green dot), missing (white dot), up (white dot).
- Shim coil temperature: 304 K (green text).

The tab **Shim** offers the possibility to change advanced LOCK & SPIN parameters and shows the complete set of shim parameters, dependent from the shim system.

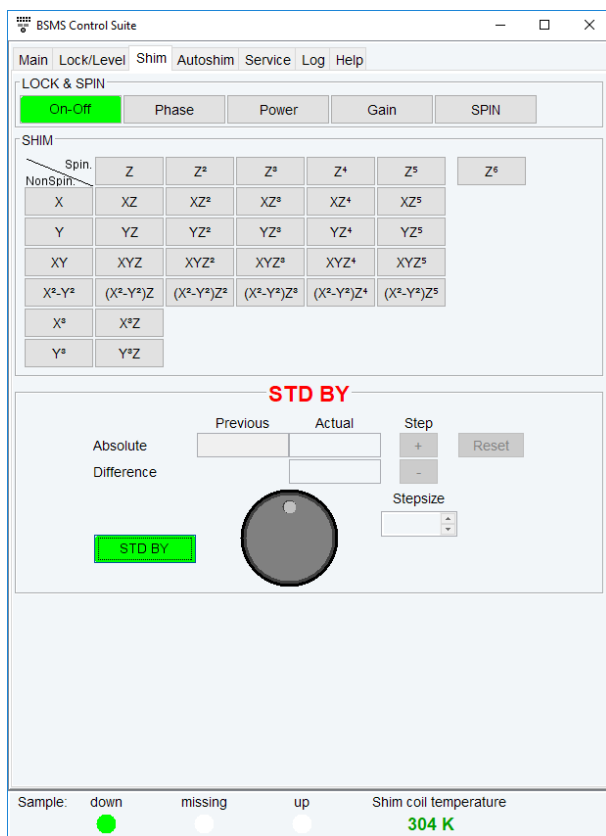
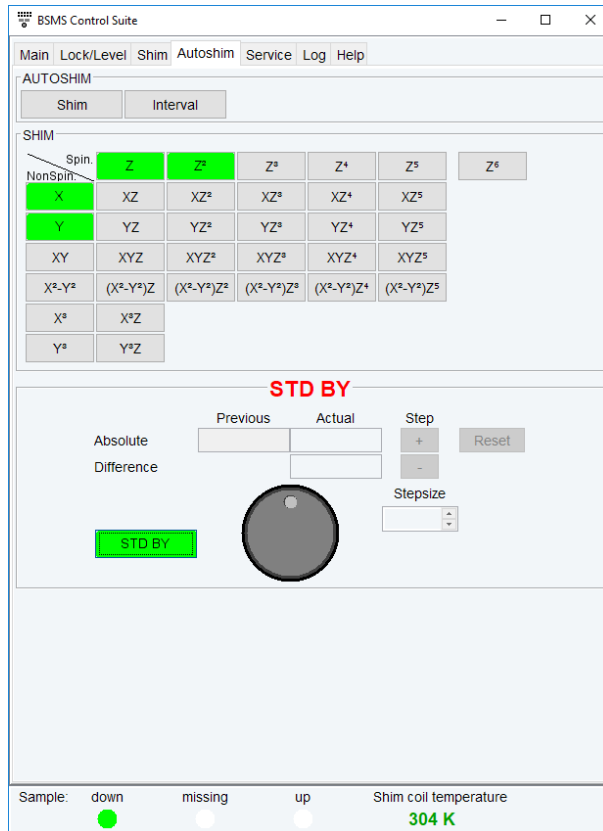


Figure 5.1: BSMS shim panel window (BoSS II shim system)

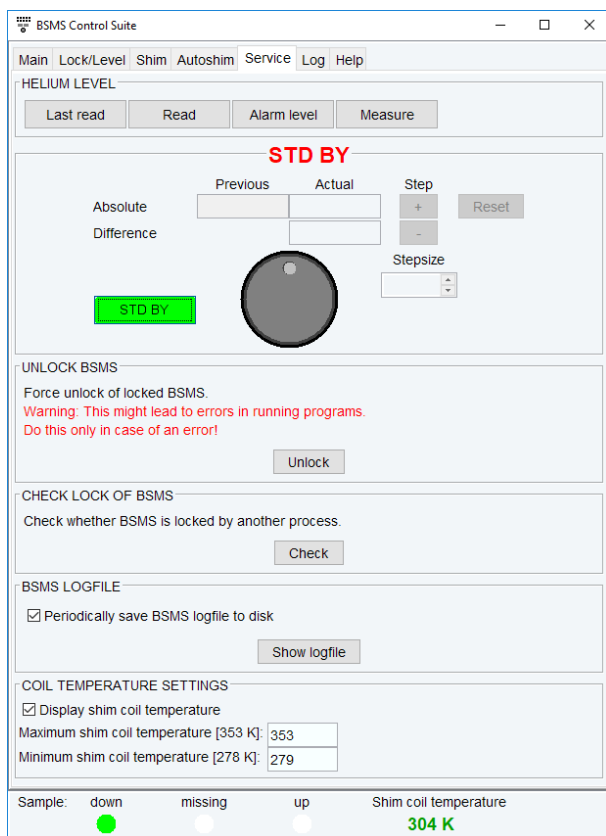
The tab **Autoshim** offers the possibility to turn the shim on or off and to select the shim gradients and their interval to be used during **autoshim**.



Please note that all shim coordinates are inactive if their absolute value is set to 0. To activate shims for **autoshim** you need to activate the absolute value higher than 0.

The tab **Service** offers some more possibilities to control and check the BSMS, e.g. Helium Level and coil temperature settings.

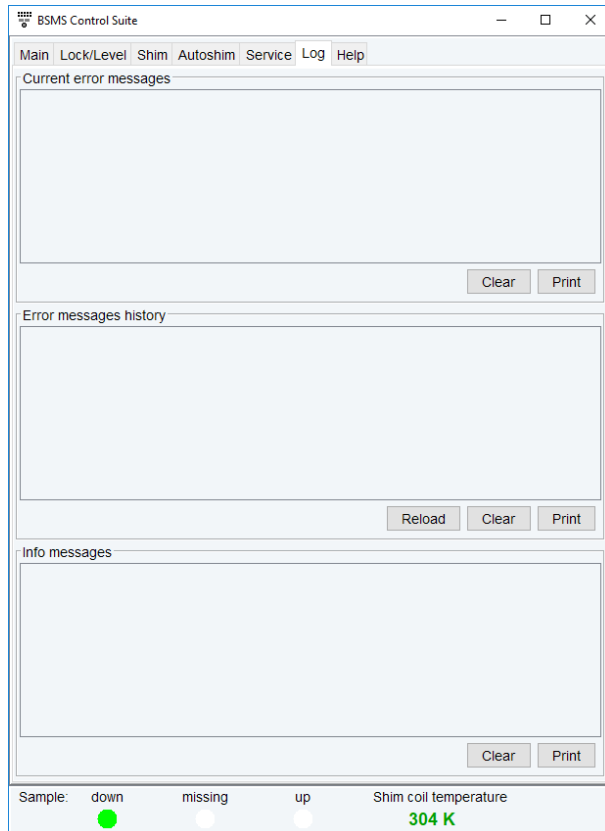
NOTICE! Please note that this service should only be used by experienced users.



The tab **Service** offers the following functionalities:

- Helium Level – check the helium level and set Alarm level
- Unlock BSMS
- Check lock of BSMS – status check
- BSMS logfile – show logfile
- Coil temperature settings – change Maximum / Minimum coil temperature

The tab **Log** shows current error messages, error messages history and info messages which can be cleared or printed:



The **Help** tab refers to detailed information about the BSMS functionalities.

See also

[edlock](#) [▶ 109], [lock](#) [▶ 117], [autoshim](#) [▶ 125]

5.3 edtune

NAME

edtune - Edit the tune file

SYNTAX

edtune [<name>]

DESCRIPTION

The command **edtune** opens a dialog box where you can edit an existing tune file or create a new one (see the next figure). The tune files you see listed here are delivered with TopSpin.

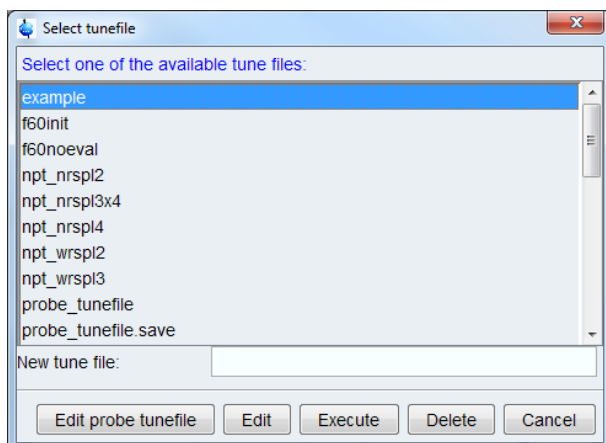


Figure 5.2: edtune

The following buttons are available:

- **Edit probe tune file**
 - Edit the probe specific tune file as it was created with **edprosol**.
- **Edit**
 - Edit the selected tune file. The file will be opened in an editable window which offers a **Save** and a **Save as** button. The latter one allows you to save the tune file under a different name, i.e. create a new tune file.
- **Execute**
 - Execute the selected tune file. This will run the command **tune**.
- **Delete**
 - Delete the selected tune file.
- **Cancel**
 - Quit the **edtune** dialog box.

Tune files are used by the **tune** command which performs automatic shimming.

- **edtune** can take one argument and can be used as follows:
 - **edtune <name>**
Edits the specified tune file. If the specified file does not exist, an error message will appear.
The format of a tune file is described for the **tune** command.

INPUT AND OUTPUT FILES

- <tshome>/exp/stan/nmr/lists/group/
 - *example* - standard tune file
 - *my_tunefile* - user defined tune file
- <tshome>/conf/instr/<instrum>/prosol/<probeID>/
 - *tunefile* - probe dependent tune file (input for **edtune** => **Probe tunefile**)

SEE ALSO

[tune](#) [► 135], [rsh](#), [wsh](#), [vish](#) [► 133], [delpar](#), [delgp](#), [delsh](#) [► 220]

5.4 rsh, wsh, vish

NAME

rsh - Read a set of shim values

wsh - Write a set of shim values

vish - View a shim file

SYNTAX

rsh [<name>]

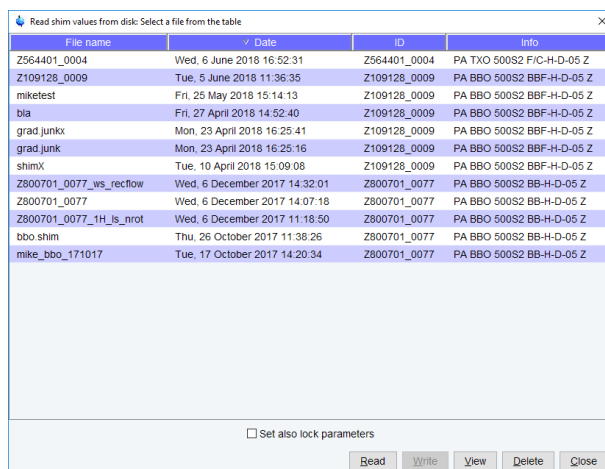
wsh [<name>]

vish [<name>]

Please note that for rsh and vish the -acqu uses the shim file form the current dataset.

DESCRIPTION

The ***sh** all open the shim dialog box when they are entered without arguments (see the next figure).



File name	Date	ID	Info
Z564401_0004	Wed, 6 June 2018 16:52:31	Z564401_0004	PA TXO 500S2 F/C-H-D-05 Z
Z109128_0009	Tue, 5 June 2018 11:36:35	Z109128_0009	PA BBO 500S2 BBF-H-D-05 Z
miketest	Fri, 25 May 2018 15:14:13	Z109128_0009	PA BBO 500S2 BBF-H-D-05 Z
bla	Fri, 27 April 2018 14:52:40	Z109128_0009	PA BBO 500S2 BBF-H-D-05 Z
grad junk	Mon, 23 April 2018 16:25:41	Z109128_0009	PA BBO 500S2 BBF-H-D-05 Z
grad junk	Mon, 23 April 2018 16:25:16	Z109128_0009	PA BBO 500S2 BBF-H-D-05 Z
shimX	Tue, 10 April 2018 15:09:08	Z109128_0009	PA BBO 500S2 BBF-H-D-05 Z
Z800701_0077_ws_rectlow	Wed, 6 December 2017 14:32:01	Z800701_0077	PA BBO 500S2 BB-H-D-05 Z
Z800701_0077	Wed, 6 December 2017 14:07:18	Z800701_0077	PA BBO 500S2 BB-H-D-05 Z
Z800701_0077_1H_Is_nrot	Wed, 6 December 2017 11:18:50	Z800701_0077	PA BBO 500S2 BB-H-D-05 Z
bbo shim	Thu, 26 October 2017 11:38:26	Z800701_0077	PA BBO 500S2 BB-H-D-05 Z
mike_bbo_171017	Tue, 17 October 2017 14:20:34	Z800701_0077	PA BBO 500S2 BB-H-D-05 Z

Figure 5.3: Read shim values

The following buttons are available:

- **Read**

Executes the command **rsh**, reading the specified shim file. When you click on a shim set, its values are loaded to the shim unit. **rsh** can also be entered on the command line with a shim file as an argument. After reading a shim file, it is usually necessary to optimize the shims, especially the Z and Z² shim. You can do that from the BSMS display (command **bsmsdisp**). **rsh** switches the autoshim function of the BSMS unit off. If you press the **AUTOSHIM** key in the BSMS display or enter **autoshim on**, the shims will be continuously optimized during the experiment.

rsh -acqu reads the shim values from the current dataset.

- **Write**

Executes the command **wsh** writing the shim values which are currently installed on the shim unit to the specified shim file. **wsh** can also be entered on the command line with a shim file as an argument.

Write shim values to disk. Select a file from the table or type a new file name

File name	Date	ID	Info
urea	Tue, 17 September 2013 17:03:43	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
tune_beg	Wed, 3 July 2013 15:51:38	55	5 mm CP-HT BB Z-GRD Z122623/0005
test	Fri, 17 January 2014 16:35:33	Z104450_0004	PA BBO 400S1 BBF-H-D-05 Z
sucrose	Tue, 4 March 2014 19:01:47	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
shintemp	Thu, 5 September 2013 14:15:29	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
pk02	Wed, 30 January 2013 11:45:57	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
pk01	Wed, 30 January 2013 11:43:22	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
pk.3d	Wed, 30 January 2013 12:15:37	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
now	Wed, 21 August 2013 12:07:17	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
kelast CPP	Thu, 1 August 2013 10:43:33	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
jic	Mon, 17 March 2014 12:00:05	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
ebatest 000	Wed, 3 July 2013 17:37:21	55	5 mm CP-HT BB Z-GRD Z122623/0005
eba_ref_z_isl_0	Thu, 4 July 2013 14:53:13	55	5 mm CP-HT BB Z-GRD Z122623/0005
eba_opt_z_isl_12	Thu, 4 July 2013 14:56:46	55	5 mm CP-HT BB Z-GRD Z122623/0005
depefirst	Thu, 31 January 2013 09:10:51	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
depebfo	Thu, 31 January 2013 15:21:58	52	5 mm PABBO BB-1H/D Z-GRD Z116098/0002
Z819001_0003_ws_reflow	Fri, 18 October 2013 17:50:38	Z819001_0003	PA TXI 400S1 H-C/N-D-05 Z
Z819001_0003_1H_is_nrot	Mon, 30 September 2013 16:33:01	Z819001_0003	PA TXI 400S1 H-C/N-D-05 Z
Z819001_0003	Fri, 18 October 2013 17:51:05	Z819001_0003	PA TXI 400S1 H-C/N-D-05 Z
Z116098_0002_ws_reflow	Tue, 4 February 2014 13:46:07	Z116098_0002	PA BBO 400S1 BBF-H-D-05 Z PLUS SP
Z116098_0002_1H_is_nrot	Tue, 4 February 2014 13:54:54	Z116098_0002	PA BBO 400S1 BBF-H-D-05 Z PLUS SP

Filename:

Read Write View Delete Close

Figure 5.4: Write Shim Values

- **View**

Executes the command **vish** opening the specified shim file with an editor. **vish** can also be entered on the command line with a shim file as an argument.

- **Delete**

Deletes the selected shim file. If the ***sh** commands are entered the command line with an argument, then they may contain wildcards; for example:

rsh a* lists all shim files beginning with “a”



Note that **rsh**, **ws** and **vish** open the dialog box with the **Read**, **Write** and **View** button activated, respectively.

INPUT FILES

- <tshome>/exp/stan/nmr/lists/bsms/
– shim files

USAGE IN AU PROGRAMS

- RSH(name)
- WSH(name)

SEE ALSO

[ed tune](#) [▶ 132], [tune](#) [▶ 135]

5.5 tune

NAME

tune -Perform automatic shimming of the magnet

SYNTAX

tune [<tunefile> | .sx]

DESCRIPTION

The command **tune** shims the magnet in an automatic procedure according to a shim definition file. This file is called the tune file and can be set up with the command **ed tune**. The command **tune** takes one argument and can be used in one of the following ways:

tune

Displays a list of available tune files (see the next figure).

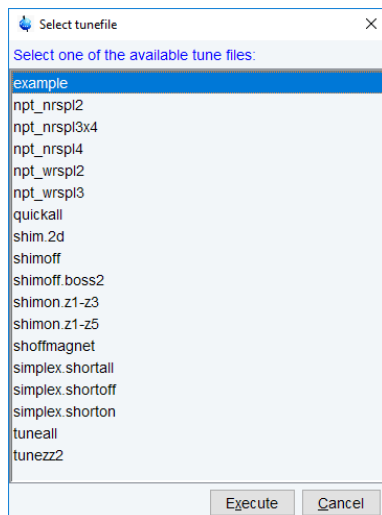


Figure 5.5: Select one of the available tune files

When you select an entry and click the **Execute** button, the corresponding tune file is interpreted and auto shimming is performed accordingly.

tune <tunefile>

Perform auto shimming according to the specified tune file.

tune .sx

Perform auto shimming according to the tune file as it is specified for the current probe. This tune file can be setup from the **ed prosol** dialog box by clicking **File | Edit Tunefile**.

An example tune file is delivered with TopSpin. You can use this as it is or modify it to your needs and store it under a different name. The statements you can use in a tune file are listed below.



Note that some of these statements are settings whereas others are commands.

Settings in a tune file:

- `USE_FIDAREA`
 - Flag indicating to use the area under the FID envelope as a criterion for field homogeneity.
- `USE_LOCKLEVEL`
 - Flag indicating to use the lock level as a criterion for field homogeneity.
- `LOCKDWELL n`
 - The number of measurements used for determining the current lock level. The measured values are averaged to suppress the effects of the noise on the lock level. Only used when `USE_LOCKLEVEL` is defined.
- `MAXLOCK m`

- The maximum lock level. Can be used to keep the lock signal from moving out of the display during the shimming procedure. The lock level is displayed at the TopSpin status line while **tune** is running.
 - DELAY *n*
 - The time (in seconds) between adjusting a shim and reading the new lock level. In the example tune file, DELAY is set to one second which is usually enough for the lock level to settle.
 - SET <shim> *w c*
 - Set the maximum step size (width) and the convergence limit for the **SIMPLEX** command. These parameters can be set for each shim separately. An example is:
- ```
SET Z1 20 3
 TIMES n
 ..
 END
```

Loop structure; all statements within the loop will be executed *n* times. Nested loops are possible to a depth of five.

### Commands in a Tune File

- ROTATION ON WAIT
  - Switches the sample rotation on, using the spin rate currently set on the BSMS unit.
- ROTATION OFF WAIT
  - Switches the sample rotation off.



Please note that these two commands are useful when switching from on-axis shims (Z1, Z2 etc ...) to off-axis shims (X, Y, XY...) since the first set (Z shims) are typically shimmed with a rotating sample and the off-axis shims (X, Y,XY ...) are adjusted with a non-rotating sample.

- RSH, RSH <filename>
  - Reads a shim file. If an argument is specified, RSH will read the corresponding shim file. If not, it will read the shim file with the name of the solvent defined by the acquisition parameter SOLVENT.
- Z *s i*, Z2 *s i*, ..., XY *s i*
  - Optimizes single shims. These commands take two arguments:
    - s* = step size; the shim increment used as long as the lock level increases
    - i* = iterations; the maximum number of steps after passing the maximum

A shim is first changed *s* units in one direction. If this increases the lock level, the shim is changed again *s* units in the same direction. This is repeated until a shim change decreases the lock level. Then the direction of change is reversed and the step size is reduced. This process is continued until one of the following criteria has been met:

- The lock level has not changed significantly during the last step.
- The maximum number of iterations (*i*) has been performed.
- The step size has been reduced to one.

Examples of shim commands are:

```
Z 10 3
```

Z2 10 3

Z3 10 3

- `SIMPLEX <shim1 shim2 etc.>`
  - Optimizes the specified shims according to the simplex algorithm which can be used for lock level and FID area shimming. SIMPLEX uses the step size and convergence limit defined by the SET statement (see above). The simplex algorithm is described in the *example* file (see INPUT FILES below).
- `AUTOSHIM ON <shim1=m, shim2=n, ...>`
  - Switches on the automatic shimming function on the shim unit after the **tune** command has finished. This command allows you to adjust the shims continuously during the entire experiment. Only the shims that are specified as arguments to the `AUTOSHIM ON` command will be optimized. For each shim, you can specify the step size used for auto shimming. If you do not specify the step size, the default value of 5 is used. An example of this command is:
- `AUTOSHIM ON Z1=2 Z2`
  - Since this command becomes effective after the **tune** command has finished, it can be specified anywhere in the tune file.
- `AUTOSHIM OFF`
  - Switches off automatic shimming on the shim unit. It makes sure that automatic shimming is switched off when it was switched on before, either from the last executed tune file or manually from the BSMS display.



Note that it would not make sense to use `AUTOSHIM ON` and `AUTOSHIM OFF` within one tune file.

- `LOCKPHASE s i`
  - Optimize the lock phase. This command takes two arguments:
    - `s` = step size
    - `i` = iterations; the maximum number of steps
  - As an alternative to the automatic shimming with **tune**, you can optimize the shims manually from the BSMS display. If the shims are far away from the optimum, you can read a standard shim set with the command **rsh** and then do manual shimming.

An alternative to the simplex procedure in **tune** is the AU program **simplex**.

## INPUT FILES

- `<tshome>/exp/stan/nmr/lists/group/`
  - *example* - tune file
- `<tshome>/conf/instr/<instrum>/prosol/<probelD>/`
  - *tunefile* - tune file for the current probe (input for **tune .sx**)

## USAGE IN AU PROGRAMS

- `TUNE(tunefile)`
  - `TUNESX`
- Eexecutes the command **tune .sx**

## SEE ALSO

[ed tune](#) [▶ 132], [rsh](#), [wsh](#), [vish](#) [▶ 133], [delpar](#), [delgp](#), [delsh](#) [▶ 220]

## 5.6 topshim

---

### NAME

**TopShim** – Automatic shimming tool

### DESCRIPTION

The command **topshim** opens the automatic shimming tool.

For further information please refer to the Gradient Shimming Manual under **Help | Manuals | Acquisition – Application Manuals | Topshim**.

### SEE ALSO

[tune](#) [► 135], [ed tune](#) [► 132], [rsh](#), [wsh](#), [vish](#) [► 133], [del par](#), [del gp](#), [del sh](#) [► 220]



## 6 Probe Commands

This chapter describes the commands which are involved in probe handling. This includes probe selection, the tuning and matching procedure and sample insert and eject.

### 6.1 **atma**

---

#### NAME

**atma** - Automatic tuning and matching of ATM probes.

#### USAGE

**atma** [exact | coarse] [high].

Type **atma ?** for a complete list of options.

#### DESCRIPTION

The command **atma** performs tuning and matching of an ATM probe. It will automatically perform the following steps:

1. Stop the sample rotation if it is on.
2. Read the nucleus with the lowest frequency as it was set up with **edasp**.
3. Determine the optimum sweep width and number of steps.
4. Tune and match the probe.
5. Repeat step 3 to 4 for all other nuclei which were set up with **edasp** in the order of increasing frequency.
6. Turn on the sample rotation if it was on before **atma** was started.

The command **atma** can be used with various options, for example:

- **atma exact** will determine the optimum tuning and matching more precisely than **atma** without an argument and will therefore be slower.
- **atma coarse** will determine the optimum tuning and matching less precisely than **atma** without an argument and will therefore be faster.
- **atma high** will start with the nucleus with the highest frequency, and tune and match the probe for each nucleus in the order of decreasing frequency.
- **atma storeWobb <x>** will automatically save the wobble curve after optimisation. **<x>** stands for the respective procno of the used dataset.

If more than one nucleus should be stored than the respectively next wobble curve n+1 will be stored in the procno number **<x+1>** (see also command **wbwr**).

Type **atma ?** for a complete list of options.

On ATM probes, **atma** can be used instead of the **wobb**. These two commands differ in the following respects:

- **atma** is fully automatic whereas **wobb** requires the user to perform the tuning and matching manually.
- **atma** automatically determines the optimal sweep width and number of steps whereas **wobb** uses the values of WBSW and WBST, respectively.

- **wobb** must be terminated with **stop** or **halt** whereas **atma** automatically finishes when optimum tuning and matching is reached. If you want to interrupt **atma**, you can do that with the command **kill**.

Automatic tuning and matching is not only convenient, it also allows you to tune and match the probe during automation. In IconNMR, you can choose to do that before each experiment, after each sample change or after each solvent change.

For more information on the tuning and matching process, see **wobb**.

**Please note:** When using an IProbe, the command might appear unresponsive due to processes that can take a few minutes:

- After installation of a new TopSpin version the atma server might install a new firmware to the IProbe electronics.
- After finishing an automatic tuning procedure, the data on the probe might need compression.

In both cases, the status is reported accordingly in the **atmm** window or the topspin status bar.

### INPUT PARAMETERS

- NUC1 - NUC4 - nuclei as defined with **edasp**

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters
- <tshome>/conf/instr/<instrum>/
  - *nuclei* - nuclei table
- <tshome>/prog/wobble/
  - *acqu\_go4* - wobble parameters
  - *Pulsprog\_X* - wobble pulse program

### SEE ALSO

[atmm \[► 142\]](#), [wobb \[► 153\]](#), [wbwr \[► 152\]](#)

## 6.2 atmm

---

### NAME

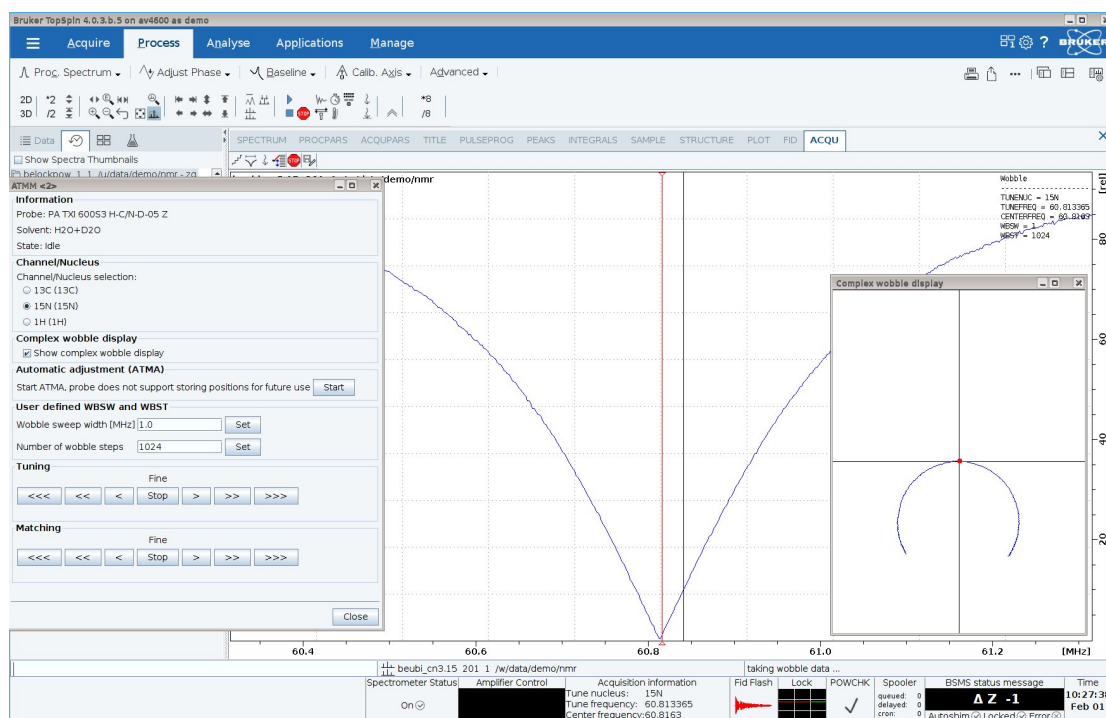
**atmm** - Manual tuning and matching of ATM probes.

### USAGE

atmm [manWbsw]

Type **atmm ?** for a complete list of options.

## DESCRIPTION



The command **atmm** is a manual tuning and matching procedure for ATM probes. It is not needed very often because ATM probes are designed for automatic tuning and matching with **atma**. Sometimes, however, the probe's resonance frequency is so far away from the optimum that **atma** would take very long to finish or would fail. In practice, this only occurs for certain nuclei at broadband probes. In that case, **atmm** allows you to manually tune and match the probe for that nucleus.

**atmm** performs the following steps:

- It reads the nucleus with the lowest frequency as it was set up with **edasp**.
  - It determines the optimum sweep width and number of steps.
  - It shows the reflected power (tuning/matching curve) in the TopSpin acquisition data field.
  - It opens the **atmm** control window from where you can:
    - See information about the connected probe and the status of the atma server.
    - Select the nucleus for which you want to tune and match the probe. By default, the nucleus with the lowest frequency is selected.
    - Start ATMA with a click on the start button which will perform an automatic tuning/matching. The positions will be stored for further use of **atma** or **atmm**.
    - Open an optional window where the complex wobble curve (real and imaginary part) is displayed in a sophisticated representation visualizing more information compared to a conventional wobble curve; this can be helpful to optimize more quickly. Instead of the normal wobble curve, a circle with a red dot is shown which has to be moved into the center of the coordinate system to achieve optimal tuning/matching.
    - Perform coarse tuning/matching on broadband probes. This is the equivalent of setting the sliders on a non ATM probe to predefined numbers.
    - Perform fine tuning/matching while observing the curve in the TopSpin acquisition data field. This is the equivalent of turning the knobs or moving the sliders on a non ATM probe. See **wobb** for a description on how to reach the optimum tuning and matching.
- During tuning and matching with the arrow keys, the positions are saved for the

current channel and nucleus combination. **atmm** will move to these positions automatically on startup if the channel and nucleus combination will be selected again after rerouting.

- Click **Close** to finish the tuning/matching process.

If **atmm** is used with the argument **manWbsw**, it does not determine the sweep width and number of steps automatically but interprets the parameters WBSW and WBST, respectively. **atmm ?** will show you a complete list of arguments.

The difference between **atmm** and **wobb** is that:

- **atmm** can only be used on ATM probes.
- **atmm**, when used without arguments, automatically determines the optimum sweep width and number of steps whereas **wobb** uses the values of WBSW and WBST, respectively.
- **atmm** allows you to optimize tuning and matching from TopSpin whereas **wobb** requires you to turn the knobs (or move the sliders) on the probe.

For more information on the tuning and matching process, see **wobb**.

**Please note:** When using an IProbe, the command might appear unresponsive due to processes that can take a few minutes:

- After installation of a new TopSpin version the atma server might install a new firmware to the IProbe electronics.
- After finishing an automatic tuning procedure, the data on the probe might need compression.

In both cases, the status is reported accordingly in the **atmm** window or the topspin status bar.

### INPUT PARAMETERS

- NUC1 - NUC4 - nuclei as defined with **edasp**
- WBSW - sweep width (only used by **atmm manwbsw**)
- WBST - number of steps (only used by **atmm manwbsw**)

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters
- <tshome>/prog/wobble/
  - *acqu\_go4* - wobble parameters
  - *Pulsprog\_X* - wobble pulse program

### SEE ALSO

[atma](#) [▶ 141], [wobb](#) [▶ 153]

## 6.3 edprobe

### NAME

**edprobe** – Edit the probe table

## DESCRIPTION

The command **edprobe** opens the probe table editor:

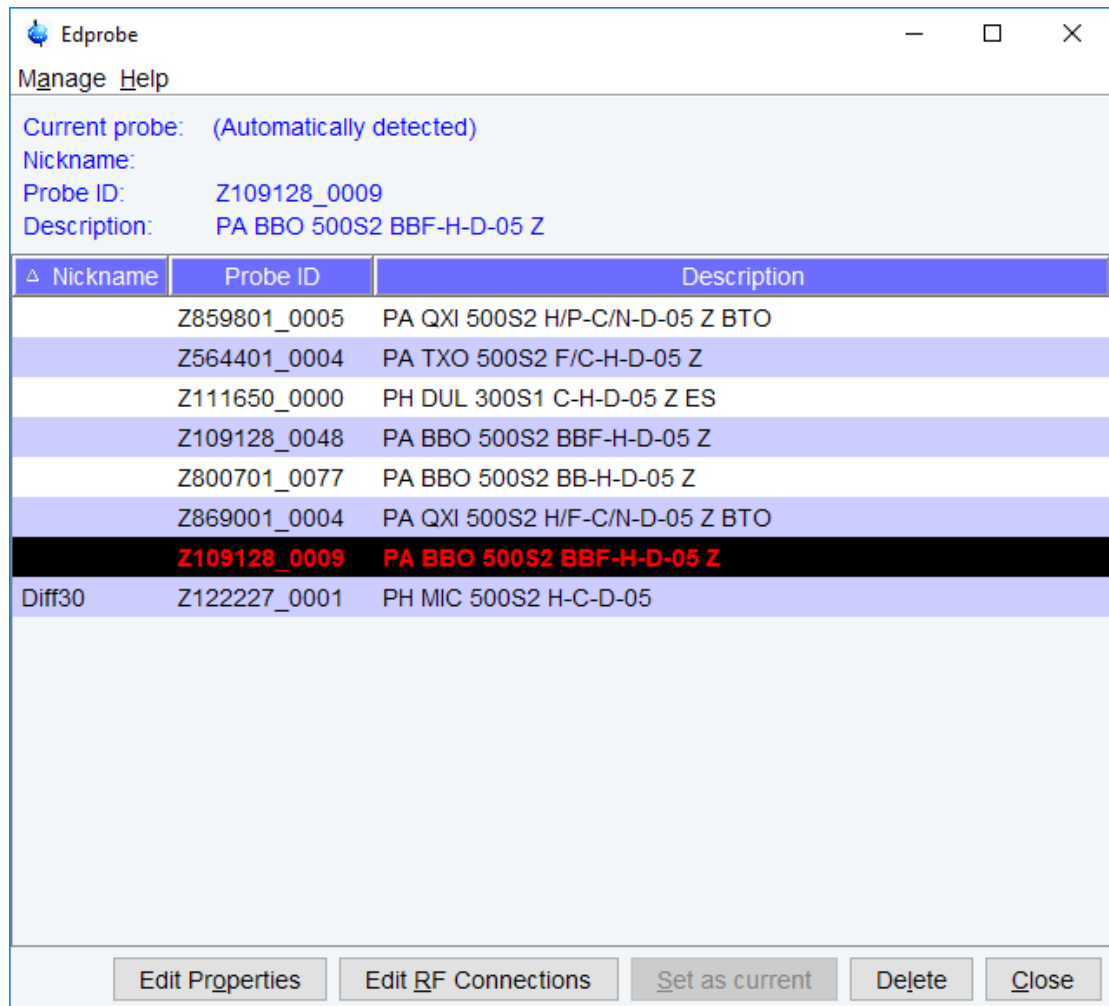


Figure 6.1: edprobe

The table has columns for Nickname (optional), Probe ID and description of configured probes. The Nickname can be freely chosen to identify a probe for the user more easily.

The entry which is defined as the current probe is highlighted. If an automatic probe detection through PICS is available, then the currently connected probe is automatically shown as the current probe. In that case the **Set as current** button is greyed out.

The probe table has a menu **Manage** in the upper left corner that offers the following commands:

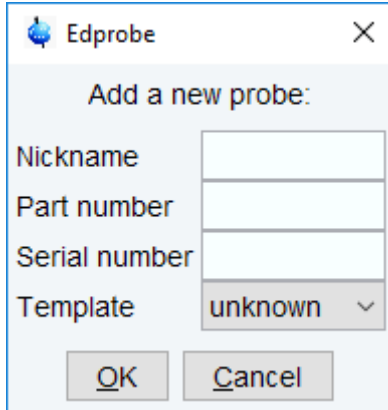
- Add a new probe**
- Import old probes**
- View Properties**
- Print**
- Flash Pics**

### Add a new probe

The probe dialog editor will be opened where you can define a new probe.

The name of the new probe will be the combination of Part number and Serial number.

With Template, one can select typical probe configurations. This simplifies the entry of the probe parameters.

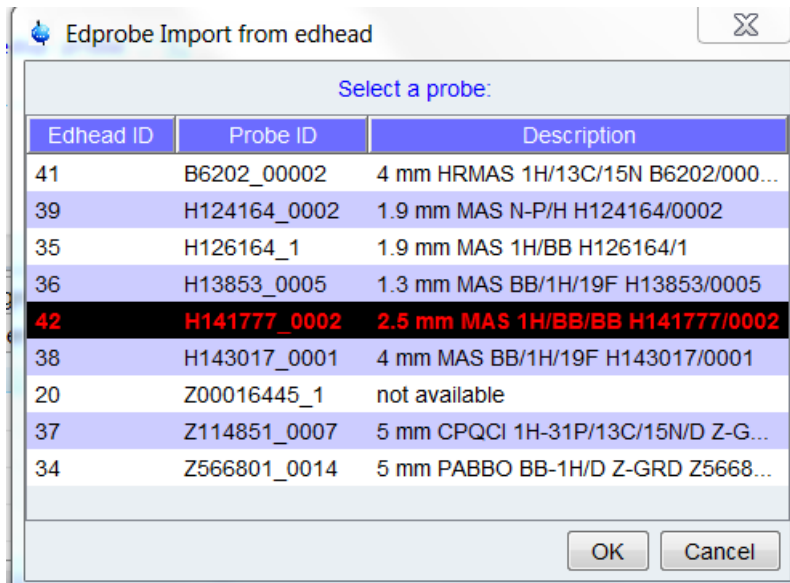
The image shows a dialog box titled "Edprobe" with a close button (X) in the top right corner. Inside the dialog, there is a section titled "Add a new probe:". Below this title, there are four input fields: "Nickname", "Part number", "Serial number", and "Template". The "Template" field is a dropdown menu currently showing "unknown". At the bottom of the dialog, there are two buttons: "OK" and "Cancel".

| Field         | Value   |
|---------------|---------|
| Nickname      |         |
| Part number   |         |
| Serial number |         |
| Template      | unknown |

Figure 6.2: Add a new probe

### Import old probes

If older (**edprobe**) definitions of probes are available in the current installation, they are listed in the import table. By selecting an entry, all settings of this probe are imported to the probe table.

The image shows a dialog box titled "Edprobe Import from edhead" with a close button (X) in the top right corner. Inside the dialog, there is a section titled "Select a probe:". Below this title is a table with three columns: "Edhead ID", "Probe ID", and "Description". The table contains several rows of data. The row with "Edhead ID" 42 is highlighted in red. At the bottom of the dialog, there are two buttons: "OK" and "Cancel".

| Edhead ID | Probe ID     | Description                        |
|-----------|--------------|------------------------------------|
| 41        | B6202_00002  | 4 mm HRMAS 1H/13C/15N B6202/000... |
| 39        | H124164_0002 | 1.9 mm MAS N-P/H H124164/0002      |
| 35        | H126164_1    | 1.9 mm MAS 1H/BB H126164/1         |
| 36        | H13853_0005  | 1.3 mm MAS BB/1H/19F H13853/0005   |
| 42        | H141777_0002 | 2.5 mm MAS 1H/BB/BB H141777/0002   |
| 38        | H143017_0001 | 4 mm MAS BB/1H/19F H143017/0001    |
| 20        | Z00016445_1  | not available                      |
| 37        | Z114851_0007 | 5 mm CPQCI 1H-31P/13C/15N/D Z-G... |
| 34        | Z566801_0014 | 5 mm PABBO BB-1H/D Z-GRD Z5668...  |

Figure 6.3: import

### View Properties

Opens the Probe Properties of the selected entry for viewing only.

View Properties of probe Z820201\_0280

Properties of probe Z820201\_0280

Probe Identity

PHNAME PA BBI 400S1 H-BB-D-05 Z

NICKNAME Nickname

PHPDID Z820201 Part number

PHPDSER 0280 Serial number

Product Info

PHTYPE HR Type of probe

PHPDECL 5.13 Engineering change level

PHPDDAT 20150827 Production date

PHPDLOC BCH Production site

PHNFREQ [MHz] 400 Nominal (1H) frequency

PHDIAM SB Probe diameter

PHATMA ☒ ATMA probe?

CYPROB ☐ Cryo probe?

Gradient System Parameters

PHGTYPE Z Type of gradient system

GRADNAME\_X name of X gradient field

GRADNAME\_Y name of Y gradient field

GRADNAME\_Z 13 name of Z gradient field

Parameters of the Z Gradient System

PGMSZ 5 Highest gradient strength in Z direction [G/cmA]

PGMCZ 10 Maximum permissible current in Z direction [A]

Temperature Parameters

PHTPTYP TypeT Type of temperature sensor

PHEATTEMPMIN [degree] -274 Minimum allowed temperature of probe heater

PHEATTEMPMAX [degree] 400 Maximum allowed temperature of probe heater

PHTPMIN [degree] -150 Minimum permissible temperature

PHTPMAX [degree] 150 Maximum permissible temperature

Temperature Controlling Gas Flow

PGFVTGASFLOWREC 400 Recommended flow at standard conditions

PGFVTGASFLOWMAX 1800 Maximum allowed flow

PGFVTGASFLOWMIN 200 Minimum recommended flow

Undo Print Close

## Print

Opens the printing dialog for the Edprobe Probes Table.

## Flash Pics

Allows to flash the PICS of the current probe

Flash PICS

Flash PICS of current probe.  
Please enter the name of the "Signed PICS File" or select the "Signed PICS File" using the "Browse" button.

**Warning: Improper use of this tool may seriously damage your probe!**

PICS file:

Figure 6.4: flashpics

This requires that the probe is connected with a PICS cable. Only digitally signed PICS files can be used to flash the probe. A new PICS file must be copied (flashed) to a probe if, for some reason, the current PICS of the probe has become corrupted or when additional parameters describing probe features become available in TopSpin.

At the bottom of the **edprobe** dialog you can select following buttons:

## Edit Properties

Opens the Probe Properties of the selected entry for editing.

Edit Properties of probe Z820201\_0280

Properties of probe Z820201\_0280

Probe Identity
Product Info
Gradient System Parameters
Temperature Parameters
Coil Parameters
Sample Parameters
Peak Powers
Available Plugins
90 deg. Pulses

Probe Identity

PHNAME

PA BBI 400S1 H-BB-D-05 Z

NICKNAME

Nickname

PHPDID

Z820201

Part number

PHPDSER

0280

Serial number

Product Info

PHTYPE

HR

Type of probe

PHPDECL

5.13

Engineering change level

PHPDDAT

20150827

Production date

PHPDLOC

BCH

Production site

PHNFRQ [MHz]

400

Nominal (1H) frequency

PHDIAM

SB

Probe diameter

PHATMA

☒

ATMA probe?

CYPROB

☐

Cryo probe?

Gradient System Parameters

PHGTYPE

Z

Type of gradient system

GRADNAME\_X

name of X gradient field

GRADNAME\_Y

name of Y gradient field

GRADNAME\_Z

13

name of Z gradient field

Figure 6.5: Edit probe properties with PICS

If the probe is connected with a PICS cable, only a few properties can be changed, see figure above. For probes without PICS, all properties can be adjusted, see figure below.

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H9775SA4\_17\_017

Edit Properties of probe Z800701\_0077

Properties of probe Z800701\_0077

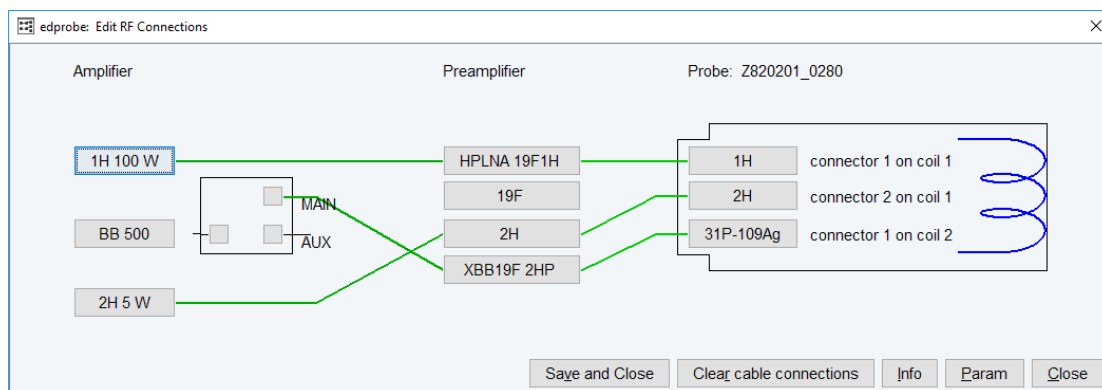
|                            |                      |                          |                                                         |
|----------------------------|----------------------|--------------------------|---------------------------------------------------------|
| Probe Identity             | PGFVTGASFLOWMAX      | 0                        | Maximum allowed flow                                    |
| Product Info               | PGFVTGASFLOWMIN      | 0                        | Minimum recommended flow                                |
| Gradient System Parameters | Protection Air       |                          |                                                         |
| Temperature Parameters     | PHCATYP              | unknown                  | Type of temperature sensor                              |
| Coil Parameters            | PHCAMIN [degree]     | -274                     | Minimum permissible temperature                         |
| Sample Parameters          | PHCAMAX [degree]     | -274                     | Maximum permissible temperature                         |
| Peak Powers                | Coil Parameters      |                          |                                                         |
| Available Plugins          | PHCGASC              | nitrogen                 | Gas compensation                                        |
| 90 deg. Pulses             | PHCOINO              | 2                        | Number of coils                                         |
|                            | Parameters of Coil 1 |                          |                                                         |
|                            | PHCH1                | 1                        | Number of connectors on coil 1                          |
|                            | PNUC1                | Edit...                  | Nuclei on coil 1                                        |
|                            | Parameters of Coil 2 |                          |                                                         |
|                            | PHCH2                | 2                        | Number of connectors on coil 2                          |
|                            | PNUC2                | Edit...                  | Nuclei on coil 2                                        |
|                            | Sample Parameters    |                          |                                                         |
|                            | PHSDIAM [mm]         | 5                        | Sample diameter                                         |
|                            | PHSDPTH [mm]         | 20                       | Maximum depth below magnetic centre                     |
|                            | PHSDPTHMIN [mm]      | 20                       | Minimum depth below magnetic centre                     |
|                            | PHSDPTHREC [mm]      | 20                       | Recommended depth below magnetic centre                 |
|                            | PHSDPTHSUP [mm]      | 20                       | Depth below magnetic centre needed for best solvent sup |
|                            | RECOMFILL [mm]       | 0                        | Recommended liquid filling height                       |
|                            | Peak Powers          |                          |                                                         |
|                            | PHPOWER              | Edit...                  | Peak powers                                             |
|                            | Available Plugins    |                          |                                                         |
|                            | PLUGPARTNO           | 0                        | Part number of plugin                                   |
|                            | PLUGSERNO            | 0                        | Serial number of plugin                                 |
|                            | PLUGACTIVE           | <input type="checkbox"/> | Plugin is active                                        |
|                            | PHPGFL               | <input type="checkbox"/> | FlowInsert plugin available?                            |
|                            | 90 deg. Pulses       |                          |                                                         |
|                            | POWCALDATA           | Show...                  | Power and width of 90 deg.pulses                        |

Undo Print Close

Figure 6.6: Edit probe properties with no PICS

## Edit RF Connections

It displays a new window where the wiring between the amplifier or preamplifier and the probe connectors can be defined, see figure below:



## Set as current

The highlighted entry will be defined as current probe. This button is only active when no automatic probe detection with PICS is available.

## Delete

The selected entry will be deleted (not possible for the currently installed probe).

## Close

Close the probe table editor.

By exiting **edprobe**, if current probe parameters have changed, the **Edit RF Connections** window is displayed where the preamplifier probe connections must be defined.

The current probe as defined with **edprobe**, is interpreted by the commands **edprosol**, **edlock**, **lock**, **lopo** and **setpre** as well as during lconNMR automation. At the end of an acquisition the current probe is stored in the acquisition status parameter PROBHD (see **dpa**).

## The input files of edprobe command:

- <tshome>/conf/instr/probehead - current probes name
- <tshome>/conf/instr/spectrometer name/<part #>\_<serial #>.par - probe parameters

## SEE ALSO

[cf \[ 51\]](#), [atma \[ 141\]](#), [atmm \[ 142\]](#), [wobb \[ 153\]](#)

## 6.4 ej, ij

### NAME

- ej** - Eject the sample from the magnet.
- ij** - Insert the sample into the magnet.

### DESCRIPTION

The command **ej** ejects the sample from the magnet. It switches on the air flow and keeps it on until it is explicitly switched off, for example with **ij**.

The command **ij** inserts the sample into the magnet. This command is used when the magnet air flow is on and the sample is floating on top of it. **ij** gradually reduces the air flow to zero so that the sample is lowered into the magnet.

As an alternative to the command **ej** and **ij**, you can also press the LIFT ON/OFF button though the BSMS display.

The SAMPLE DOWN indicator in the shimming panel of the BSMS display is lit when the sample is positioned correctly in the probe. The SAMPLE UP indicator is lit when the sample has reached the top of the magnet. The SAMPLE MISSING indicator is lit if the sample is somehow positioned between the magnet top and the probe, either moving up or down or being stuck. The latter can happen, for instance, when the air flow is too high.

## USAGE IN AUTOMATION

EJ

IJ

## SEE ALSO

[ro](#) [ 151]

## 6.5 ro

---

### NAME

**ro** - Switch the sample rotation on or off

### SYNTAX

**ro** [ acqu | on | off | off wait ]

### DESCRIPTION

The command **ro** switches the sample rotation on or off. When entered without arguments, it opens a dialog box (see the next figure).

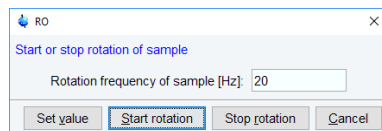


Figure 6.7: **ro**

Here, you can set the rotation frequency and start/stop the rotation.

**ro** takes up to two parameters and can be used as follows:

- **ro on**  
Switches the sample rotation on with the spin rate currently set through the BSMS display (visible when you press the SPIN RATE key).
- **ro acqu**  
Sets the spin rate to the value of the acquisition parameter RO, then switches rotation on and waits for 60 seconds. If spin rate has not been reached within that time, an error message appears.
- **ro off**  
Switches the sample rotation off.
- **ro off wait**  
Switches the sample rotation off and waits until the rotation has reached zero. During the waiting time the BSMS unit cannot be accessed by other commands.
- **ro <value>**  
Sets the acquisition parameter RO to <value>.

As an alternative to the command **ro**, you can press the SPIN ON/OFF, and SPIN RATE keys through the BSMS display (command **bsmsdisp**)

### INPUT PARAMETERS

- RO - sample rotation frequency (input for **ro acqu**)

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters

### USAGE IN AU PROGRAMS

- ROT  
Executes the command **ro acqu**.
- ROTOFF  
Executes the command **ro off wait**.

### SEE ALSO

[ej, ij](#) [▶ 150]

## 6.6 **wbwr**

### NAME

**wbwr** - save wobble curve to disk

### DESCRIPTION

The command **wbwr** saves the wobble curve to disk.



Please note that the command is only valid in the wobble mode (first enter command **wobb**).

**wbwr** prompts the user to enter a PROCNO which will be used to store the wobble curve.

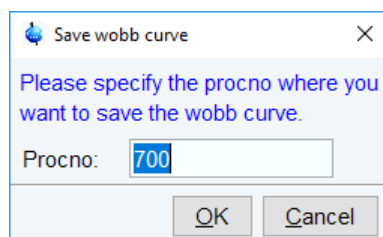


Figure 6.8: *wbwr*

As an alternative to **wbwr** entered on the command line, the button can be clicked in the TopSpin toolbar.

The wobble curve is stored as processed data (1r) and not as raw data (fid.). This provides the additional option of using standard processing tools like e. g. multiple display.

In addition, **wbwr** can directly be entered together with an additional parameter denoting the PROCNO that should be used, i.e. "**wbwr 4**".

### OUTPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/<procno>/

- 1r - the wobble curve
- procs - processing status bar

## SEE ALSO

[wobb](#) [ 153]

6.7 **wobb**

## NAME

**wobb** - Manual tuning and matching of the probe.

## USAGE

**wobb** [high][ext50][raw][all][f1][f2][f3][f4]

## DESCRIPTION

The command **wobb** allows you to manually tune and match the probe. It opens the wobble window showing the wobble curve (see the next figure).

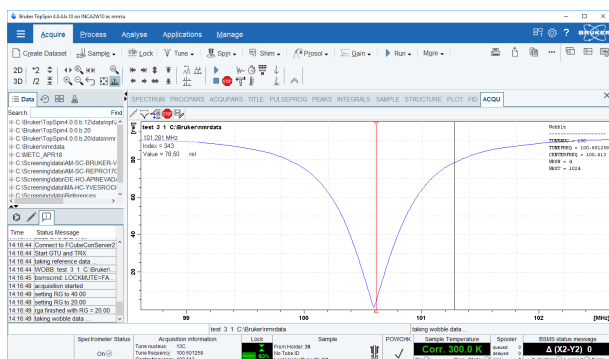


Figure 6.9: **wobb**

The buttons have the following functions:



Change the number of wobble steps [**wbst**].



Change the wobble sweep width [**wbsw**].



Change the wobble frequency.



Switch to the next channel/nucleus (if available).



Stop the wobble procedure.

Turn the tuning and matching knobs on the probe until the wobble curve is exactly in the middle and its minimum reaches the zero line.

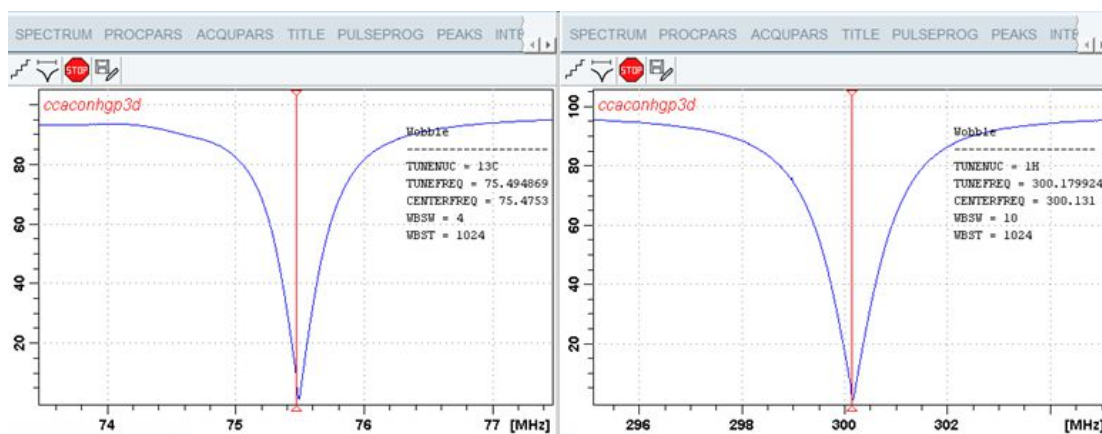
An NMR probe must be tuned and matched because it is a resonance circuit. If its resonance frequency and impedance are the same as the transmitter frequency and impedance, respectively, the full transmitter power is transferred to the probe. However, if either or both are different, part of the transmitter power is reflected by the probe. This results in a longer 90° pulse or, for a given pulse length, a smaller flip angle.



Note that a multi nuclear probe has a resonance circuit for each nucleus and each nucleus must be tuned and matched separately.

The command **wobb** is normally used without argument. It can, however, be used with arguments. For example:

- **wobb high**  
Starts with the nucleus with the highest frequency and continues in the order of decreasing frequency.
- **wobb ext50**  
Uses an external 50 ohm resistor as a reference.
- **wobb f1**  
Starts with frequency channel f1. It continues with the next higher frequency or, if the argument **high** is also used, with the next lower frequency.
- **wobb f2**  
Starts with frequency channel f2. It continues with the next higher frequency or, if the argument **high** is also used, with the next lower frequency.
- **wobb f<x> f<y>**: simultaneous wobbling of channels F<x> and F<y> in edasp. For WBSW the respective array entries are used, i.e. WBSW[0] for channel F1, WBSW[1] for channel F2 etc. If WBSW[x] is 0 then WBSW[0] is used as a fallback.
- **wobb all**: simultaneous wobbling of all channels in edasp using the respective WBSW entries.
- **wobb wbst 1024 f1 wbsw 4.5 f2 wbsw 60**: simultaneous wobbling of channels f1 and f2 with WBST=1024, and f1 using 4.5MHz and f2 using 60MHz for WBSW






The **wobb** command allows you to optimize both the probes resonance frequency (tuning) and impedance (matching). It sends a low power RF signal to the probe and sweeps that signal over a certain frequency range. The number of steps (frequencies) within that range is defined by the acquisition parameter WBST. The width of the frequency range is defined by WBSW. The center frequency depends on the nucleus; SFO1 for NUC1, SFO2 for NUC2 etc. The deviation of the probe impedance from the nominal 50 ohm is shown as function of the frequency in the TopSpin data field. This is the so called wobble curve. At the probes resonance frequency, the curve shows a dip, the minimum reflected power. Tuning the probe means adjusting its resonance frequency until it reaches SFO1. Matching the probe means adjusting its impedance until the reflected power reaches zero.

The entire wobble procedure involves the following steps:

- Stop the sample rotation if this is on, for example with **ro off**, or by pressing the SPIN ON/OFF button through the BSMS display.
- Setup the nucleus or nuclei for the current experiment with **edasp**.

This will automatically set the parameters SFO1, SFO2 etc.

- Click **Acquire | Observe fid window** or enter **acqu** to switch to the TopSpin acquisition menu. If, however, tuning and matching is observed on the preamplifier, this step can be skipped (see below).
- Enter **wobb**. The wobble curve will appear in the TopSpin data field showing a dip at a certain frequency. At the center of the data field, you will see a vertical line. If you do not see the dip, it probably lies outside of the data field. In that case, you should click the  button or enter **wbchan** to increase the sweep width. You can do this while **wobb** is running.
- When the dip is visible, you can start tuning and matching as follows:
  - Turn the tuning knob until the dip lies across the vertical line.
  - Turn the matching knob until the dip has reached a minimum. Matching influences tuning, so the dip probably moves away from the center.
  - Turn the tuning knob until the dip lies at the center again. Tuning influences matching, so the dip probably moves up again.
  - Turn the matching knob until the dip reaches a minimum again.
  - Continue this process until the dip lies exactly across the vertical line and reaches the x-axis.
- In case of a multi nuclei experiment, you have to switch to the next nucleus. For multiple channel experiments (2D, 3D etc.) tuning and matching of the channels (e.g.  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ) interdependent. The command **wobb all** will work on all nuclei in parallel. Note that **wobb** automatically starts with the nucleus with the lowest basic frequency. You can switch to the nucleus with the next higher frequency in two possible ways:
  - Press **Channel Select** at the HPPR. This will automatically select the nucleus with the next higher frequency.
  - Click  or enter **wbchan** in TopSpin. Answer the question "Do you want to change the nucleus" with **yes**.
  - Repeat step 5 / 153] for the current nucleus.
- If your experiment involves more than two nuclei, repeat step 6 / 153] for each further nucleus.
- Click  or enter **stop** on the command line to finish the wobble procedure.

A probe has a tuning knob (labeled **T**) and matching knob (labeled **M**) for each resonance circuit. Most probes have two, one for  $^1\text{H}$  and one for X-nuclei. When the tuning knob reaches the end of its range before the probe is properly tuned, you should turn it to the middle of its range, adjust matching, then tuning, then matching etc. A similar procedure can be used if the matching knob reaches the end of its range.

The process of tuning and matching can also be followed on the HPPR preamplifier. Some people find that more convenient and it is necessary when the computer screen is not visible from the position of the probe. The horizontal row of LED's indicates tuning, the vertical row indicates matching. When you turn the tuning or matching knob at the probe, you will see how the number of lit LED's changes. The probe is perfectly tuned when only one LED (a green one) is lit. The same holds for matching. In practice, proper tuning and matching means that only green LED's are lit. If the LED update seems to be very slow, this might be caused by the time consuming update of the wobble curve in the TopSpin acquisition display.

In that case, you can simply click  to close the wobble window.

Broadband probes usually have sliders for tuning and matching rather than turning knobs. These have the advantage that their positions are numbered. The default slider positions for each nucleus are usually written on cards that are kept with the probe. When wobbling is started with these default values, only some fine tuning and matching is required.

The probe resonance frequency and impedance is dependent on the sample. This can be a problem in automation, where several samples are measured but the probe is only matched and tuned on one of them. Bruker ATM probes support automatic tuning and matching which can be preformed on every sample during automation (see description of the commands **atmm** and **atma**).

### INPUT PARAMETERS

- Set by the user with **eda** or by typing **wbst**, **wbsw** etc.:
  - WBST - number of wobble steps
  - WBSW - wobble sweep width
- Set by the user with **edasp** or **eda** => NUC1:
  - NUC1 - NUC4 - the nuclei for which the probe is tuned and matched
  - SFO1 - SFO4 - irradiation frequency

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters
- <tshome>/prog/wobble/
  - *acqu\_go4* - wobble parameters
  - *Pulsprog\_X* - wobble pulse program

### SEE ALSO

[atma](#) [► 141], [atmm](#) [► 142], [edasp](#) [► 162]

# 7 Parameter Handling Commands

This chapter describes commands which are involved in parameter handling. This involves the setting of acquisition parameters, probe/solvent dependent parameters and nuclei assignment. Furthermore, the usage of predefined parameters sets is discussed.

## 7.1 ased

### NAME

**ased** - Edit acquisition parameters used in pulse program

### DESCRIPTION

The command **ased** opens a dialog box with the acquisition parameters which are used for the current experiment (see the next figure).

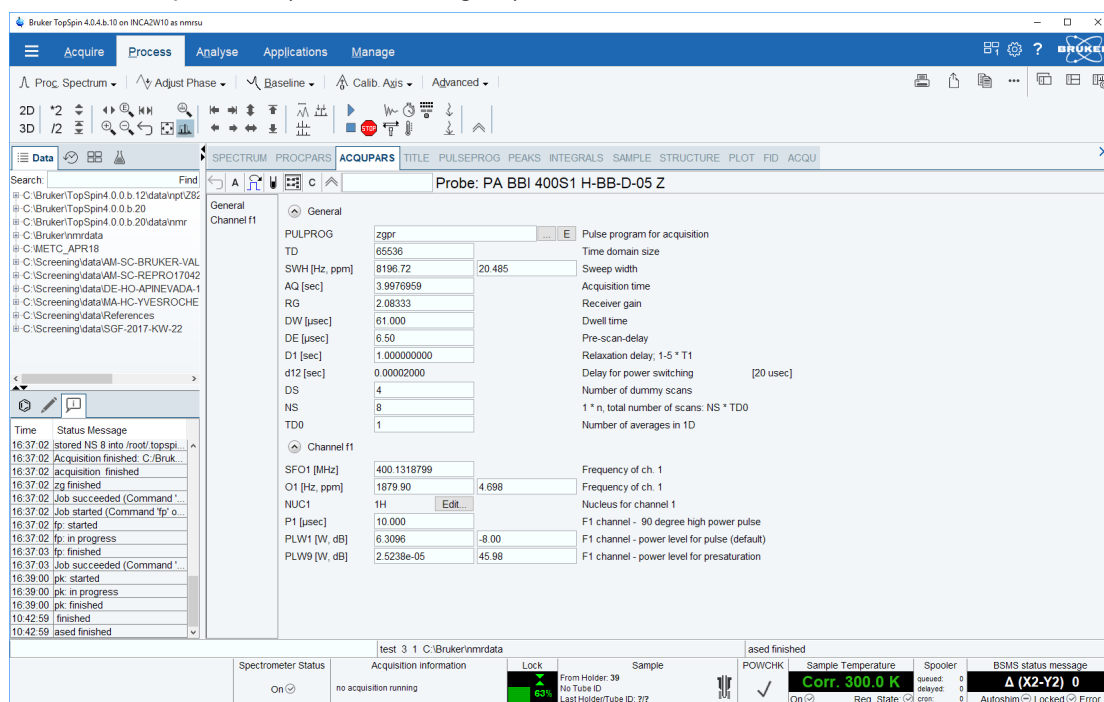





Figure 7.1: ased


This means that **ased** shows much less parameters then **eda** which shows all acquisition parameters. Entering **ased** on the command line is equivalent to clicking the **AcquPars** tab and then clicking the  button.

The following buttons are available:

 Undo the last modification (unused for status parameters).

 Switch to all acquisition parameters.

 Force parse of the pulse program.

 Set probe/solvent dependant parameters.



Open the nuclei and routing table.



Create a multi-receiver or a multi-dataset acquisition.

In front of the probe name the search function allows to go to a specific parameter.

**ased** compiles and interprets the pulse program defined by PULPROG. For pulses, delays and constants, the parameter description in the right column of the **ased** window is taken from the comment section at the end of the pulse program.

### INPUT AND OUTPUT PARAMETERS

- For all experiments:
  - PULPROG - pulse program used for the acquisition.
  - TD - time domain; number of raw data points.
  - NS - number of scans.
  - DS - number of dummy scans.
  - SWH - spectral width in Hz.
  - AQ - acquisition time in seconds.
  - RG - receiver gain.
  - DW - dwell time.
  - DE - pre-scan delay.
- For each frequency channel defined with **edasp**:
  - NUCx - nucleus for channel x.
  - SFOx - irradiation frequency for channel x.
- All delays, pulse lengths, power levels etc. defined in the pulse program, e.g.:
  - D[1] - relaxation delay.
  - P[1] - 90° pulse length.
  - PL[1] - power level for pulse.
  - PCPD[1] - CPD pulse length.

### INPUT FILES

- <tshome>/exp/stan/nmr/lists/pp/ (primary source) or <dir>/data/<user>/nmr/<name>/<expno>/lists/pp (fallback if not found in primary source)
  - The pulse program defined by PULPROG
- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters

### OUTPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters

### SEE ALSO

[eda](#) [► 160], [edcpul](#) [► 167]

## 7.2 dpa

### NAME

**dpa** - Display the acquisition status parameters

### DESCRIPTION

The command **dpa** displays the acquisition status parameters (see the next figure).

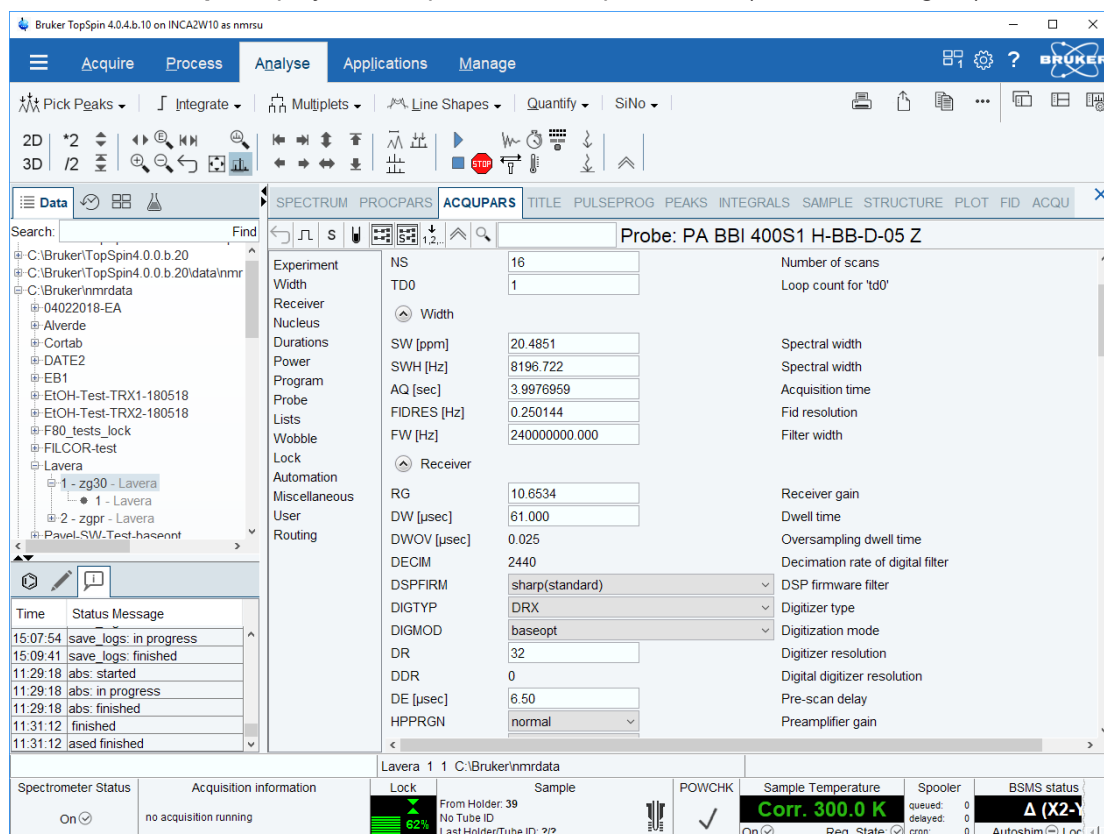





Figure 7.2: dpa

These are set by acquisition commands and represent the status of the raw data. Entering **dpa** on the command line is equivalent to clicking the **AcquPars** tab and then clicking the **S** button.


The following buttons are available:


 Undo the last modification (unused for status parameters).


 Show pulse program parameters .

 Switch to acquisition parameters.

 Set probe/solvent dependent parameters.

 Open and set the nuclei and routing.

 Show the status of the nuclei and routing information (**edasp-s**).

 Collapse all submenus.

# Parameter Handling Commands



Read shim values from current dataset (**rsh shimvalues**).



Search for the parameter specified in the search field.

Acquisition status parameters can also be viewed by entering their names on the command line. For example:

- **s ns**  
Displays the acquisition status parameter NS.
- **s td**  
Displays the acquisition status parameter TD.

On multidimensional data, the parameter values for each direction are shown.

## INPUT FILES

- `<dir>/data/<user>/<name>/nmr/<expno>/`
  - *acqus* - acquisition status parameters

On 2D and 3D data the files *acqu2s* and *acqu3s* are used for the indirect directions, respectively (see also chapter [Parameter Files](#) [ 15]).

## SEE ALSO

[eda](#) [ 160], [dpa](#) [ 159]

## 7.3 eda

### NAME

**eda** - Edit acquisition parameters.

### DESCRIPTION

The command **eda** opens a dialog box in which you can set all acquisition parameters (see the next figure).

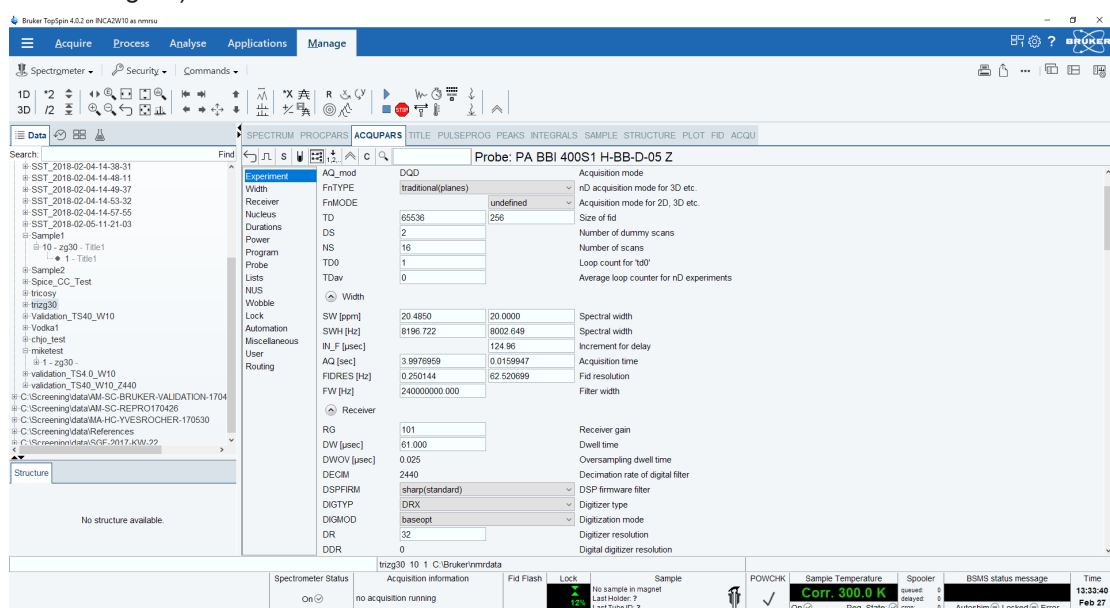


Figure 7.3: eda


Entering **eda** on the command line is equivalent to clicking **AcquPars** in the tab bar of the data window.

The following buttons are available:


 Undo the last modification. Can be used repeatedly.


 Show pulse program parameters.


 Switch to acquisition status parameters.


 Set probe/solvent dependant parameters.

 Open and set the nuclei and routing.

 Show the status of the nuclei and routing information (**edasp-s**).

 Change raw dataset dimensionality (parameter **PARMODE**).



 Collapse/expand all parameter sections.

 Search for the parameter specified in the search field.

Inside the parameter editor, you can do the following actions:

- Select an acquisition parameter submenu, e.g. **Experiment**, at the left of the dialog box. The submenu is highlighted and the corresponding parameters will appear in the right part of the dialog box.
- Click in a parameter field, e.g. TD, to set the parameter value. It is automatically stored.
- Hit the **Tab** key to jump to the next parameter field.
- Hit **Shift-Tab** to jump to the previous parameter field.
- Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.



Note that the   buttons to the right of the PULPROG parameter allow you to show the pulse program list or edit the current pulse program, respectively. This applies to all parameters that refer to a filename.

Parameters can also be set by entering their names on the command line. A dialog window will appear where you can enter the parameter value(s). For example:

**td**

On a 1D data set.

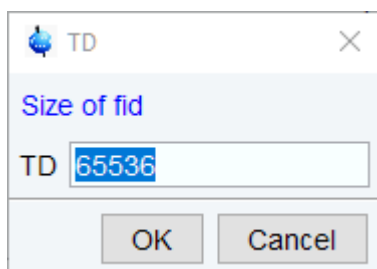


Figure 7.4: TD - Size of fid

or on a 2D data set:

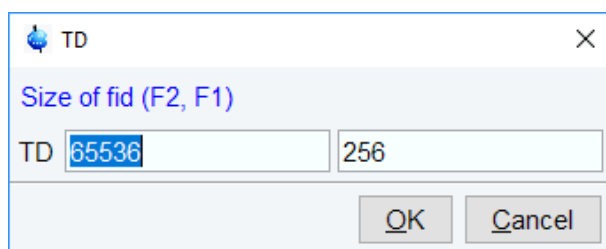


Figure 7.5: TD - Size of fid (F2, F1)

Alternatively, you can specify the parameter value as an argument on the command line, For example;

**td 8k**

The time domain will be set to 8k.

### INPUT AND OUTPUT PARAMETERS

All acquisition parameters.

#### INPUT FILES

- `<tsHOME>/classes/prop/`
  - *pared.prop* - parameter properties file.
- `<tsHOME>/exp/stan/nmr/form/`
  - *acqu.e* - format file for **eda**.

#### INPUT AND OUTPUT FILES

- `<dir>/data/<user>/<name>/nmr/<expno>/`
  - *acqu* - acquisition parameters for the acquisition (direct) direction.
  - *acqu2* - acquisition parameters for F1 (2D) or F2 (3D) indirect direction.
  - *acqu3* - acquisition parameters for the F1 direction (3D).

#### SEE ALSO

[dpa](#) [ 159], (edp)

## 7.4 edasp

### NAME

**edasp** - Set up nuclei and spectrometer routing

### DESCRIPTION

The command **edasp** allows you to set up the nuclei and the spectrometer routing for the current experiment. It opens the routing table showing the current nuclei selection and amplifier routing. Here you can specify the nucleus or nuclei to be used for the experiment. For the f1 logical frequency channel, you can click the NUC1 button and select a nucleus from the appearing list. The basic frequency, BF1, is automatically set. Then you can specify the frequency offset; OFSH1 for 1H or OFSX1 for X nuclei. The irradiation frequency SFO1 is automatically calculated as the sum of the basic frequency and frequency offset.



Note that the parameters NUC1, BF1 and SFO1 also appear in **eda** but cannot be set from there.

However, the frequency offset (OFSH1 or OFSX1) appears in **eda** as O1 and can be set from there. In a multi nuclear experiment, you can set up the parameters for channel f2, f3 etc. in the same way as described for f1.

The routing table also shows the spectrometer routing. The hardware elements which have been detected when the spectrometer was configured (with **cf**) will appear in this list. When you select a nucleus for a certain channel, the default routing is automatically set. Normally, this can be left as it is. Only in very special cases it is useful to change it. The routing table consists of the following stages:

Channel---FCU---Amplifier---Swibox/I ---Swibox/O---Preamplifier

You can set up the routing by connecting an element from one stage to an element of the next stage. A connection can be installed or removed by clicking the two elements involved. The routing must follow the following rules:

- Between the logical frequency channels and FCU's any combination is allowed but only one to one.
- An FCU can be connected to one amplifier only but an amplifier can be connected to multiple FCU's. Furthermore, FCU1 can only be connected to the first three amplifiers and FCU2 can only be connected to the first four amplifiers.
- The first four amplifiers are automatically connected to switchbox input in a fixed way. These connections cannot be changed.
- Between the switchbox input and switchbox output, any connection is allowed but only one to one.
- Between the switchbox output and the Preamplifier modules, any connection is allowed but only one to one. Make sure that the cables are connected accordingly.
- The output of the fifth and sixth amplifier must be connected directly to the preamplifier modules. Any combination is allowed but only one to one and only to preamplifier modules which are not connected to a switchbox output.

Advance spectrometers which are used for solid state experiments usually contain high power amplifiers with two output stages:

- A low power output: typically 150 W for 1H or 300 W for X nuclei.
- A high power output: typically 1000 W for 1H or X nuclei.

The second output appears as an extra stage in the routing table to the right of the switchbox. If you use the second output stage, the switchbox is always bypassed.

If you make a routing connection which is not allowed, you will get a message that it is illegal. You must remove it before you can save the routing table. Some connections are allowed but not recommended. In that case, you only get a warning.

At the bottom of the routing table you will find the following buttons:

- SAVE - save the routing table and quit.
- SWITCH F1/F2 - exchange the F1 and F2 nucleus including the frequency and frequency offset.
- SWITCH F1/F3 - exchange the F1 and F3 nucleus including the frequency and frequency offset.
- DEFAULT - set the default amplifier routing for the current nuclei.
- CANCEL - quit without saving any changes.
- PARAM - shows the routing parameters.

In a 2D dataset, NUC1 has a different function in the two directions. In F2, it works like in 1D experiments; it opens the routing table. In F1, it opens the nuclei list and allows you to select the nucleus for this direction. The same principle holds for 3D data; in F3, NUC1 opens the routing table, in F2 and F1 it opens the nuclei list.

The spectrometer routing is stored under the current dataset in the acquisition parameters FCUCHAN, RSEL, SWIBOX, PRECHAN and HPMOD (see the description of these parameters). These can be viewed by clicking the PARAM button in the routing table.



Note that these parameters appear in **eda** and can be set from there.

This, however is not very common as setting them from the routing table is much more convenient. In Bruker parameter sets (see **rpar**), the routing parameters have been set according to the configured hardware. This corresponds to the routing that will be set by clicking the **default** button in the routing table.

The connections between the Switchbox output and the Preamplifier modules are fixed; they cannot be changed. However, if you start **edasp** with the argument **setpreamp**, you can change these connections or remove them all by clicking **Clear preamplifier connections**. If you make any changes here, you must make sure that the cables at the spectrometer are connected accordingly. The command **edasp setpreamp** is implicitly called as a part of spectrometer configuration (command **cf**).

### INPUT AND OUTPUT PARAMETERS

Set graphically from **edasp** by connecting routing elements:

- FCUCHAN - logical frequency channel - FCU connections.
- RSEL - FCU - amplifier connections.
- SWIBOX - Switchbox input - Switchbox output connections.
- PRECHAN - Switchbox output - Preamplifier module connections.
- HPMOD - high power amplifier - Preamplifier module connections.

### INPUT AND OUTPUT FILES

- `<dir>/data/<user>/<name>/nmr/<expno>/`
  - *acqu* - acquisition parameters.
- `<tshome>/conf/instr/<INSTRUM>/`
  - *specpar* - routing parameters.

### SEE ALSO

[edsp \[ 94\]](#), [eda \[ 160\]](#), [cf \[ 51\]](#), [expinstall \[ 99\]](#)


## 7.5 getprosol

### NAME

**getprosol** - Get probe and solvent dependent parameters

### DESCRIPTION

The command **getprosol** reads the probe and solvent dependent parameters (the prosol parameters) and copies them to the corresponding acquisition parameters. Entering **getprosol** on the command line is equivalent to clicking the **AcquPars** tab and then clicking

the  button. The relations between the prosol and acquisition parameters are shown in table [Table 7.1 \[ 165\]](#). These are the default relations which apply to most standard high resolution experiments. Protein, DNA/RNA, LC-NMR and several other types of experiments require different relations which are defined in the files, *triple*, *triple\_na*, *lcnmr*, etc.,

respectively (see INPUT FILES). To use relations other than default, the so called relations file must be specified in the pulse program. You can do that by editing the pulse program (with **edpul** or **edcpul**) and adding the line:

```
prosol relations=<filename>
```

before the actual pulse sequence. To look at an example, you can enter **edpul lc2** or **edpul zgesgp**.



Note that the file *default*, for default relations can, but does not need to be specified in the pulse program.

| Description                          | edprosol      | eda        |
|--------------------------------------|---------------|------------|
| F1 90° hard pulse length             | P90[F1]       | P[0], P[1] |
| F1 180° hard pulse length            | P90[F1]*2     | P[2]       |
| F2 90 ° hard pulse length            | P90[F2]       | P[3]       |
| F2 180° hard pulse length            | P90[F2]*2     | P[4]       |
| F1 Tocsy spin lock 60° pulse length  | PTOC[F1]*0.66 | P[5]       |
| F1 Tocsy spin lock 90° pulse length  | PTOC[F1]      | P[6]       |
| F1 Tocsy spin lock 180° pulse length | PTOC[F1]*2    | P[7]       |
| F1 Roesy spin lock pulse length      | PROE[F1]      | P[15]      |
| Gradient 1 pulse length              | P_grad1       | P[16]      |
| F1 Tocsy trim pulse length           | P_mlev        | P[17]      |
| Gradient 2 pulse length              | P_grad2       | P[19]      |
| F3 90° hard pulse length             | P90[F3]       | P[21]      |
| F3 90° hard pulse length             | P90[F3]*2     | P[22]      |
| F1 HSQC trim pulse length            | P_hsqc        | P[28]      |
| F2 Roesy spin lock pulse length      | PROE[F2]      | P[31]      |
| F1 90° hard pulse power level        | PL90[F1]      | PL[1]      |
| F2 90° hard pulse power level        | PL90[F2]      | PL[2]      |
| F3 90° hard pulse power level        | PL90[F3]      | PL[3]      |
| F1 Tocsy spin lock power level       | PLTOC[F1]     | PL[10]     |
| F1 Roesy spin lock power level       | PLROE[F1]     | PL[11]     |
| F2 CPD power level                   | PLCPDP[F2]    | PL[12]     |
| F2 Second CPD (bilev) power level    | PLCPD2[F2]    | PL[13]     |
| F3 CPD power level                   | PLCPDP[F3]    | PL[16]     |
| F2 Homodecoupling power level        | PLHD[F2]      | PL[24]     |
| Gradient recovery delay              | D_grad        | D[16]      |
| F2 CPD pulse length                  | PCPDP[F2]     | PCPD[2]    |
| F2 CPD pulse length                  | PCPDP[F3]     | PCPD[3]    |

Table 7.1: Default relations between prosol and acquisition parameters

## Usage Of Getprosol With Command Line Options

The command **getprosol** (get probe and solvent dependent parameters from the edprosol table) can be called with three options:

- The nucleus.
- P90, the value for 90° hard pulse length.
- PL90, the value for 90° hard pulse power level.

The existing prosol parameterset, set up by **edprosol**, is not modified.

**getprosol Nuc P90 PL90** recalculates standard hard power levels with:

$PLx = 20 \cdot \log(Px/P90)$  and the standard soft power levels PLSH1 - PLSH16 by:

$PLSHx = 20 \cdot \log(\text{integFac} \cdot Px / \text{totRot} \cdot (P90/90.0))$  where integFac (=SHAPE\_INTEGFAC) and totRot (SHAPE\_TOTROT) are read from the shapes <TOPSPINHOME>/exp/stan/nmr/lists/wave/PNSHx

and

<TOPSPINHOMME>/exp/stan/nmr/lists/wave/Gaus1.100 (e.g.)

## INPUT AND OUTPUT PARAMETERS

See table [Table 7.1](#) [▶ 165].

### INPUT FILES

- <tshome>/conf/instr/<instrum>/prosol/relations
  - *default* - relations file for most experiments
  - *triple* - relations file for Protein experiments
  - *triple\_na* - relations file for DNA experiments
  - *lcnmr* - relations file for LC-NMR
  - etc.
- <tshome>/conf/instr/<instrum>/prosol/<probeID>/<solvent>
  - *nucleus.channel.amplifier* - prosol parameters

### OUTPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters
  - *relations* - copy of the input relations file

## SEE ALSO

[edprosol](#) [▶ 84], [eda](#) [▶ 160],

[setprosol](#)

## 8 Pulse and AU Program Commands

This chapter describes commands for the setup of pulse programs, gradient programs, CPD programs etc. Furthermore, it describes the setup of various lists which can be used in acquisition like variable pulse or variable delay lists.

### 8.1 edcpul, edpul

#### NAME

**edcpul** - Edit the current pulse program.

**edpul** – Edit any pulse program.

#### SYNTAX

edcpul [<name>]

edpul [<name>]

#### DESCRIPTION

The command **edcpul** opens the TopSpin editor showing the current pulse program (see the next figure). The current pulse program is defined as the pulse program of the foreground dataset as defined by the acquisition parameter PULPROG.

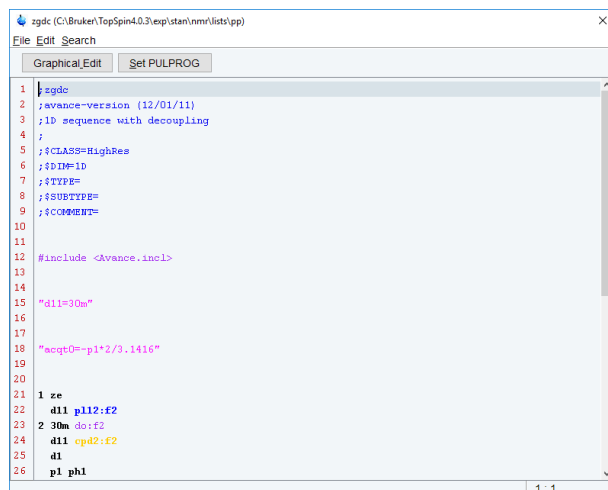


Figure 8.1: edcpul

Bruker pulse programs are opened in **view** mode which means they cannot be modified. The dialog **File** menu offers you the following functions:

- **Open**

This will open the **edpul** dialog where you can open any available pulse program. The current pulse program is automatically highlighted.

## Pulse and AU Program Commands

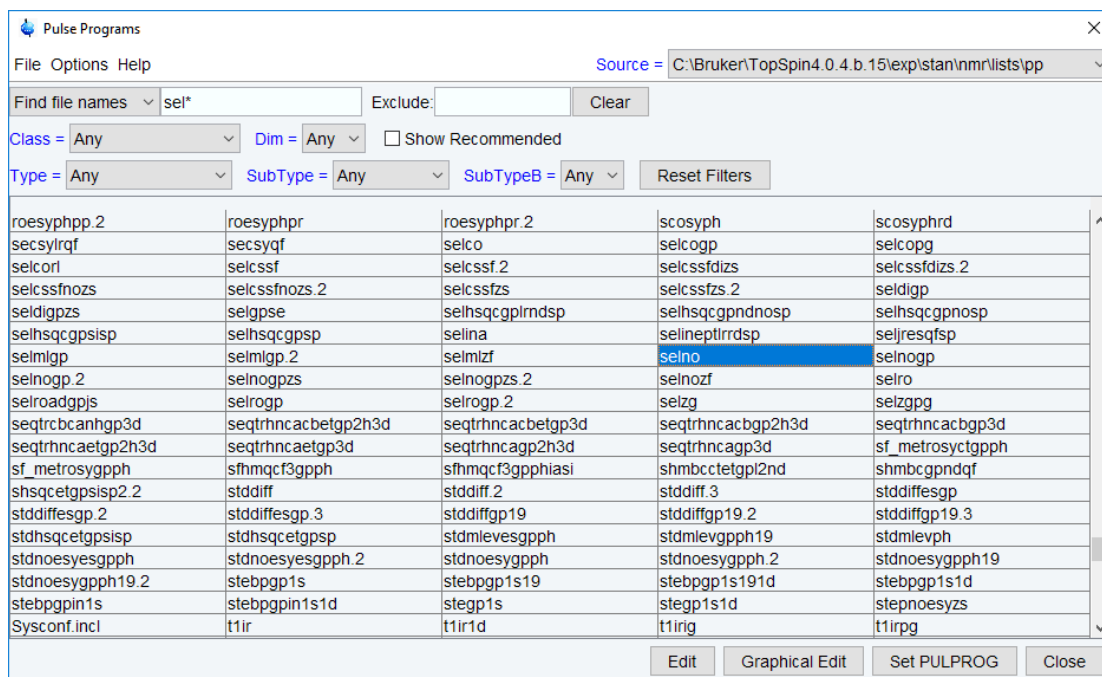
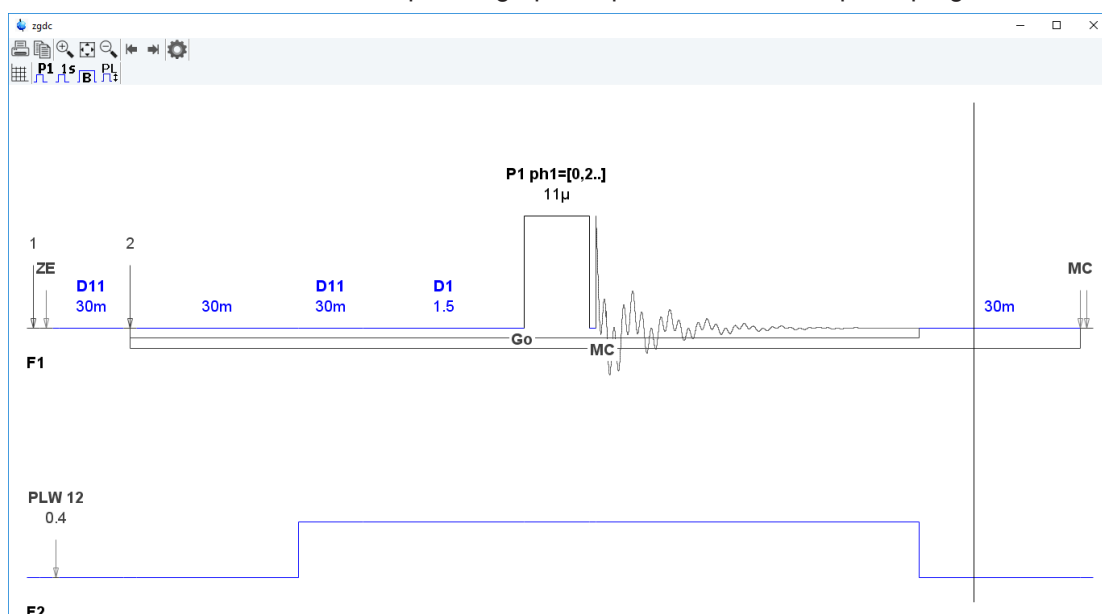


Figure 8.2: **edpul**: list of pulse programs

- **Save as...**  
Allows you to save the pulse program under a different name
- **Print**  
This will print the pulse program

The button **Graphical Edit** opens a graphical presentation of the pulse program:



All parameters as set in the current dataset are provided in the graphical display.

The button **Set PULPROG** writes the pulse program name to the acquisition parameters.

User defined pulse programs are opened in **edit** mode and can be modified. The dialog **File** menu offers you the following extra functions:

- **New**

Allows you to open a new pulse program.

- **Save**

Allows you to save the pulse program under the same name

Besides the File menu, the dialog offers the **edit** and **search** menu with common edit/search functions.

## INPUT PARAMETERS

To be set with **eda** or by typing **pulprog** :

- PULPROG - the current pulse program (input of **edcpul**)

## INPUT FILES

- <tshome>/exp/stan/nmr/lists/pp
  - Bruker and user defined pulse programs
- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters

## OUTPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters (output of **edcpul** <name>)

## SEE ALSO

[edgp](#) [► 169], (edcpd)

## 8.2 edgp

### NAME

edgp - Edit gradient programs

### SYNTAX

edgp [<name>]

### DESCRIPTION

The command **edgp** allows you to list, create or edit gradient programs. If you enter **edgp** without arguments, a list of all gradient programs is displayed (see the next figure).

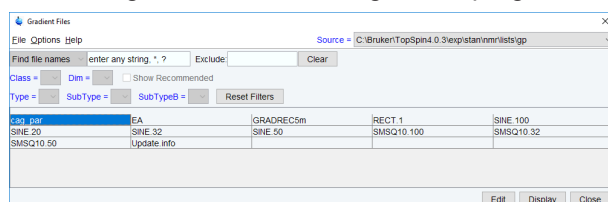


Figure 8.3: *edgp*

This shows a list of all Bruker and/or User gradient programs and allows you to edit or delete them.

To list Bruker gradient programs:

- Click **Options => Bruker defined**

To list User gradient programs:

- Click **Options => User defined**

To list all gradient programs:

- Click **Options => All defined**

To edit the selected gradient program:

- Double-click the gradient program or select the gradient program and click **Edit**. The gradient program will be shown in an editor and can be saved by clicking **Save**. To save it under a different name, click **Save as ...**

To create a new gradient program:

- Click **File --> New** and write the gradient program in the appearing editor

or

- Double-click an existing gradient program, modify the contents to your needs and store it under a different name by clicking **Save as ...**

To delete a gradient program

- Click **Delete** and click **OK** in the warning dialog.

If you enter the command with an argument, i.e. **edgp <name>**, the gradient program <name> is opened or, if it does not exist, it is created. The argument may contain wildcards, e.g. **edgp a\*** displays a list of all gradient programs which start with a.

Bruker gradient programs must be installed with the command:

**expinstall** before they can be opened with **edgp**.

**edgp** uses the editor which is defined in the TopSpin User Preferences. To change it, enter **set**, click **Miscellaneous** and select or change the editor.

### INPUT AND OUTPUT FILES

- <tshome>/exp/stan/nmr/lists/gp/\*
  - gradient programs

### SEE ALSO

[edcpul](#) [▶ 167], (edpu)l, [expinstall](#) [▶ 99]

## 8.3 edlist, dellist

---

### NAME

**edlist** - Edit various lists.

**dellist** - Delete various lists.

### SYNTAX

**edlist** [<type> <list> ]

**dellist** [<type> <list>]

## DESCRIPTION

The command **edlist** opens a dialog box with the **Edit...** option selected:

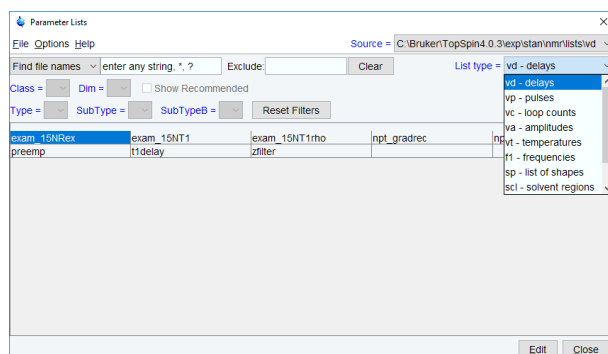


Figure 8.4: **edlist**

Just select the desired **List type** and click **OK**. The available files of the chosen list type appear and can be edited. To create a new list file:

- Open an existing file, edit it and click **Save as ...** to save it under a different name.
- or
- Enter a name in the field **New file**, click **OK**, enter the list in the appearing editor and click **OK**.

Lists types that can be edited with **edlist** are shown in the table [Table 8.1 \[ 171\]](#). They are used by the acquisition, for example, a **vd** list is read by the pulse program statement **vd**.

A variable delay list can be set up and used as follows:

- Create a variable delay list with **edlist**.
- Set the acquisition parameter **VDLIST** to the name of that list.
- Specify the **vd** statement in the pulse program.

Other lists can be used in a similar way. They typically contain one value per line and the number of lines is unlimited. The type of the list that is interpreted is determined by the type of pulse program statement. The list name is determined by an acquisition parameter.



Note, however, that **SREGLST** is a processing parameter.

| List type  | Description             | Defined by parameter | Read by pulse program statements |
|------------|-------------------------|----------------------|----------------------------------|
| <b>vd</b>  | delay list              | VDLIST               | vd, ivd, vdidx                   |
| <b>vp</b>  | pulse list              | VPLIST               | vp, ivp, vpidx                   |
| <b>vc</b>  | counter list            | VCLIST               | lo to x times c, ivc             |
| <b>va</b>  | amplitude list          | VALIST               | define list<power>               |
| <b>vt</b>  | temperature list        | VTLIST               | RVTLIST, VT, IVTLIST, DVTLIST    |
| <b>f1</b>  | frequency list (Avance) | FQLIST               | fq1, fq2, fq3 etc.               |
| <b>sp</b>  | list of shapes          | SPNAM                | list<shape>                      |
| <b>scl</b> | scaling region list     | SREGLST              |                                  |

| List type    | Description         | Defined by parameter | Read by pulse program statements |
|--------------|---------------------|----------------------|----------------------------------|
| <b>phase</b> | variable phase list | PHLIST               | list<phase>                      |
| <b>masr</b>  | MAS spin rate list  |                      | AU prog. Multimas                |
| <b>gp</b>    | Gradient Files      | GPNAM                | list<gp>                         |

Table 8.1: Lists used in acquisition



RVTLIST, VT, IVTLIST, DVTLIST:

Note that these are AU program macros rather than pulse program statements.

## Delay Lists

Delay lists contain any number of delay values with the corresponding units, e.g.:

10u

5m

2s

where u = microseconds ( $\mu$ s), m = milliseconds and s = seconds. They are interpreted by the pulse program statements:

`vd` - read value from the current position in the delay list

`ivd` - increment the delay list position to the next value

`"vdidx=n"` - set the index to position *n* in the delay list

## Pulse Lists

Pulse lists contain any number of pulse length values with the corresponding units, e.g.:

10u

20m

where u = microseconds and m = milliseconds. They are interpreted by the pulse program statements:

`vp` - read value from the current position in the pulse list

`ivp` - increment the pulse list position to the next value

`"vpidx=n"` - set the index to position *n* in the pulse list

A variable pulse list can only be used for hard pulses, not for shaped pulses.

## Counter Lists

A variable counter list contains any number of loop counter values, e.g.:

4

7

20

They are interpreted by the pulse program statement:

`lo to x times c`

Where *x* is a pulse program label and *c* is the value at the current position of the counter list

`ivc`

increment the counter list position to the next value

### Variable Amplitude (power) Lists

A variable amplitude list contains any number of power values, e.g.:

```
-6.0
0.0
3.0
6.0
```

The entries represent attenuation values in dB.

The usage of a VA list is different from pulse and delays lists. You must define the statement by which a VA list is accessed in the pulse program. Such a statement can have any name, for example the name `vanam` is used in the examples below. The suffixes `.inc`, `.dec` and `.res` can be used to increment, decrement and reset the lists position, respectively. Furthermore, the caret operator (^) allows you to read a list value and increment the list position with one statement. The following pulse program entries illustrate the use of a variable amplitude list:

```
define list<power> vanam = <$VALIST>
```

definition of the power list

```
d1 vanam:f2 vanam.dec
```

set the power to the current value of the list and decrement the index

```
d1 vanam[2]:f3
```

set the power to the second value of the list

```
"vanam.idx = vanam.idx + 3"
```

increment the list index by 3

```
d1 vanam^:f4
```

set power to the current value of the list increment the index

As an alternative to using a list defined by the parameter VALIST, you can explicitly define a variable amplitude (power) list filename or even the list values in the pulse program. The following examples illustrates such definitions:

```
define list<power> vanam=<my_filename>
```

```
define list<power> vanam={10 30 50 70}
```



Note that the second definition does not require a list file.

Note that variable amplitude lists can only be accessed using define statements as described above. The statement `va` does not exist. More information on using variable amplitude lists can be found under:

**Help | Manuals | Programming Manuals | Pulse Programming**

### Temperature Lists

A variable temperature list contains any number of temperature values (in Kelvin), e.g.:

```
300
320
340
```

Temperature lists are interpreted by the AU program macros:

- RVTLIST  
Open the temperature list defined by VTLIST
- VT

Read value from the current position in the temperature list and set the temperature unit accordingly.

- IVTLIST

Increment the current position in the temperature list to the next value.

- DVTLIST

Decrement the current position in the temperature list to the previous value.



Note that temperature lists are only interpreted by AU program macros, not by pulse program statements.

### Frequency Lists

Frequency lists contain the irradiation frequency preceded by the letter O on the first line (optional) and any number of frequency offset values on subsequent lines, e.g.:

```
O 500.13
```

```
3000
```

```
3150
```

```
3200
```

They are interpreted by pulse program statements like:

```
30m fq1:f1
```

Read the current value from the list defined by FQ1LIST to channel f1

```
d1 fq2:f1
```

Read the current value from the list defined by FQ2LIST to channel f1

```
d11 fq3:f2
```

Read the current value from the list defined by FQ3LIST to channel f2



Note that the `fq1`, `fq2` etc. statements must be specified with a delay. In contrast to the `vd` and `vp` statements, they automatically increment the current position in the list to the next value.

In the above example, the offset values in the list are added to the frequency specified on the first line, independent of the channel. If, however, the first line would be omitted, the offset values in the list are added to the values of SFO1, SFO2 etc. for the respective channels.

### Shape Lists

Shape lists are handled in the same way as Amplitude lists. The pulse program statement:

```
define list<shape> shl = <$VALIST>
```

will read the file name provided in the parameter VALIST from the shape directory `<tshome>/exp/stan/nmr/lists/sp`.

Alternatively, you can use the pulse program statement:

```
define list<shape> shl = <shapelist>
```

which will read the file shapelist from the shape directory `<tshome>/exp/stan/nmr/lists/sp`.

Note that more details on shape lists can be found under **Help | Manuals | Programming Manuals | Pulse Programming**

Scaling Region Lists

scl lists are used in the context of integration and are described in **Help | Manuals | Acquisition & Processing References | Proc. Commands & Parameters**

## Phase Lists

Phase lists are handled in the same way as Amplitude lists. The pulse program statement:

```
define list<phase> Phlist1 = <myphaselist>
```

will read the file myphaselist from the phase directory *<tshome>/exp/stan/nmr/lists/phase*.

Alternatively you can use the pulse program statement:

```
define list<phase> Phlist2 = <$PHLIST>
```

which will read the file name provided in the parameter PHLIST from the phase directory *<tshome>/exp/stan/nmr/lists/phase*.

Note that more details on phase lists can be found under **Help | Manuals | Programming Manuals | Pulse Programming**

### Masr Lists

MASR lists contain any number of MAS spin rate values in Hz, e.g.:

3000

3500

4000

4500

They are interpreted by the AU program **multimas**. This AU program will ask you if you want to use a list or enter the start and increment value interactively. If you choose the former (default), it will offer you the available MASR lists.

There are alternative ways of defining and using lists in acquisition. Rather than using a predefined statements like *vd*, you can define your own statement in the pulse program to access a certain list. For example, the statements:

```
define list<delay> vdnam = <$VDLIST>
```

```
define list<delay> vdfil = <my_file>
```

```
define list<delay> vdval = {0.1 0.2 0.3 0.4}
```

Allows you to use the statements *vdnam*, *vdfil* and *vdval* to read a value from a delay list. The use of lists via define statements is fully described above for the variable amplitude lists. More information on user defined lists can be found under:

**Help | Manuals | Programming Manuals | Pulse Programming**

## Gradient Programs

Gradient Programs lists are handled in the context of the parameter GRADIENT in the acquisition parameter list.

Note that more details on gradient files can be found in **Help | Manuals | Programming Manuals | Pulse Programming**

- **edlist** can be used in one of the following ways:
  - **edlist** - opens the edit/delete dialog box
  - **edlist <type>** - displays all entries of the list type *<type>*
- **dellist** opens the same dialog box as **edlist** expect that the Delete option is selected. When you select a **List Type**, and click **OK**, the available files of that type appear. You can click one or more entries to mark them for deletion. Clicking the **Delete** button deletes all marked entries.

## INPUT AND OUTPUT FILES

- *<tshome>/exp/stan/nmr/lists*
  - *vd* - variable delay lists
  - *vp* - variable pulse lists

- *vc* - variable counter lists
- *va* - variable amplitude lists
- *vt* - variable temperature lists
- *f1* - frequency lists
- *sp* – variable shape file lists
- *scl* - scaling region files
- *phase* – variable phase list
- *masr* - MASR rotation values
- *gp* – gradient programs

### SEE ALSO

[edlist](#), [dellist](#) [► 170]

## 9 Acquisition Commands

This chapter describes all commands involved in data acquisition. This includes parameter optimization, the actual data acquisition and stopping a running experiment. Most experiments which involve a single acquisition are started with the command **zg** and run until they are finished. Other experiments involve multiple acquisitions executed with an AU program or with IconNMR.

### 9.1 aqguide

#### NAME

**aqguide** - Open the Acquisition Guide.

#### DESCRIPTION

The command **aqguide** opens the TopSpin Acquisition Guide (see the next figure). This contains a workflow for acquiring data, especially suited for new or occasional users. In **Automatic mode**, the Acquisition Guide will simply execute an acquisition command when you click the corresponding button. This requires the acquisition parameters to be set correctly. In interactive mode (**Automatic mode** unchecked), the Acquisition Guide will, at each step, open a dialog box offering you the available options and required parameters.

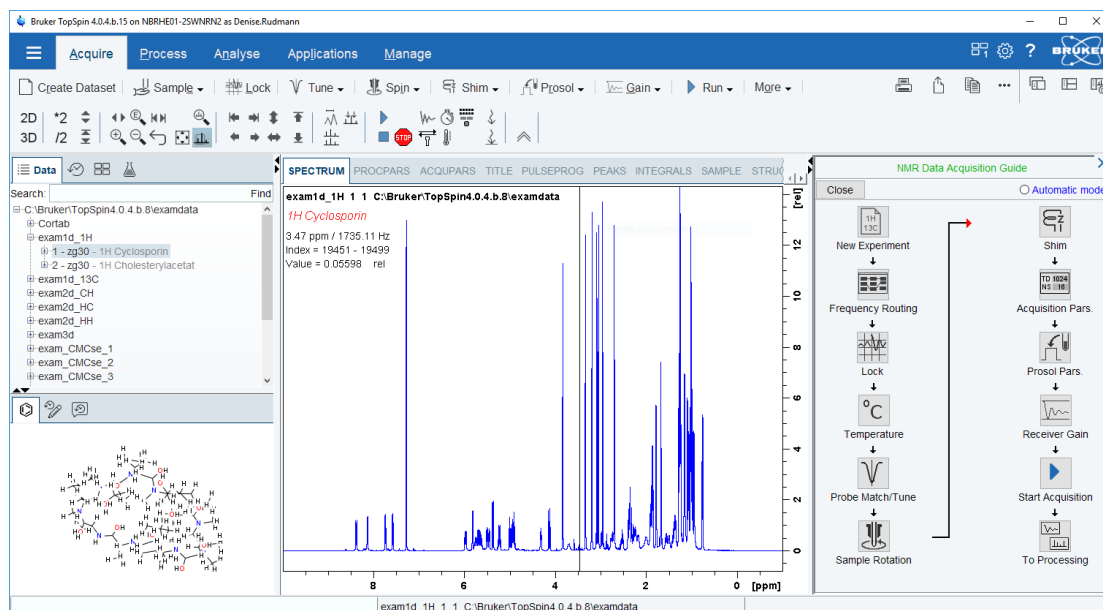


Figure 9.1: aqguide

#### SEE ALSO

(prguide, t1guide, solaguide)

### 9.2 expt

#### NAME

**expt** - Display the experiment time

## DESCRIPTION

The command **expt** calculates and displays the experiment time for the current data set (see the next figure).

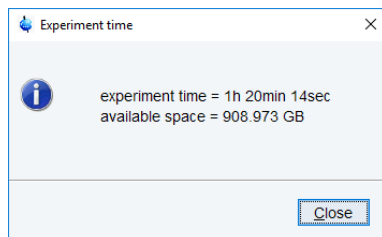


Figure 9.2: **expt**

If this exceeds the time you have available, you can reduce the number of scans (parameter NS) until the experiment time is acceptable.

Alternatively, the acquisition time (parameter AQ) can be reduced, modifying accordingly parameters SW and TD. Avoid truncation of the signal. Also D0 (relaxation delay) can be reduced). In this case take care not to saturate (overflow) the receiver, in case of too fast pulsing (complete relaxation should still occur).

For 2D experiments, the resolution in the indirect dimension F1 can be reduced (TD1 parameter), as long as the resolution remains sufficient (sometimes a compromise has to be made between all these possibilities).

For 2D and 3D experiments, **expt** also compares the file size of the raw data with the available disk space.

**expt** can also be executed by clicking the  button in the toolbar.

## INPUT PARAMETERS

- NS - number of scans
- AQ - acquisition time in seconds

## SEE ALSO

[zg](#) [ 195], [gs](#) [ 179]

## 9.3 go

### NAME

**go** - Perform an acquisition, adding to existing data

### DESCRIPTION

The command **go** starts an acquisition on the current dataset adding to possibly existing raw data. It works like **zg**, except that it does not overwrite existing data. If raw data already exist, **go** will add the new data to them. This is, for example, useful if the signal to noise of your spectrum is too low and you want to acquire additional scans. If no data exist, **go** has the same result as **zg**.



If you have stopped an acquisition with **halt** or **stop**, you can, in principle, continue it with **go**. Note, however, that the acquisition might have been stopped in the middle of a phase cycle and **go** starts a new phase cycle. Therefore, if you want to be able to stop and continue an acquisition, we recommend to use the commands **suspend** and **resume** (see the description of these commands).



Note that if you enter **halt** or **stop** during a 2D or 3D acquisition it might stop in the middle of a second or third direction increment (see above). However, this problem only occurs when you use the `wr` statement to write the data to disk. If you use the `mc` statement, the **go** command continues a 2D or 3D acquisition at the position where it was stopped. **Caution:** if you increment or decrement any pulses, delays or phases within the acquisition loop, you must do that within one of the `mc` arguments `F1PH`, `F1QF` etc., for example:

```
d1 mc #1 to 1 F1PH(id0, ip1)
```

Most acquisitions are started with **zg** and run until they have finished. As such, the command **go** is not used very often. It is, however, used in some Bruker AU programs like **noediff**, **noemult**, **deptyc** and **multicyc**.

Note the difference between the TopSpin command **go** and the pulse program statement `go` (See pulse programming manual).

## INPUT AND OUTPUT PARAMETERS

See **zg**

## INPUT AND OUTPUT FILES

See **zg**

## USAGE IN AU PROGRAMS

- **GO**

## COMMAND LINE OPTIONS

|                                                         |                                                                      |
|---------------------------------------------------------|----------------------------------------------------------------------|
| <code>-D &lt;define&gt;</code>                          | set precompiler directive <code>&lt;define&gt;</code>                |
| <code>-scaleByRg</code>                                 | divide the fid by the receiver gain                                  |
| <code>-scaleByNs</code>                                 | divide the fid by the number of scans                                |
| <code>rgAdjust</code>                                   | adjust receiver gain during dummy scans                              |
| <code>interactive</code>                                | allow parameter change during runtime of experiment                  |
| <code>o1calib</code>                                    | used for the O1 calibration experiment                               |
| <code>o1calib &lt;stepsize&gt; &lt;rangesize&gt;</code> | calibration of O1 with specified stepsize and rangesize (both in Hz) |
| <code>-help</code>                                      | print help message                                                   |

## SEE ALSO

[zg](#) [► 195], [suspend](#) [► 190], [resume](#) [► 189]

## 9.4 gs

### NAME

**gs** - Interactive parameter optimization during acquisition.

## DESCRIPTION

The command **gs** opens a dialog box that consists of two panels. In the left panel, you can adjust parameters interactively during an acquisition (see the next figure). The right panel shows the FID display window where the fid is continuously updated showing the effect of each parameter change (see the figure [Figure 9.4 \[p. 181\]](#) display).

**gs** repeatedly executes the current pulse program but only up to the first `go=n` or `rcyc=n` statement. Therefore, **gs**:

- Does not accumulate data.
- Does not interpret the phase list.
- Does not write data to disk.

The dialog box only shows the parameters which are typically set during **gs** like irradiation frequencies and offsets, pulse lengths and power levels. By default, the irradiation frequency Offset is selected for adjustment. You can adjust the indicated parameter by putting the cursor on the slider, pressing the left mouse button and moving the mouse. Alternatively, you can click above or below the slider bar. The slider sensitivity can be changed from the **Sensitivity** field. The following parameters can be changed from the **gs** dialog box:

- SFO1 - SFO8 - irradiation frequency for channel f1- f8.
- O1 - O8 - irradiation frequency offset for channel f1- f8.
- PL[0-63] - square power levels.
- AMP[0-31] – amplitude.
- PHCOR[0-31] - reference phases.
- PH\_ref - receiver phase correction.
- RG - receiver gain.
- P[0-63] - pulse lengths.
- D[0-63] – delays.

Frequency, Offset and Square Power appear for each channel that has been setup with **edasp**.

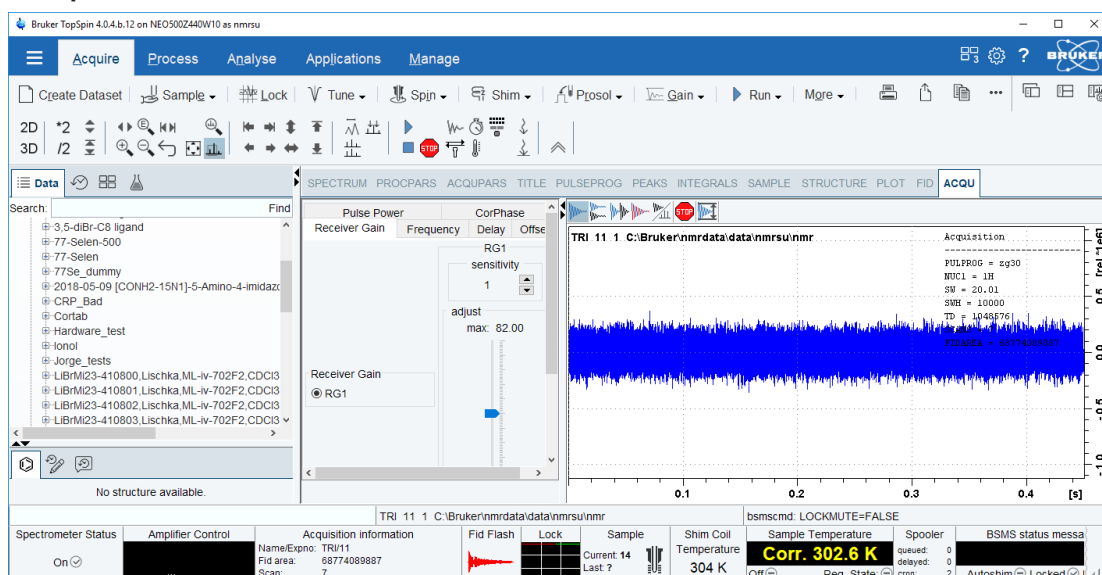


Figure 9.3: gs



Note that moving the RG slider causes an exponential change in the receiver gain. The effect of changing RG will be shown immediately in the FID display. For all other parameters in the above list, the effect of a change will be shown after one or two scans.

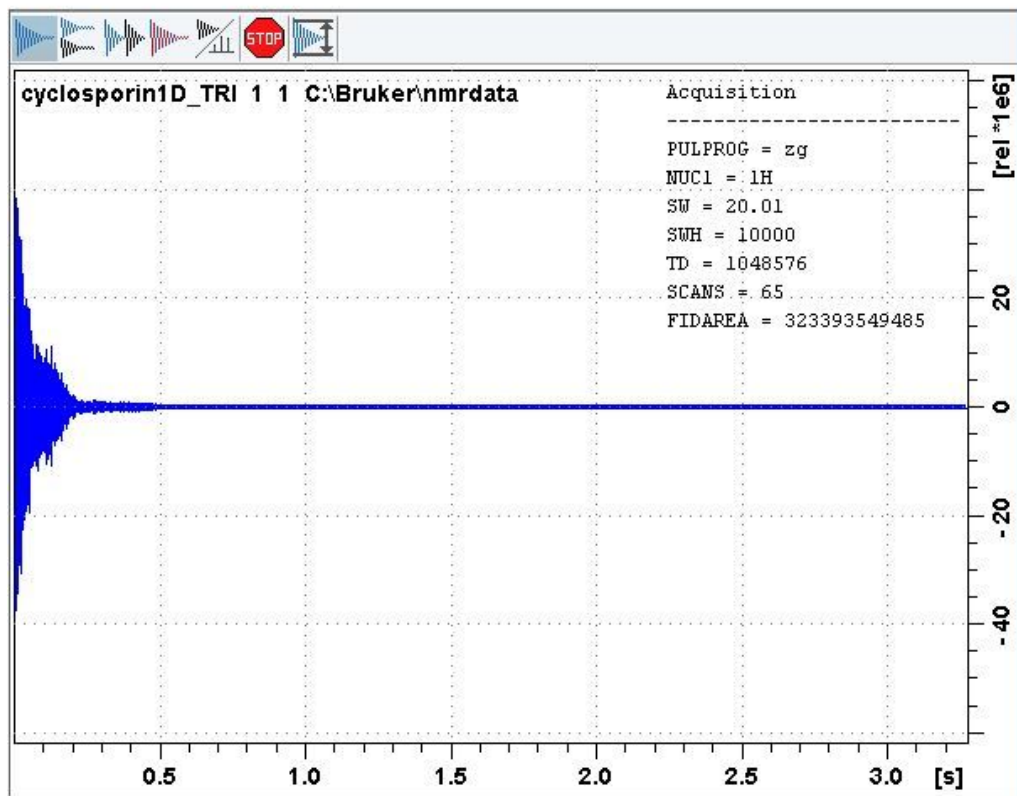


Figure 9.4: Fid display

The buttons of the FID window have the following functions:



Show FID in shuffled mode.



Show FID in unshuffled mode, vertically arranged.



Show FID in unshuffled mode, horizontally arranged.



Show FID in unshuffled mode, interleaved.



Switch between FID and spectrum.



Stop the acquisition [**stop**].



Use current FID as reference for scaling [**\_noscale**]



The button toggles between FID and real time spectrum display and provides two extra buttons:



Real time FT settings.



Toggle calculation of peak width at 50%, 5.5% and 1.1% height (Shown as status parameters).

The GS dialog box also contains the following buttons:

The screenshot shows the 'Receiver Gain' section of the GS dialog box. The 'Receiver Gain' tab is selected, and 'RG1' is chosen. A vertical slider is used to adjust the gain, with a current value of 22.60 displayed at the bottom. The slider has a maximum value of 72.60 and a minimum value of 0.25. At the bottom of the dialog are buttons for 'Save', 'Save all', 'Restore', 'Restore all', and 'Stop'.

- **Save** - save the parameter that was changed last.
- **Save all** - save all changes.
- **Restore** - restore the parameter that was changed last.
- **Restore all** - restore all changes.
- **Stop** - stop the acquisition and leave the **gs** dialog box.

If you click **Stop** without having saved your changes, **gs** shows you the changed parameters and allows you to select the ones to be saved.

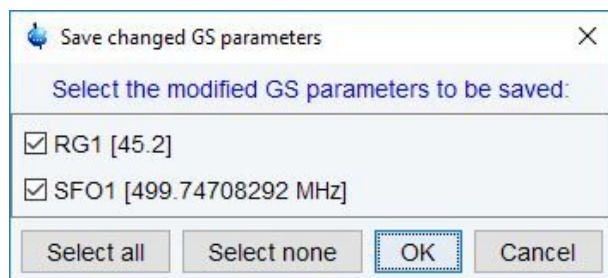


Figure 9.5: Save changed GS parameters

## INPUT AND OUTPUT PARAMETERS

See the parameter list above.

## INPUT AND OUTPUT FILES

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *acqu* - acquisition parameters

## SEE ALSO

[zg](#) [▶ 195], [go](#) [▶ 178], [rga](#) [▶ 189]

## 9.5 halt

### NAME

**halt** - Halt the acquisition after the current scan.

### DESCRIPTION

The command **halt** stops the acquisition after the current scan and writes the data to disk. It is the regular command to stop a running acquisition.



Note that **halt** does not complete the current phase cycle.




As an alternative to entering **halt** on the command line, you can click the button of the TopSpin toolbar or in the acquisition window toolbar. If, for some reason, a running or hanging acquisition cannot be stopped with **halt**, you can try the **stop** command. If that does not work either, you can use **kill**. This command will show all active processes and you can click the **go** module to stop the acquisition.

The command **halt** can even be entered with an optional parameter as command **halt <1...-NS>** (please note that <1...-NS> must be integer and > 0). If <1...-Ns> is defined the execution of **halt** is delayed until the total number of scans reaches a multiple of <1...-NS>. This option is useful if a fid with a complete phase cycle should be stored to disk.



Please note that the command **halt** and its arguments does only work with AVANCE II and newer spectrometers.

As an alternative to typing **halt <1...-NS>** in the command line the button can be used from

the TopSpin toolbar with this button: 

This button opens the following dialogue:

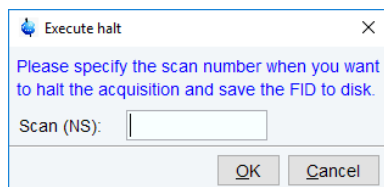


Figure 9.6: Execute halt

### OUTPUT PARAMETERS

All acquisition parameters

### OUTPUT FILES

#### In a 1D Dataset:

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *fid* - raw data
  - *acqus* - acquisition parameters

#### In a 2D Dataset:

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *ser* - raw data
  - *acqus* - F2 acquisition status parameters
  - *acqus2s* - F1 acquisition status parameters

#### In a 3D Dataset:

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *ser* - raw data
  - *acqus* - F3 acquisition status parameters
  - *acqus2s* - F2 acquisition status parameters
  - *acqus3s* - F1 acquisition status parameters

### SEE ALSO

[stop](#) [► 190], [zg](#) [► 195], [go](#) [► 178], [rga](#) [► 189], [wobb](#) [► 153]

## 9.6 iconnmr

### NAME

**IconNMR** - User interface for automation and routine spectroscopy.

**DESCRIPTION**

The command **iconnmr** starts the icon driven user interface IconNMR for routine spectroscopy and automation:

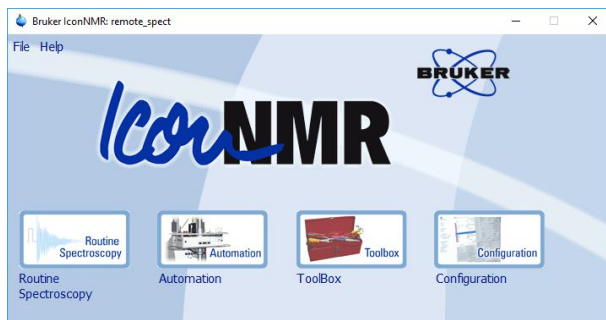


Figure 9.7: IconNMR

It is fully described in the IconNMR manual. The online version of this manual can be opened by clicking **Help | Manuals | Automation and Data Publishing | IconNMR Automation Interface**.

## 9.7 ii

---

**NAME**

**ii** - Initialize spectrometer interface.

**DESCRIPTION**

The command **ii** initializes the spectrometer interface. It tries to access all hardware parts of the spectrometer that are needed for the current experiment and loads the acquisition parameters.

**ii** must be executed once, when the spectrometer has been switched off.

For AVANCE spectrometers it is possible to effectuate a restart of the hardware controllers with the command **ii restart**. This may be helpful if a hardware failure has blocked the system.

**INPUT PARAMETERS**

All acquisition parameters.

**USAGE IN AU PROGRAMS**

- **ii**

**SEE ALSO**

[zg \[► 195\]](#)

## 9.8 popt

---

**NAME**

**popt** - Open the parameter optimization window.

**DESCRIPTION**

The command **popt** allows you to optimize acquisition parameters like pulses and delays (see the next figure).

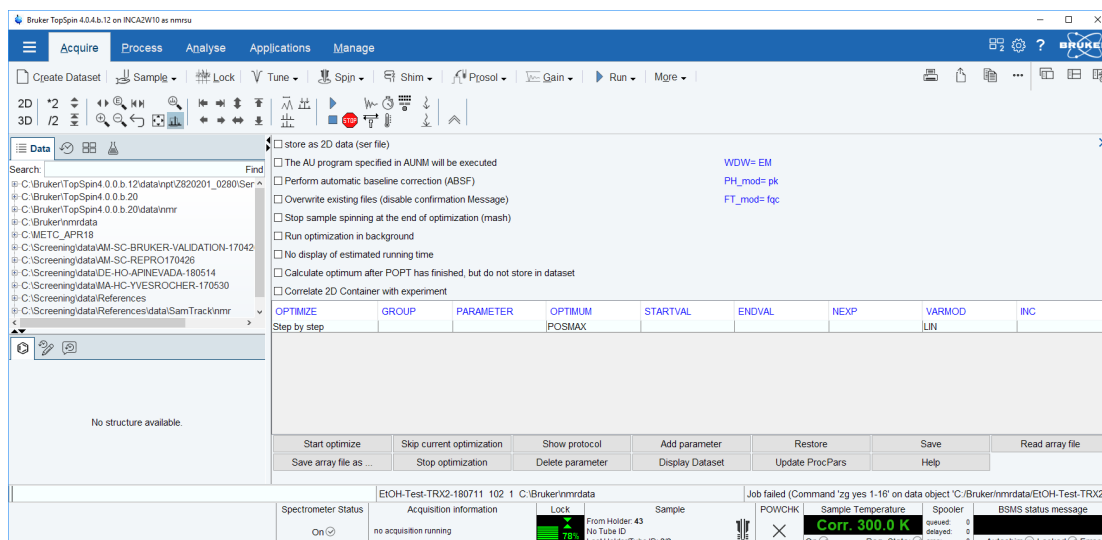


Figure 9.8: *popt*

Before you start an optimization, you must run one acquisition with the acquisition parameters as they are (not optimized) and process the data. On the resulting spectrum, you must define the spectral range (a peak or group of peaks) to be used for optimization. To do that, click-hold the left mouse button at one edge of the desired region and drag the cursor to the other edge. The TopSpin display will automatically be adjusted to show the selected region only. You must now store this region with a right-mouse click in the spectrum window and select **Save Display Region to ...** or by entering **dpl1**.

The **popt** dialog box allows you to create an entry for each parameter you want to optimize. By default, it shows only one entry; more parameters can be added by clicking the button **Add parameter**. Furthermore the following fields are offered:

- **OPTIMIZE** : Optimization of the parameters in the group.
  - **Step by Step**

The parameters of a group are optimized one after the other. NEXP can be different for each parameter. The total number of experiments is the sum of the NEXP value of each parameter. The result of each parameter optimization is stored in a separate PROCNO.
  - **Simultaneous**

The parameters of a group are optimized simultaneously. NEXP must be the same for each parameter and represents the total number of experiments. The result of the parameter optimization is stored in one PROCNO.
  - **Array**

The parameters of a group are optimized according to an N-dimensional array (N is the number of parameters in a group). NEXP can be different for each parameter. The total number of experiments is the product of the NEXP value of each parameter. The result of the parameter optimization is stored in one PROCNO.
  - **No Optimization**

The parameter is not optimized.
- **GROUP**: group number. Optimization starts with the lowest group number.
- **PARAMETER**: The parameter to be optimized. If **OPTIMIZE** is set to **No Optimization**, the parameter will be stored as comment in the optimization setup.
- **OPTIMUM**: Optimization criterion (see below).
- **STARTVAL**: First value of the parameter.
- **ENDVAL**: Last value of the parameter.

- **NEXP**: Number of experiments.
- **VARMOD**: Parameter variation mode: linear or logarithmic.
- **INC**: Parameter increment value. Unused for VARMOD = log.

The optimization criterion OPTIMUM can take the following values:

- POSMAX - the maximum value of a positive peak.
- NEGMAX - the maximum value of a negative peak.
- ZERO - zero intensity of a peak.
- MAGMAX - the maximum magnitude value of a peak.
- MAGMIN - the minimum magnitude value of a peak.

At the bottom of the dialog box you will find the following buttons:

- **Start optimize** - start the optimization for all checked parameters.
- **Skip current optimization** - stop the optimization for the current parameter.
- **Show protocol** - show the optimization result. A dialog appears with a list of protocol files:
  - *popt.protocol* : the entire optimization result.
  - *popt.protocol.999* : the optimization result in PROCNO 999.
  - *popt.protocol.998*: the optimization result in PROCNO 998.
  - etc.
- **Add parameter** - add a parameter entry.
- **Restore** - restore the last saved optimization setup.
- **Save** - save the current optimization setup to current dataset EXPNO.
- **Read array file** - read optimization setup.
- **Save array file as..** - save current optimization setup for general usage.
- **Stop optimization** - stop the optimization for all checked parameters.
- **Delete parameter** - delete the selected parameter.
- Display Dataset – Display the current dataset
- Update ProcPars – Update Processing Parameters
- **Help** - open the **popt** help page.

Clicking the button **Start optimize** will start the optimization process.



Note that it runs on the current dataset. For each parameter/group, a series of acquisitions will be performed. The result of this is a series of spectra (actually spectral regions) that are displayed in one screen and show the optimum parameter value. They are stored as one or more processed data files under the current dataset name and experiment number, but under different processing numbers. For the first parameter/group that is optimized this is PROCNO 999, for the second parameter/group PROCNO 998 etc. As such, you must start **popt** on a dataset with PROCNO < 900. The result will also be stored in the so-called protocol file (see OUTPUT FILES)

*Please note that the **popt** command is especially useful for 90° pulse length calibration.*

***TO Do: Beispiel***

*But also for pulse power optimization or any other pulse (decoupling, indirect pulses etc.) popt can be a useful tool.*

At the top of the dialog box you will find the following check buttons:

- **Store as 2D data (ser file).**

If checked, the result of the optimization (a series of 1D spectra) will be stored as a 2D dataset in EXPNO 899. However, if the source dataset PROCNO is greater than 100, the EXPNO of the destination 2D data will be

PROCNO - 100.

- **The AU program specified in AUNM will be executed.**

If checked, the AU program defined by AUNM will be executed instead of the command **zg**.

- **Perform automatic baseline correction (ABSF)**

If checked, the output data will be baseline corrected with **absf**.



Note that this command corrects the selected region (determined by the processing parameters ABSF1 and ABSF2).

- **Overwrite existing files (disable confirmation message).**

If checked, the output PROCNO, if it exists, will be overwritten without warning.

- **Stop sample spinning at the end of optimization (mash)**

- **Run optimization in background**

If checked, the foreground dataset will remain the same during the optimization. If it is not checked, the TopSpin display will change to PROCNO 999 where the optimization result is displayed.

- **No display of estimated running time**

- **Calculate optimum after POPT has finished, but do not store in dataset**

- **Correlate 2D Container with experiment**

To the right of the above check buttons, the current values of the parameters WDW (window multiplication mode), PH\_mod (phase correction mode) and FT\_mod (Fourier Transform mode) are displayed.

If you want to rerun an optimization, you must first return to the starting PROCNO.

### INPUT FILES

- <tshome>/exp/stan/nmr/lists/popt/
  - <name> - parameter optimization setup for general usage (input of **Read array file..**)
- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters
  - *popt.array* - parameter optimization setup (input of **Restore**)
  - *popt.protocol* - parameter optimization result (input of **Show protocol**)
- <dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/
  - *proc* - processing parameters
- <tshome>/prog/au/bin/
  - *poptau* - AU program that runs the optimization (executable)
  - *popthalt* - AU program that halts the current optimization (executable)

## OUTPUT FILES

- `<tshome>/exp/stan/nmr/lists/popt/`
  - `<name>` - parameter optimization setup for general usage (output of **Save array file as..**)
- `<dir>/data/<user>/nmr/<name>/<expno>/pdata/999`
  - `1r` - processed data containing the optimization result of the first parameter/group
- `<dir>/data/<user>/nmr/<name>/<expno>/pdata/998`
  - `1r` - processed data containing the optimization result of the 2<sup>nd</sup> parameter/group
- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - `popt.array` - parameter optimization setup (output of **Save**)
  - `popt.protocol` - parameter optimization result (output of **Start optimize**)
- `<dir>/data/<user>/nmr/<name>/899/`
  - `ser` - 2D raw data containing the optimization result

## SEE ALSO

[gs](#) [► 179], [zg](#) [► 195]

## 9.9 resume

---

## NAME

**resume** - Resume a suspended acquisition.

## DESCRIPTION

The command **resume** resumes an acquisition that has been suspended.

An acquisition can be suspended with the command **suspend**. When this is entered, the acquisition holds as soon as the pulse program statement `suspend` or `calcsuspend` is encountered. If the pulse program does not contain such a statement, **suspend** has no effect. Alternatively, an acquisition can be suspended with the pulse program statement `autosuspend` or `calcautosuspend`. They automatically hold the acquisition, without user interaction. The command **resume** continues acquisition that was suspended, either automatically or with the command **suspend**.

For more information on the `suspend` pulse program statements click:

**Help | Manuals | Programming Manuals | Pulse Programming**

A resumed acquisition does not start with dummy scans. This can be a problem if the recycle delay is shorter than 4 times the T1 value of the measured nucleus.



Note that the suspend information is temporarily stored on the spectrometer hardware, not on the workstation disk. As soon as you enter **stop** or **halt**, or switch off the spectrometer, the suspend information is lost and the acquisition cannot be resumed.

## SEE ALSO

[suspend](#) [► 190], [zg](#) [► 195], [go](#) [► 178]

## 9.10 rga

---

## NAME

**rga** - Automatic receiver gain optimization.

## DESCRIPTION

The command **rga** automatically optimizes the receiver gain. It performs an acquisition with varying receiver gain and finally sets it just below the value where no overflow occurs. In fact, **rga** repeatedly executes the current pulse program but only up to the first `go=n` or `rcyc=n` statement.

If you already know the proper value for the receiver gain, you can simply set RG in **eda** or by typing **rg** on the command line.

## OUTPUT PARAMETERS

- can be viewed with **eda** or by typing **rg**:
  - RG - receiver gain

## USAGE IN AUTOMATION

- RGA

## SEE ALSO

[gs \[► 179\]](#), [zg \[► 195\]](#), [go \[► 178\]](#)

## 9.11 stop

---

### NAME

**stop** - Stop the acquisition immediately


### DESCRIPTION

The command **stop** stops the acquisition immediately without writing the data to disk.



Note that in most 1D experiments, the data are only written at the end of the acquisition and using **stop** would cause a complete loss of data. As such, it is used in case of emergency. To stop a normal acquisition the **halt** command is used.



Instead of entering **stop** on the command line, you can also click the  button in TopSpin tool bar or in the acquisition window toolbar.

If, for some reason, a running or hanging acquisition cannot be stopped with **halt** or **stop**, you can use **kill**. This command will show all active processes and you can click the **go** module to stop the acquisition.

## SEE ALSO

[halt \[► 183\]](#), [zg \[► 195\]](#), [go \[► 178\]](#), [rga \[► 189\]](#), [wobb \[► 153\]](#)

## 9.12 suspend

---

### NAME

**suspend** - Suspend a running acquisition.

**DESCRIPTION**

The command **suspend** allows you to hold a running acquisition. When it is entered, the acquisition holds as soon as the pulse program statement `suspend` or `calcsuspend` is encountered. If the pulse program does not contain such a statement, **suspend** has no effect. Alternatively, an acquisition can be suspended with the pulse program statement `autosuspend` or `calcautosuspend`. They automatically hold the acquisition, without user interaction. The command **resume** continues acquisition that was suspended, either automatically or with the command **suspend**.



Note that the suspend information is temporarily stored on the spectrometer hardware, not on the workstation disk. As soon as you enter **stop** or **halt**, or switch off the spectrometer, this information is lost, and the acquisition cannot be resumed.

Standard Bruker pulse programs do not contain any `suspend` statements. Therefore, **suspend** can only be used with user defined pulse programs which contain a `suspend` statement at a certain position.

**SEE ALSO**

[resume](#) [► 189], [zg](#) [► 195], [go](#) [► 178]

## 9.13 topguide

---

**NAME**

**topguide** - Open the *TopGuide* acquisition and processing tool

**DESCRIPTION**

The command **topguide** opens a guided acquisition and processing tool: *TopGuide*. This tool is a guide for setting up and processing NMR experiments. As the name implies, it is an interactive guide, which guides the user through the necessary and important steps after the insert of a new sample (tuning & matching the sample, locking, shimming) and the following process of running a basic 1H 1D (reference) experiment. After these initial steps it offers a database with the basic 1D and 2D NMR experiments and helps the user to set those up.

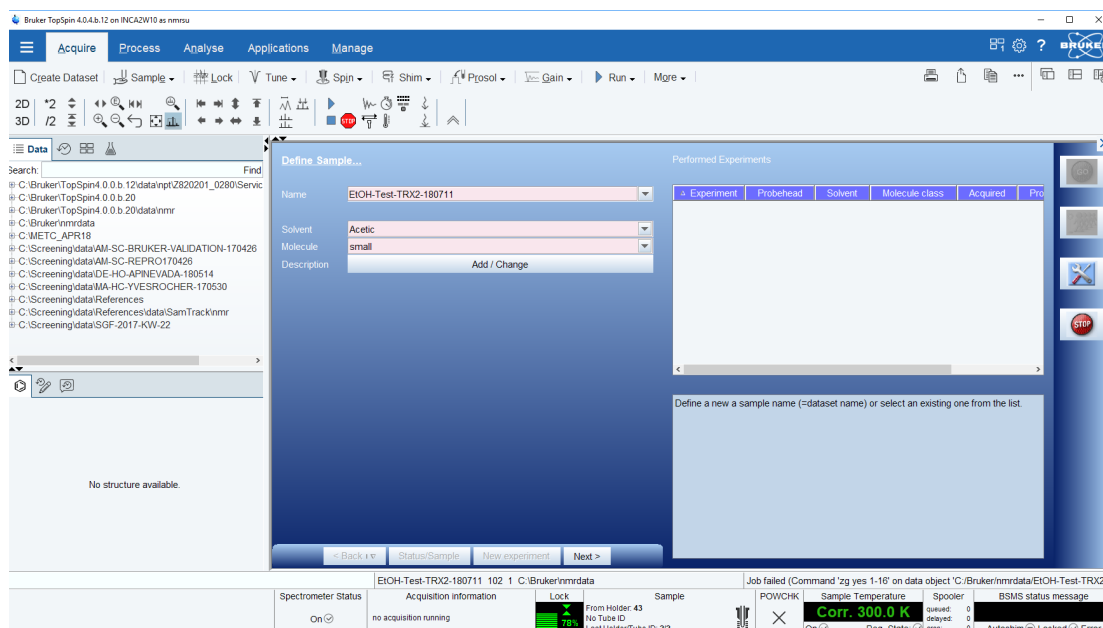


Figure 9.9: topguide

The special user interface of *TopGuide* guides the user through all the steps and decisions the user has to make. Each item within the user interface has its own help context. The help text describes the action the user has to take, gives explanations for parameters, provides explanations for procedures and/or some background information.

*TopGuide* keeps track of the experiments which were run using *TopGuide* and stores this information in a database. For each sample (i.e. Name) the status window (Performed Experiments) shows the list of experiments which are setup (Acquisition no) or done (Acquisition yes) and if processing has been done or not (Processing yes/no). The status list provides an easy way to access these datasets: a simple left click will load the dataset into the upper part of the window, a right click pops up a context menu which gives access to either acquisition or processing parameters or some other dataset related commands.

On the right is a tool bar with 4 buttons for the basic operation. **GO** starts the acquisition on the current dataset. The spooler mechanism (acquisition queue) enables the user to run more than 1 experiment in a row. It is an option and the user should enable auto-queuing in the **Preference** dialog. If enabled, all acquisition commands are automatically send into this queue. The **Queue** button offers the possibility to use the queue even if auto-queuing is disabled or to delay the start of an acquisition by entering a certain start time. The **Tools** button gives access to preferences and some other options and to leave *TopGuide* (**Quit**). **STOP** will stop the current acquisition and will disable the spooler. This is meant to be used as an emergency stop. If the user wants to end a running acquisition in a defined manner, he should type **halt** instead of **stop** (or **halt 8** on AVANCE II and newer spectrometers). **halt** will finish the current scan and writes the acquired data to disk.

## General Concept of TopGuide

If a new sample should be measured some initial set up steps are strongly advised: tuning & matching the probe to the sample susceptibility, locking and shimming. *TopGuide* will lead the user through these initial steps by either doing all this automatically or giving help information for manual operation. The automatic execution, of course, depends on the hardware configuration. A probe equipped with ATMA and a Z-gradient coil allows this. Without this hardware, some manual steps are required and the user is guided through manual tuning & matching and/or manual shimming. If a Z-gradient is present, *TopGuide* assumes that automatic gradient shimming is set up and it will be used by *TopGuide*. *TopGuide* caches the information about these steps executed, so further measurements (within the same *TopGuide* session) on the same sample will not ask for this again, unless the user changes the nucleus to be measured. If, for example, a  $^1\text{H}, ^{13}\text{C}$ -HSQC had been

measured and therefore *TopGuide* knows that the probe is tuned to  $^1\text{H}$  and  $^{13}\text{C}$ , and you now want to run a  $^1\text{H},^{15}\text{N}$ -HSQC (let's assume you have a BBI probe and therefore this is possible), *TopGuide* will request to tune & match again, now to  $^{15}\text{N}$  instead of  $^{13}\text{C}$ .

The use of *TopGuide* to setup new experiments is based on a recorded  $^1\text{H}$  1D spectrum. This proton spectrum is used to determine the signal to noise ratio (S/N) for this sample. *TopGuide* will select the highest signal in the spectrum (solvent peaks are automatically excluded), but the user may select a different peak/area for the S/N calculation. This may be of interest if the highest signal doesn't belong to the investigated compound in the case of mixtures or impurities. The determined S/N is used to estimate the number of scans (NS) for further experiments, to obtain a spectrum with reasonable S/N.

*TopGuide* provides a database with basic 1D and 2D experiments. *TopGuide* will only offer those experiments, which may be run on the current hardware, i.e. if the current probe doesn't have a gradient, *TopGuide* will not offer any experiment using gradients, but if the probe is equipped with a gradient, *TopGuide* will preferably offer experiments using gradients. If the current probe is a  $^{13}\text{C}/^1\text{H}$  dual probe, *TopGuide* will not offer any  $^{15}\text{N}$  experiment. There are some more filter criteria based on the field strength. *TopGuide* doesn't use parameter sets like IconNMR. Therefore, *TopGuide* will never show the same experiments as you would see in the listing of parameter sets, it will always show recommended experiments.

Before an additional experiment is performed, *TopGuide* will ask you to determine the spectral width (SW) to be used in the proton dimension. It will pre-select the region with peaks found in the reference spectrum. You may change this to your needs but be aware that for homonuclear 2D measurements this SW will be applied to the indirect dimension as well. If you select a region which cuts off some signals, you may get folding of these peaks in the indirect dimension of a homonuclear 2D. The information about your selected SW is stored together with the reference spectrum and will be used in all further  $^1\text{H}$  dimensions for this sample.

The database contains reasonable acquisition and processing parameters for all experiments in it. Some parameters are fixed (typical coupling constants), some are dynamic and are chosen based on the molecular size (like relaxation times or NOESY mixing times), the field strength (TD) or the actual experiment (different SW for  $^{13}\text{C}$  in HSQC and HMBC).



#### Tools Button

The **Tools** button gives access to some preferences and options.

**Data Directory:** the user can select the data directory where the NMR data is stored (disk unit). The initial setting depends on how *TopGuide* has been started. If you start *TopGuide* on a loaded dataset, it will keep that disk unit, if you start with no active dataset this will open a new window and the data path defaults to the TopSpin installation directory (i.e. C:\Bruker\TopSpin under Windows or /opt/topspin under Linux).

**User:** if additional IconNMR users are defined, you can login as one of those.

**Preferences:** you can enable or disable **auto-processing**. Depending on this setting newly acquired data is automatically processed with default processing parameters and options, or not.

**Protected acquisition:** this means that once an FID or SER file has been acquired it is protected by TopGuide, you are not allowed to overwrite it. The start of a new acquisition on a dataset with an existing FID/SER file will automatically create a new dataset (i.e. expno).

**Protected processing:** the same protection as described above is applied to processed data. Existing ones are not overwritten, but instead a new procno is created.

**Import reference:** Setting up experiments with *TopGuide* requires a reference 1D spectrum, which is measured with *TopGuide* by default. If a 1D spectrum has already been recorded outside of *TopGuide* and you want to use this one as a reference for further experiments, you can import it into *TopGuide*. The import searches all expnos of the current dataset and displays the available 1D 1H spectra.

### SEE ALSO

[zg \[ 195\]](#), [halt \[ 183\]](#), [go \[ 178\]](#), [stop \[ 190\]](#)


## 9.14 tr

### NAME

**tr** - Transfer data to disk during the acquisition.

### DESCRIPTION

The command **tr** transfers (writes) data to disk during a 1D acquisition. This is, for example, useful if you want to do a Fourier transform and view the spectrum before the acquisition has finished. Another reason to use **tr** is to save the currently acquired scans of a long term acquisition. This avoids losing all data in case of a power loss.

As an alternative to entering **tr** on the command line, you can click the  button of the TopSpin toolbar.

The command **tr** can even be entered with an optional parameter as command **tr <1...-NS>** (please note that <1...-NS> must be integer and > 0). If <1...-NS> is defined the execution of **tr** is delayed until the total number of scans reaches a multiple of <1...-NS>. This option is useful if a fid with a complete phase cycle should be stored to disk.

As an alternative to typing **tr <1...-NS>** in the command line the button can be used from

the TopSpin toolbar with this button: 

This button opens the following dialog:

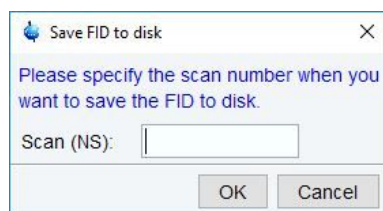


Figure 9.10: Save FID to disk

### OUTPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *fid* - 1D raw data
  - *acqus* - acquisition status parameters

### SEE ALSO

[zg \[ 195\]](#), [go \[ 178\]](#)

## 9.15 **xaua, xaup**

---

### NAME

**xaua** - Execute the AU program specified with AUNM

**xaup** - Execute the AU program specified with AUNMP

### DESCRIPTION

The commands **xaua** and **xaup** execute the AU program which is specified by the parameters AUNM and AUNMP, respectively. In all Bruker parameter sets, these parameters are set to relevant Bruker AU programs. For example, in the parameter set PROTON, AUNM = au\_zg and AUNMP = proc\_1d. When parameter sets are used in automation (IconNMR), the AU programs specified by AUNM and AUNMP perform the acquisition and the processing, respectively.

For details on writing, compiling, and executing AU programs please refer to the TopSpin AU Programming manual (click [Help](#) | [Manuals](#) | [Programming Manuals](#) | [AU Programming](#)).

### INPUT PARAMETERS

- Set by the user with **eda** or by typing **aunm** :
  - AUNM - acquisition AU program name for **xaua**
- Set by the user with **edp** or by typing **aunmp** :
  - AUNMP - processing AU program name for **xaup**

### INPUT FILES

- <tshome>/exp/stan/nmr/au/src/
  - AU program source files (only input if the AU program is not compiled yet)
- <tshome>/prog/au/bin/
  - AU program binary executables
- <dir>/data/<user>/<name>/nmr/<expno>/
  - *acqu* - acquisition parameters (input file for **xaua**)
- <dir>/data/<user>/<name>/nmr/<expno>/pdata/<procno>/
  - *proc* - processing parameters (input file for **xaup**)

### USAGE IN AU PROGRAMS

- XAUA
- XAUP
- XAUPW
 

XAUPW waits until the AU program has finished before the next statement is executed whereas XAUP doesn't. XAUA works like XAUPW in this respect.

### SEE ALSO

(xau, edau, delau), [expinstall](#) [ 99], (compileall, cplbruk, cpluser)

## 9.16 **zg**

---

### NAME

**zg** - Perform an acquisition, overwriting possibly existing data

## DESCRIPTION

The command **zg** performs an acquisition on the current dataset. A new data window will appear showing the currently acquired FID:



Figure 9.11: zg

While an acquisition is running the buttons of the ACQU window have the following functions:



Show FID in shuffled mode.



Show FID in unshuffled mode, horizontally arranged.



Show FID in unshuffled mode, vertically arranged.



Show FID in unshuffled mode, interleaved.



Switch between FID and spectrum.



Halt the acquisition [**halt**].



Stop the acquisition [**stop**].



The button toggles between FID and real time spectrum display and provides two extra buttons:



Real time FT settings.

Clicking this button opens the following dialog window:

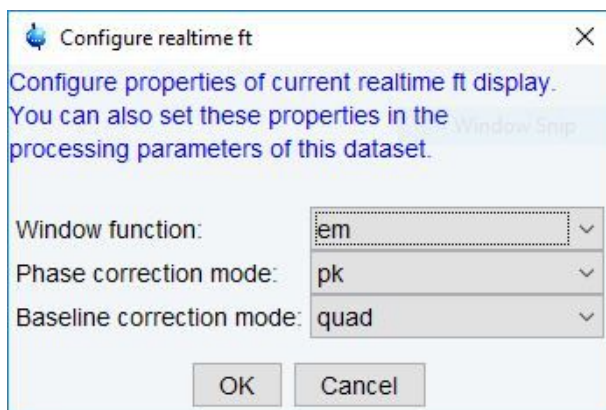


Figure 9.12: Configure realtime spectrum display parameters



Toggle calculation of peak with at 50%, 5.5% and 1.1% height. (Shown as status parameters)

The command **zg** performs the following sequence of actions:

- Read the acquisition parameters.
- Compile the pulse program defined by the acquisition parameter PULPROG.
- Execute the pulse program. For most pulse programs this involves:
  - The acquisition of DS dummy scans.
  - The acquisition of NS real scans, accumulating the data.
  - Storing the accumulated data to disk.
- Update the acquisition status parameters

### Acquisition Sequence

Before you can start an acquisition with **zg**, you will normally have to prepare the experiment. This typically involves the following command sequence:

- **edprobe** [▶ 144] - define the current probe.
- **edprosol** - define the probe and solvent dependent parameters.
- **new** - define a new dataset and make it the current dataset.
- **rpar** - read a standard parameter set for the desired experiment.
- **getprosol** - get the probe and solvent dependent parameters.



**Please note that the new command offers the possibility to read a parameter set and to execute getprosol. A separate rpar and getprosol command is then not necessary.**

- **lockdisp** - open the lock display window.
- **lock** - lock the magnetic field.
- **wobb** or **atma** - tune and match the probe (**atma** only for ATM probes).
- **edasp** - set up nuclei (NUC1, NUC2 etc.) and the spectrometer routing
- **ased** or **eda** - adjust the acquisition parameters to your needs.
- **zg** - acquire the data.

## Pulse Program

The type of experiment is mainly determined by the pulse program. A simple 1D Bruker pulse program is `zg`, which contains the following lines:

```
1 ze ;zero memory, reset scan counter and phase lists,
 ;enable dummy scans, label 1

2 d1 ;relaxation delay with length D1, label 2
 p1 ph1 ;pulse with length P1 and phase ph1
 go=2 ph31 ;sample TD points with phase ph31, loop to 2
 ; times NS+DS

 wr #0 ;write the data to the current dataset
exit ;end of the pulse program

ph1=0 2 2 0 1 3 3 1 ;phase program (list) used for the RF pulse
ph31=0 2 2 0 1 3 3 1 ;phase program (list) used for the receiver
```

The RF pulse `p1` is executed on the default channel (`f1`) with the default power level (`PL1`). The loop to label 2 will be performed `NS` times to accumulate this number of scans. The `wr` statement lies outside of this loop which means the data are only written to disk once, at the end of the experiment.

Furthermore, an information window will appear showing the current scan, the total number of scans and the residual experiment time.

The purpose of dummy scans is to reach steady state conditions concerning  $T_1$  relaxation. This is necessary whenever the recycle delay of the experiment is shorter than 4 times the  $T_1$  value of the measured nucleus. Furthermore, dummy scans can be used to establish a stable temperature. This is especially important in decoupling experiments where the irradiation high power increases the sample temperature. The number of dummy scans is determined by the acquisition parameter `DS`. In the pulse program, the `ze` statement explicitly enables the `go` statement to perform dummy scans. In contrast, the `zd` statement disables the execution of dummy scans.

## Transfer to Disk

In most 1D experiments, the acquired data are written to disk only once, at the end of the experiment. You can, however, use the command `tr` to write data to disk while the acquisition is running. This is, for example, useful if you want to do a Fourier transform and view the spectrum after a few scans. Another reason to use `tr` is to save the currently acquired scans of a long-term experiment. This avoids losing all data in case of a power loss. In multidimensional experiments, the `wr` statement is part of a loop, and is executed for each increment in the indirect direction(s).




Note that in many pulse programs the `wr` statement has been replaced by the `mc` statement which performs both the disk write and loop back function.

## Multidimensional Data

`zg` allows you to perform 1D or multi-dimensional acquisition. The dimensionality of the data is determined by the pulse program. If this contains an `if` and/or `st` statement, `zg` assumes a 2D or 3D dataset. Furthermore, if the pulse program contains a nested loop with loop counters `td1` and `td2`, `zg` assumes a 3D dataset. Finally, the acquisition parameter `PARMODE` is evaluated. If the value of `PARMODE` is not consistent with the pulse program, `zg` will display a warning but allow you to continue the acquisition. 1D data are stored a file named *fid* under the experiment number (`expno`) of the current dataset. 2D and 3D data are

stored in a file named `ser` in the same directory. The pulse program is not limited to 3D and allows you to acquire data in 4 or more directions. TopSpin 2.0 and newer supports processing of nD data. Datasets up to dimension 5 have been tested by Bruker.


### Stopping Acquisition

Normally, an acquisition will run until it has finished. If, however, you want to interrupt it, you can do that by clicking the  button or entering the command **halt**. This will finish the current scan, write the data to disk and then stop the acquisition.



Note that **halt** finishes the current scan but not the current phase cycle.



Clicking the  button or entering the command **stop** immediately stops the acquisition. It does not finish the current scan or write the data to disk. If, for some reason, **halt** and **stop** do not work, you can use the command **kill** to stop the acquisition.

When an acquisition has finished but the signal to noise is insufficient, you can accumulate additional scans. Just set the parameter NS to the number of extra scans and enter **go**. This command does not overwrite the existing data but adds the extra scans to them. **Caution: go** works correctly if the previous acquisition has finished normally but should not be used if this has been interrupted with **halt** or **stop** (see the description of **go**).


### Preventing Data Overflow

1D raw data are, if necessary, stored as double precision (64-bit) data. If, based on the number of scans and the current accumulated signal, data overflow is expected to occur, data are transferred to the computer that controls the spectrometer, i.e. an automatic **tr** command is executed. Here the data are stored in 64-bit double precision format. The acquisition status parameter DTYPA shows whether data are stored as integers (DTYPA = int) or doubles (DTYPA = double).



Note that processed data are always stored as integer data.

### Preventing Data Overwrite

**zg** overwrites possibly existing raw data. Each user can configure TopSpin to get a warning about existing data or not. Click on the Preferences icon  | **Acquisition** and make sure that the entry **Overwrite existing FID without inquiry (ZG safety off)** is not checked.



Note the difference between **zg** and **go**. The latter command does not overwrite existing data but adds new data to them.

After a manually performed acquisition has finished, it is normally processed with processing commands like **em**, **ft**, **apk** etc. Processing commands are described in the Processing Reference Manual.

The command **zg** is automatically executed by AU programs that contain the ZG macro. Examples of these are **au\_zg\***, **au\_getl\*** and **multizg**. Furthermore, **zg** is automatically executed when experiments are started from the automation interface IconNMR.



Note that an acquisition always runs in background which means that TopSpin can do other tasks simultaneously. You can change the focus to a different data window and process data there. This is actually what happens all the time during an automation sequence performed by IconNMR.

## Pulse Programming

TopSpin is supplied with a large number of pulse programs from simple 1D to sophisticated multidimensional experiments. Furthermore, you can write your own pulse programs with the **edpul** command using the Bruker pulse programs as an example. For a detailed description of the pulse program syntax click:

**Help | Manuals | Programming Manuals | Pulse Programming Manual**

Python programs and pulse programs can be integrated. Python programs can calculate pulse program parameters such as delays, pulses, phases and shapes using Python, and generate or execute a pulse program by executing a Python program.

(cf . **Help | Manuals | Programming Manuals | Pulse Programming With Python**).

## Command Spooling/Queuing

**zg**, like other acquisition commands, is automatically queued. This allows you to enter multiple **zg** commands, for example on different datasets. Queued commands can be viewed in the Spooling field of the acquisition status bar. Automatic command spooling as well as the display of the spooling field in the status bar can be enabled/disabled in the User Preferences



(command **set**).

## INPUT PARAMETERS

All acquisition parameters as described in chapter [TopSpin Parameters \[ 13\]](#) of the Acquisition Reference Manual.

## OUTPUT PARAMETERS

All acquisition status parameters as described in chapter [TopSpin Parameters \[ 13\]](#) of the Acquisition Reference Manual.

## INPUT FILES

### 1D Data

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *acqu* - acquisition parameters

### 2D Data

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *acqu* - acquisition parameters direct direction (F2)
  - *acqu2* - acquisition parameters indirect direction (F1)

### 3D Data

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *acqu* - acquisition parameters direct direction (F3)
  - *acqu2* - acquisition parameters indirect direction (F2)
  - *acqu3* - acquisition parameters indirect direction (F1)

**All Data**

- `<tshome>/exp/stan/nmr/lists/` (primary source) or `<dir>/data/<user>/nmr/<name>/<expno>/lists` (fallback if not found in primary source)
  - `pp/<PULPROG>` - the pulse program defined by PULPROG
  - other list files (e.g. shapes, CPD programs as well as frequency, loopcounter, delay, or pulse lists) in their respective subfolders
- `<tshome>/conf/instr/<curinst>/`
  - `scon2` - spectrometer parameters (created with **edscon**)

**OUTPUT FILES****1D Data**

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - `fid` - raw data
  - `acqus` - acquisition status parameters

**2D Data**

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - `ser` - raw data
  - `acqus` - acquisition status parameters direct direction (F2)
  - `acqus2s` - acquisition status parameters indirect direction (F1)

**3D Data**

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - `ser` - raw data
  - `acqus` - acquisition status parameters direct direction (F3)
  - `acqus2s` - acquisition status parameters indirect direction (F2)
  - `acqus3s` - acquisition status parameters indirect direction (F1)

**All Data**

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - `Pulseprogram.precomp` - the precompiled pulse program
  - `audita.txt` - acquisition audit trail
  - `scon2` - spectrometer parameters
  - `dslist` - dataset list (output if a `wr #n` or `wr ##` statement is used)
  - `cag_par` - rotation matrices for gradients used for imaging
- `<dir>/data/<user>/nmr/<name>/<expno>/lists`
  - used list files (e.g. shapes, CPD programs as well as frequency, loopcounter, delay, or pulse lists) in their respective subfolders

**USAGE IN AU PROGRAMS**

- ZG

**COMMAND LINE OPTIONS**

|                                |                                                       |
|--------------------------------|-------------------------------------------------------|
| <code>-D &lt;define&gt;</code> | set precompiler directive <code>&lt;define&gt;</code> |
|--------------------------------|-------------------------------------------------------|

|                                |                                                                      |
|--------------------------------|----------------------------------------------------------------------|
| -scaleByRg                     | divide the fid by the receiver gain                                  |
| -scaleByNs                     | divide the fid by the number of scans                                |
| rgAdjust                       | adjust receiver gain during dummy scans                              |
| interactive                    | allow parameter change during runtime of experiment                  |
| o1calib                        | used for the O1 calibration experiment                               |
| o1calib <stepsize> <rangesize> | calibration of O1 with specified stepsize and rangesize (both in Hz) |
| -help                          | print help message                                                   |

### SEE ALSO

[go](#) [► 178], [gs](#) [► 179], [rga](#) [► 189], [wobb](#) [► 153], [atma](#) [► 141], [suspend](#) [► 190], [resume](#) [► 189]

# 10 Temperature Commands

This chapter describes commands which configure, control or monitor the temperature unit. Temperature units which are delivered with Bruker spectrometers are often referred to as a eurotherm; the make of most units. They are used to warm up or cool down the NMR sample and keep it at a certain temperature during the experiment.

## 10.1 edte

### NAME

**edte** - Edit the temperature parameters

### DESCRIPTION

The command **edte** opens a dialog box from which the temperature unit can be controlled (see the next figure).

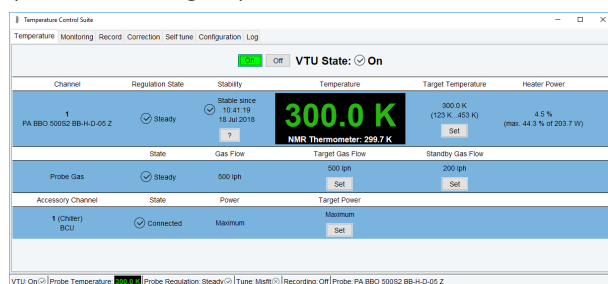


Figure 10.1: **edte**

The functionality of this window is described in a separate manual that can be opened from the TopSpin window by clicking:

**Help | Manuals | Technical Manuals | Temperature Regulation**

Or from the **edte** window by clicking:

**Help | Edte Users Manual**

### SEE ALSO

[teget, te2get](#) [ 203], [teset, te2set](#) [ 204]

## 10.2 teget, te2get

### NAME

**teget** - Get the temperature from the temperature unit.

**te2get** - Get the second temperature from the temperature unit.

### DESCRIPTION

The command **teget** gets the temperature from the temperature unit and stores it in the acquisition status parameter TE.

The command **te2get** gets the so called second temperature from a temperature unit with two regulators. The value is stored in the acquisition status parameter TE2. Temperature units with two regulators are, for example, used in BEST NMR where the first regulator controls the sample temperature and the second regulator controls the inlet capillary temperature.

### OUTPUT PARAMETERS

- *TE* - demand temperate on the temperature unit.
- *TE2* - demand second temperate on the temperature unit.

### OUTPUT FILES

- `<dir>/data/<user>/nmr/<name>/<expno>/`
  - *acqus* - acquisition status parameters

### USAGE IN AU PROGRAMS

- TEGET
- TE2GET

### SEE ALSO

[edte](#) [► 203], [teset](#), [te2set](#) [► 204]

## 10.3 teset, te2set

---

### NAME

**teset** - Set the temperature on the temperature unit.

**te2set** - Set the second temperature on the temperature unit.

### SYNTAX

`teset [<temperature>]`

`te2set [<temperature>]`

### DESCRIPTION

The command **teset** sets the temperature on the temperature unit. It takes one argument and can be used as follows:

#### **teset**

Sets the temperature to the value of the acquisition parameter TE. Before you enter **teset** without argument you must set TE to the desired temperature, in Kelvin, either from **eda** or by typing **te** on the command line.

#### **teset <temperature>**

Sets the temperature to the specified value.

The command **teset** is, for example, used in the AU programs **au\_zgte** and **multi\_zgvt**.

The command **te2set** works like **teset** except that it sets the so called second temperature to the value of the acquisition parameter TE2. This value is set on the second regulator of a temperature unit with two regulators. Such units are, for example, used in BEST NMR where the first regulator controls the sample temperature and the second regulator controls the inlet capillary temperature.

### INPUT PARAMETERS

- TE - demand temperature on the temperature unit (input of **teset**).
- TE2 - demand second temperature on the temperature unit (input of **te2set**).

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters

### USAGE IN AU PROGRAMS

- TESET
- TE2SET
- VT executes the command **teset <vt\_list\_index>**

### SEE ALSO

[edte](#) [► 203], [teget](#), [te2get](#) [► 203]




# 11 MAS Commands

## 11.1 MasDisp

### 11.1.1 Accessing the User Interface

The user interface can be accessed in different ways:

- Enter **masdisp** at the TopSpin prompt.
- Click **mas** in the TopSpin **Acquisition** tab.
- Click the **MAS spin rate** icon  on the TopSpin acquisition status bar at the bottom of the TopSpin window.

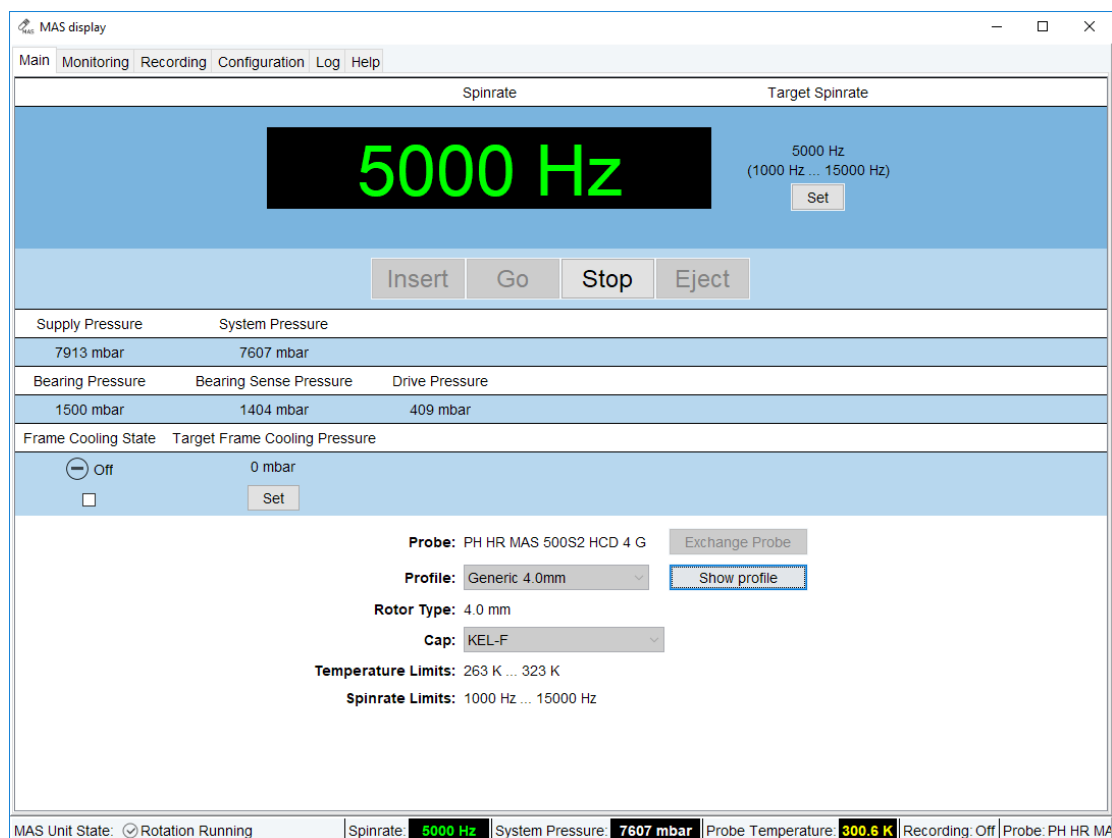


Figure 11.1: The Main Tab of the TopSpin MAS User Interface.

### 11.1.2 Masdisp Overview

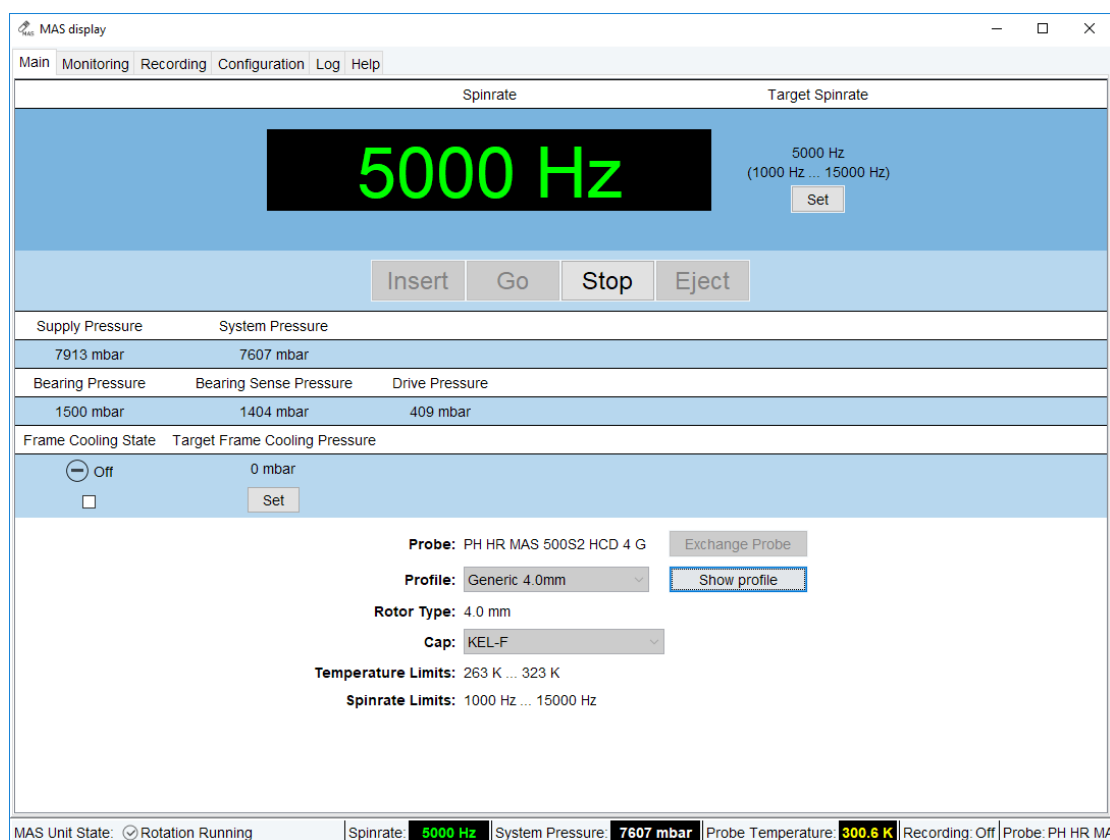
The user interface supplies the following tabs:

- **Main**: Main window for routine operation.
- **Monitoring**: Display of spin rate and pressure settings or readings.
- **Recording**: Writing and (graphical) inspection of record files.
- **Configuration**: Settings for displaying stability information and for window handling.

- **Log:** Display of MAS unit notifications and error messages.
- **Help:** Display of information about setting up and using the MAS unit.

A status line is located at the bottom of the window. It displays the current state (rotation on/off), the spinning stability, the current spinning speed, the system pressure, and the probe temperature as monitored and controlled by the variable temperature control unit.

## 11.1.3 The Main Tab of the TopSpin MAS User Interface



### 11.1.3.1 Overview

Most of the MAS operation is controlled from the **Main** menu. It shows the following information (see the figure above) from top to down:

- Current and desired spin rate.
- Buttons for insert, eject, spinning, and stopping the rotor.
- Supply pressure and internal operation pressure readings of the MAS unit.
- Actual pressure settings for bearing, sense of bearing, and drive.
- Frame cooling state and pressure setting.
- Settings for probe, profile, rotor type, cap material, temperature limits, and spin rate limits.

At startup the following settings are displayed: probe, profile (this defines the regulation parameters and others), rotor type, cap material, temperature limits, and lower and upper spinning frequency limits. Except for the cap material usually no user input is required

because the probe is set according to the *current probe* as defined by the **edprobe** command. The profile and rotor type are automatically chosen according to the probe. Temperature limits and frequency limits are defined by the cap material, the profile and the current probe, respectively and cannot be changed independently.

### 11.1.3.2 Probe and Profile Selection

---

For standard operation the user does not need to select the probe and corresponding profile. At startup the main tab will show the current probe as set by **edprobe**. A suitable profile (this defines the regulation parameters as well as maximum and minimum spinning frequencies) is automatically loaded. The user may change the probe by clicking on the **Exchange probe** button – the NMR super-user password is required for this. The probe cannot be changed while a rotor is spinning. The profile may be changed as well by choosing one of the available profiles from a drop-down list. Usually, the default profile will be the correct one, special profiles may be set for dedicated applications like slow spinning). Details of the current profile may be inspected by clicking the **Show profile** button.

### 11.1.3.3 Rotor and Cap Type Selection

---

The rotor is set according to the selected probe, this cannot be changed. The cap type may be selected from a drop-down menu, the default setting is *Kel-F* for 4 mm and 7 mm rotors and Vespel for smaller diameter ones. The cap material defines the allowed temperature range and maximum spinning speed. For further information please refer to the SB-MAS Operation Manual under **Help | Manuals | Acquisition – Application Manuals | SB-MAS**.

### 11.1.3.4 Temperature Limits and Spin Rate Limits

---

The displayed temperature limits are set according to the probe and cap material settings. The display is for information only, the limits cannot be changed on their own. The same holds true for the spin rate limits, which are set according to the probe, profile, and cap material. If, e. g., a lower temperature limit is required the rotor must be equipped with suitable cap. If, e. g., slower spinning is desired a suitable profile needs to be chosen.

### 11.1.3.5 Rotor Handling

---

#### 11.1.3.5.1 Insertion and Removal

---

Rotor insertion and removal are performed by clicking the **Insert** or **Eject** button, respectively. The unit will perform the necessary steps according to the probe type like applying insert and eject air, stator flipping for probes equipped with a flip type stator etc. The **Eject** button is enabled as long as no rotation is running even when no sample is in the system. Both the **Insert** and the **Eject** button are inactive during sample spinning.

#### 11.1.3.5.2 Spinning and Stopping

---

The target spin rate is shown on the top right side of the **Main** window together with the allowed spin rate range. The user may set the spin rate by clicking the **Set** button, this will open a small window in which the desired value may be typed. Changing the target frequency is always possible but not during the start and stop rotation phases. Entries outside of the allowed range cannot be set. Spinning is started or stopped by clicking the **Go** button or **Stop** button, respectively. The **Go** button is inactive before **Insert** is applied at least once. The **Stop** button is inactive if the rotor does not spin. The current spin rate is shown on the upper left side of the **Main** window, a color code is used to indicate regulation status:

- Green color indicates that the rotor is spinning at the desired spinning speed with a defined tolerance (this is set in the **Configuration** tab, see [The Configuration Tab of the TopSpin MAS User Interface \[▶ 214\]](#)).
- Red color indicates deviations from the desired spin rate.

Such deviations occur during normal operation when the rotor is spun up or down, or the spinning speed is changed. They may as well indicate a problem like instable spinning due to an imbalanced rotor or strong fluctuations of the supply pressure. In case the spinning stability is lost a corresponding message will be displayed just below the display of the current spin rate. The user may delete this message by clicking the **Reset** button on its right side, see the next figure. The color code may be changed by the user in the **Configuration** tab of the TopSpin user interface.

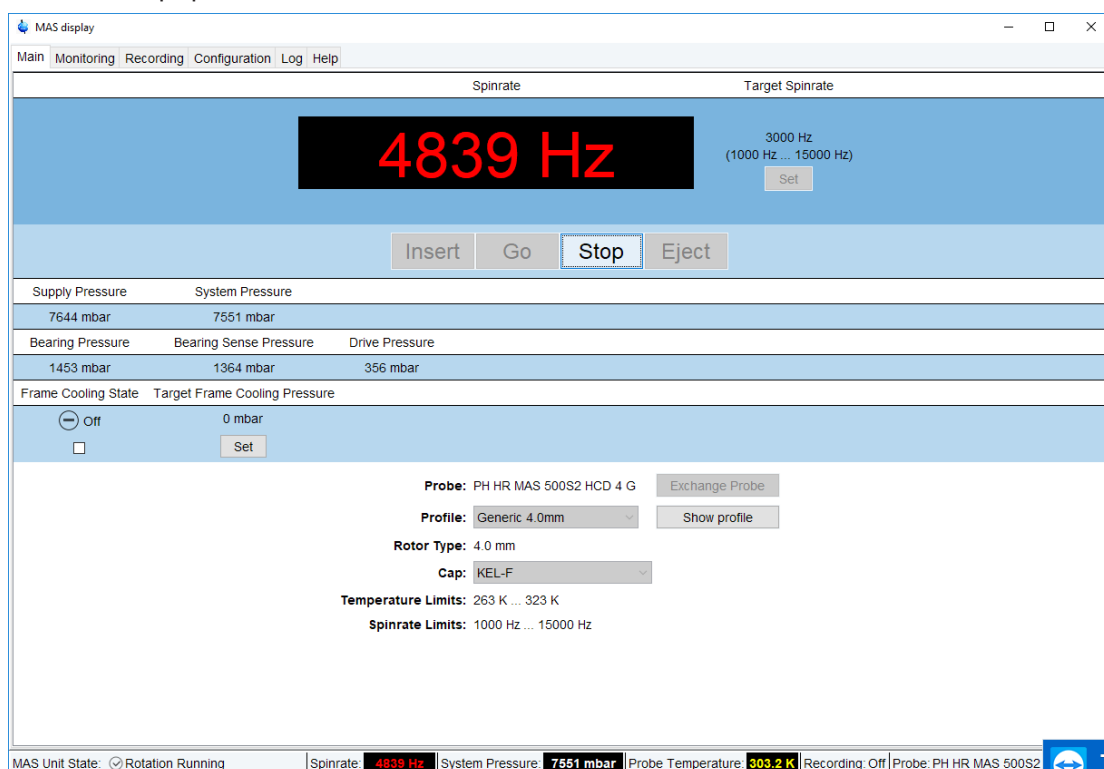


Figure 11.2: The **Main** Tab of the TopSpin MAS User Interface in Case of Instable Spinning.



Please note that on Avance spectrometers up to the III HD architecture, a MAS II Unit may be installed. On these units, insertion and ejection of the sample may be performed through their built-in digital panel. Avance Neo spectrometers are always delivered with MAS III units that are handled only through the TopSpin MAS user interface or its webpage.

## 11.1.3.6 Pressure Display

### 11.1.3.6.1 Supply Pressure and System Pressure

The supply pressure is the pressure of the gas supply for the MAS unit. This pressure is reduced to the system pressure in the unit which in turn is used to set bearing, drive, etc. The internal pressure has to be adjusted on the pressure regulator near the gas tank.

### 11.1.3.6.2 Bearing Pressure, Bearing Sense Pressure, and Drive Pressure

The bearing and drive pressures are set by the MAS unit according to the probe, profile, rotor and cap material, and desired spinning speed. Both pressures are set by the MAS unit and displayed in the main window. The display is for information only, the values cannot be changed. The bearing pressure is used to put the rotor in levitation to cancel any mechanical resistance (friction force etc.). The drive pressure is set to the value needed to obtain sufficient tangential airflow that arrives on the fins of the rotor cap to reach the desired spinning speed. The bearing sense pressure is measured at the probe directly for safety purposes: The MAS unit supervises the bearing sense pressure constantly and stops the spinning if its value drops below a certain cutoff limit. This is intended to prevent a rotor damage caused by a loss of bearing pressure between MAS unit and probe. Such a loss may, e. g., occur if the MAS hoses or joints are not tight or damaged.

### 11.1.3.7 Frame Cooling

The frame cooling is a stream of ambient temperature gas which is applied to the probe's frame. This is intended as a cooling of the electric parts in high RF and high duty cycle experiments. It is as well used to keep the probe's electric parts at ambient temperature in high or low temperature experiments. Frame cooling is switched on by ticking the corresponding check box. The target frame cooling pressure may be set by clicking the **Set** button and typing in the desired value.

The frame cooling may be used for other purposes, e. g. for transfer line cooling.



Please note that at high spinning speed (typically close to the maximum rotor dependent spinning speed), the rotor may heat up. In such cases cooling is required to keep the sample at a suitable temperature.

## 11.1.4 The Monitoring Tab of the TopSpin MAS User Interface



### 11.1.4.1 Purpose

---

This tab is provided for information purposes. It supplies a graphical display of the spin rate and pressure settings or readings as a function of time, see the figure above.

### 11.1.4.2 Configuration

---

The user may define the displayed parameters by ticking the corresponding checkboxes in the **Configure** section of the tab. The parameter list may be shown or hidden by clicking the **Down arrow** / **Up arrow** button, respectively, on top of window (left to **Configure**). The following settings can be made.

- General: Update interval in seconds.
- Parameters.
- Spin rate: Target and actual spin rate.
- Pressures: Supply pressure and system pressure.
- Bearing/Drive pressure

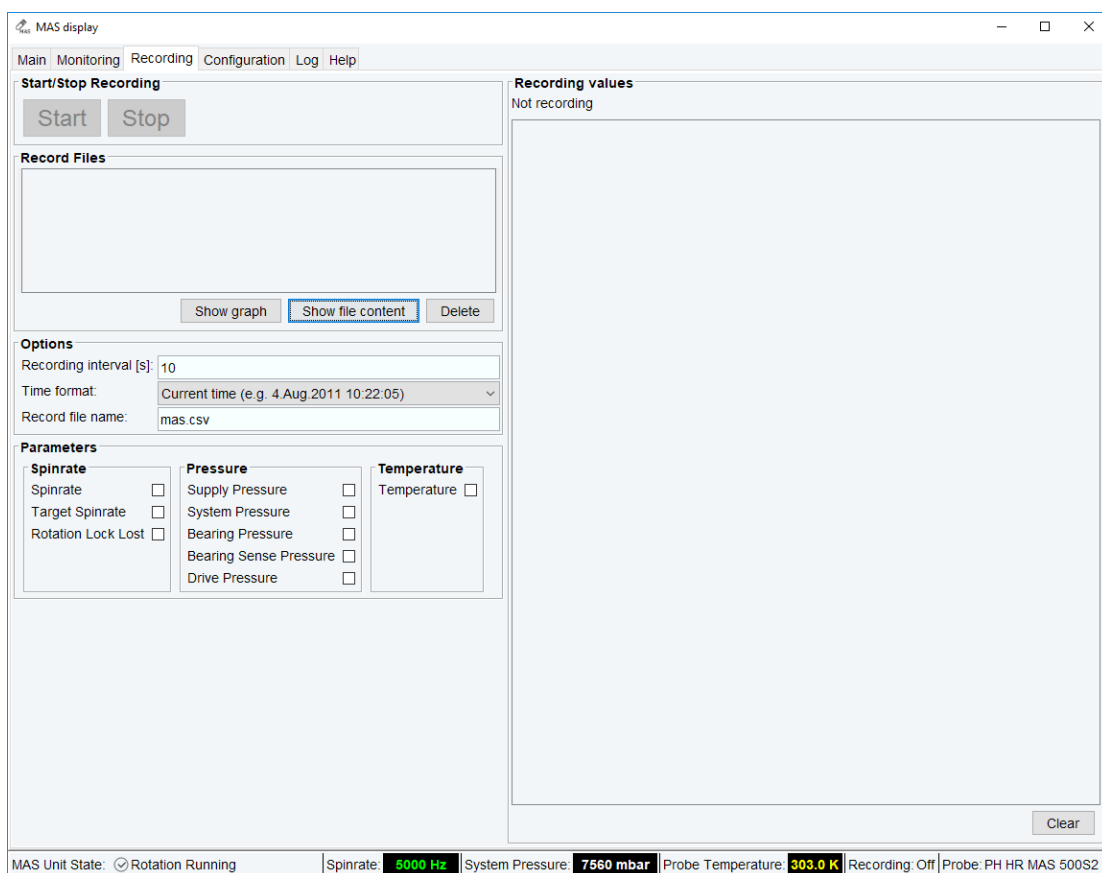
If the **Auto scale** check box is marked the vertical and horizontal axes will constantly be rescaled to fit to the actual spin rate and pressure settings or readings. The **Overview** mode is similar to the TopSpin overview mode for spectra display, if the corresponding box is checked the full curve will always be shown on top of the actual display.

### 11.1.4.3 Graphical Display

---

For each of the parameter groups described above a separate graph will be shown (if no parameter of the corresponding group is selected, no graph will be shown). Each display has got icons similar to the TopSpin icons for expanding/compressing the horizontal or vertical scales. If the **Overview** mode is set (see above) the full curve will always be shown on top of the current display.

### 11.1.5 The Recording Tab of the TopSpin MAS User Interface



#### 11.1.5.1 Purpose

The user may write and inspect record files in which spin rate and pressures settings and readings of the MAS unit are stored at defined time steps (see the figure above).

#### 11.1.5.2 Defining the Recorded Parameters

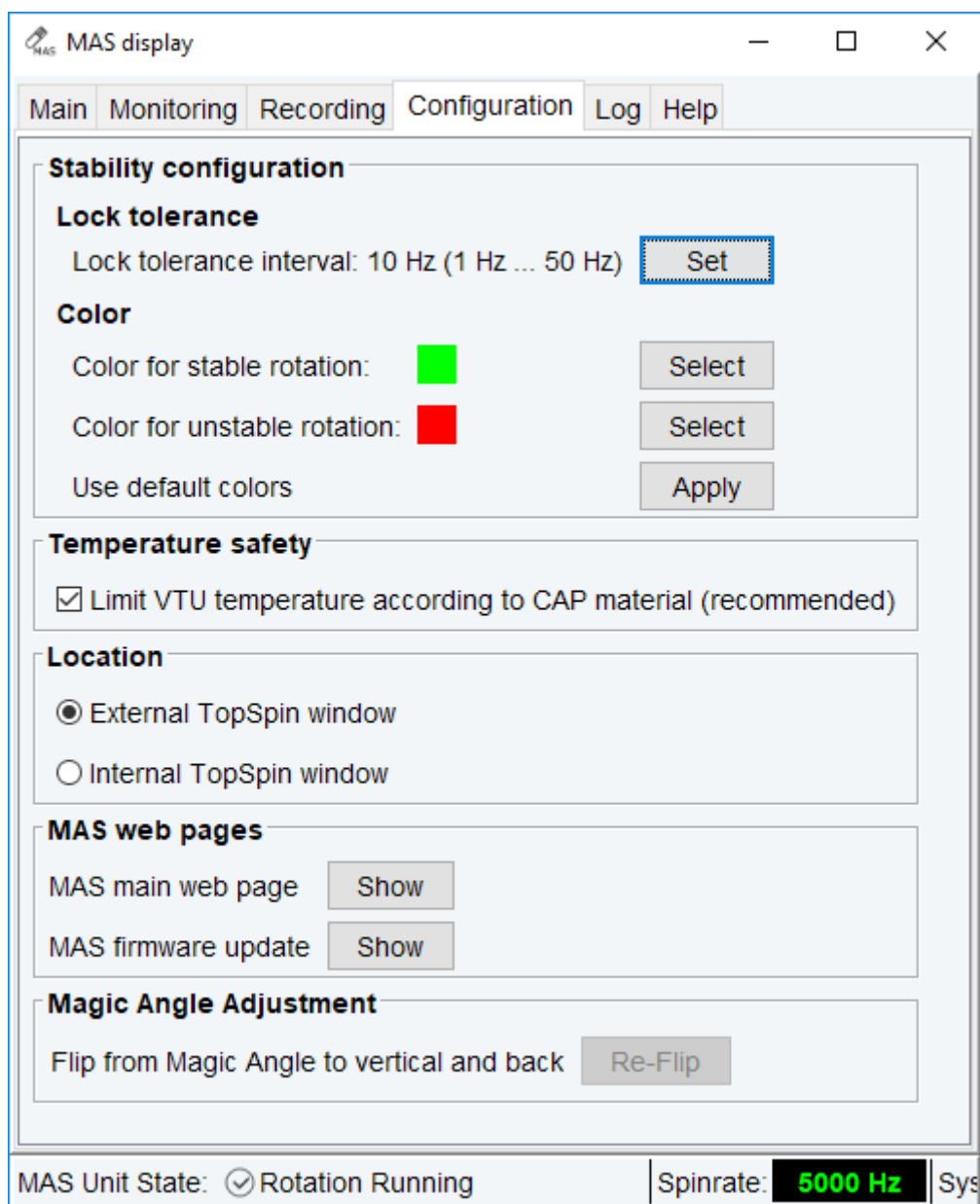
The left side of the **Recording** tab is for user input and for the start of stop of the recording. The following sections are given:

- **Start/Stop Recording:** The user may start or stop the recording by clicking the appropriate button.
- **Record files:** This shows a list of previously written record files. The file content may be displayed graphically (button **Show graph**) or edited (button **Show file content**). The user may delete files by clicking the **Delete** button. The user will be prompted to confirm the deletion.
- **Options.** Here the recording interval and the time format are set and the user may define a suitable record file name. Record files are stored in the XXX directory.

#### 11.1.5.3 Monitoring of the Recorded Parameters

On the right side of the **Recording** window the last recorded lines written to file are displayed. The user may inspect these lines e. g. to check the proper choice of parameters and time interval. The display may be cleared by clicking the **Clear** button.

## 11.1.6 The Configuration Tab of the TopSpin MAS User Interface



### 11.1.6.1 Purpose

This tab allows some settings for the graphical appearance of the TopSpin MAS interface. It is not intended to configure the MAS unit. For the latter purpose, however, a link to the MAS unit's web page is supplied.

### 11.1.6.2 Settings

The following sections are available:

**Stability Configuration:**

- Lock tolerance: the *spinning speed lock tolerance interval* defines the maximum deviation of the actual spin rate from the target spin rate which is regarded as acceptable for stable spinning. The default value is  $\pm 5$  Hz, the user may change this to smaller or larger figures. It cannot be changed while a rotation is starting or stopping.



The spinning speed lock tolerance limit is only a monitoring parameter, it has no impact on the spinning regulation. It is used for the spinning speed color code, the stability indicator in the TopSpin MAS interface status bar, and the *Rotation Lock Lost* entry of the record files.

**Color**

- Color for stable rotation: This is the color for the spin rate display for stable spinning, the default color is green, the user may choose a different color by clicking the **Select** button.
- Color for unstable rotation: This is the color for the spin rate display if spinning is unstable, the default color is red, the user may choose a different color by clicking the **Select** button. Red color appears also during the rotation starting and stopping phase.
- Use default colors: This button may be clicked to undo any user choices and return to the default color scheme.

**Location**

- External TopSpin window: The MAS user interface will show up in a separate window which may be handled independently of the main TopSpin window.
- Internal TopSpin window: The MAS interface will be incorporated into the main TopSpin window.

**MAS web pages**

- MAS main web page: Clicking the **Show** button will open a web browser and display the main MAS unit web page.
- MAS firmware update: Clicking the **Show** button will open a web browser and display the MAS unit web page for firmware update.

**Magic Angle Adjustment**

Please note that for MAS probes, the Magic Angle ( $54.7^\circ$  with respect to the vertical B0 main magnetic field) must be adjusted accurately with a KBR rotor. For detailed information please refer to the Solids User Manual (Help | Manuals | Acquisition – Application Manuals | Solids).

**11.1.7 The Log Tab of the TopSpin User Interface****11.1.7.1 Purpose**

This tab allows to inspect, print, or clear notifications, error messages and information supplied by the MAS unit.

**11.1.7.2 Categories**

The following categories are displayed:

- MAS Unit Notifications.
- Current error messages.
- Error message history: The **Reload** button updates the display to include the most recent entries.
- Info messages.

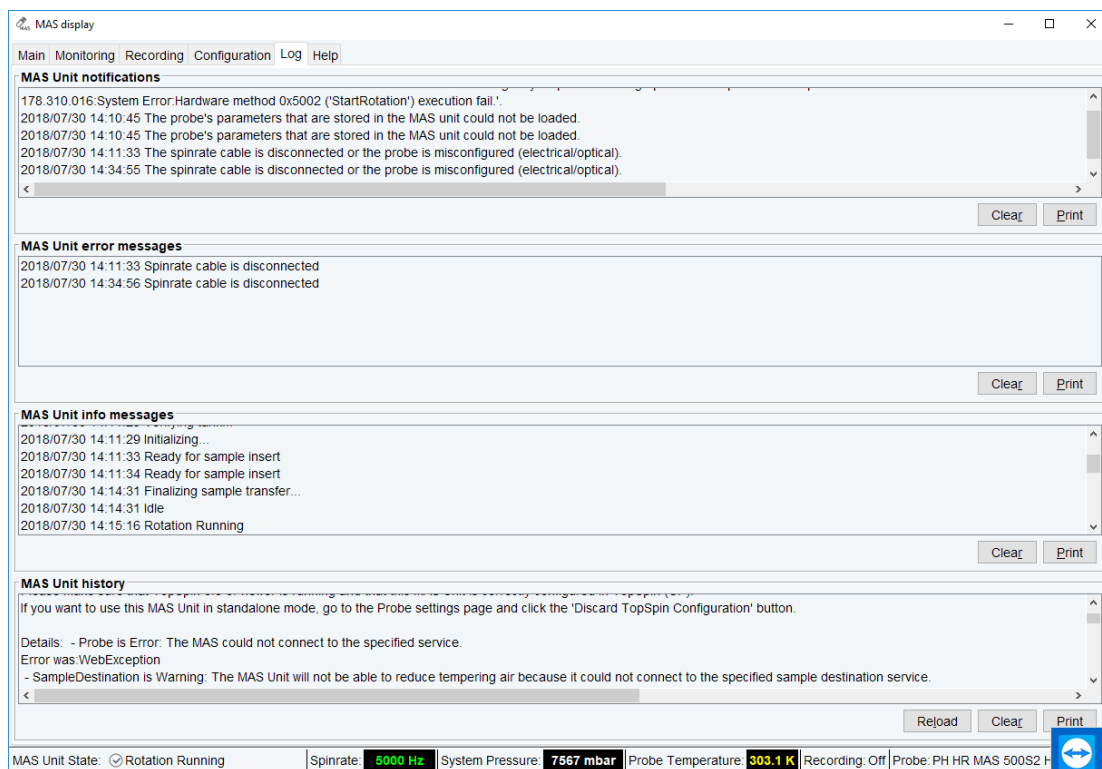


Figure 11.3: The Log Tab

To print a message category:

- Click the **Print** button.

To empty a message category:

- Click the **Clear** button.

## 11.1.8 The Help Tab of the TopSpin User Interface

This tab provides access to the MAS unit manual.

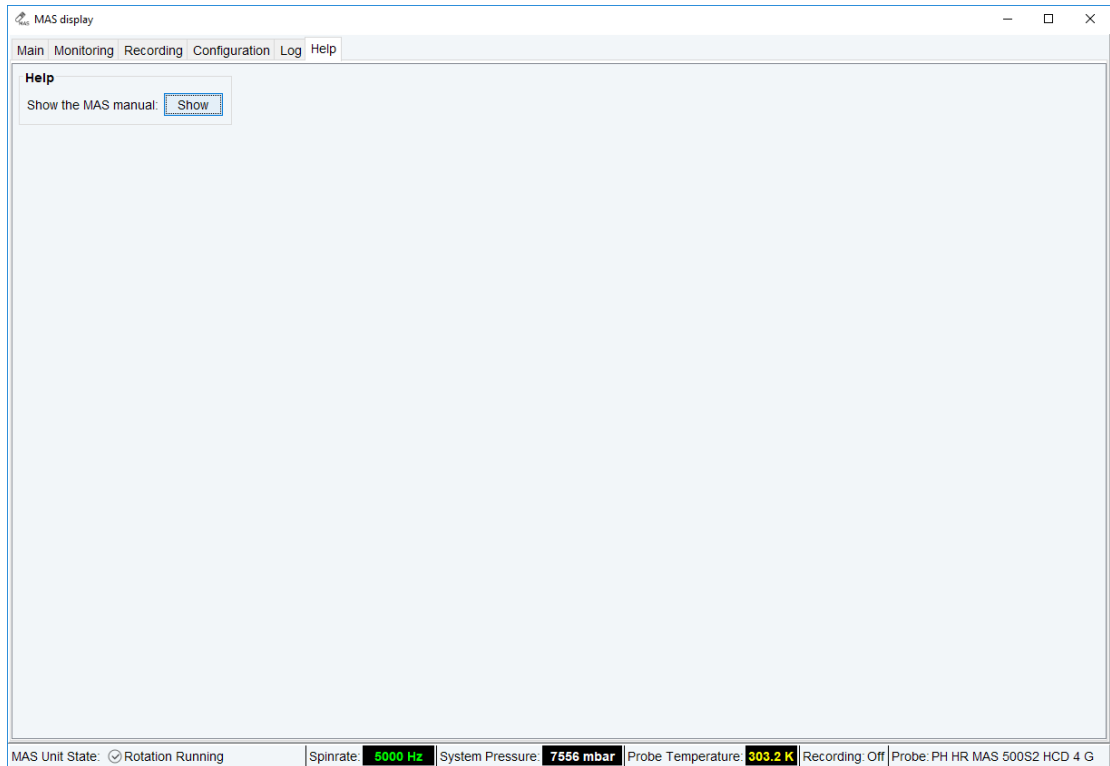


Figure 11.4: The **Help** Tab



## 12 Miscellaneous

This chapter describes TopSpin commands that are somehow acquisition related and have not been described in previous chapters.

### 12.1 **account**

---

#### NAME

**account** - Show acquisition accounting statistics

#### DESCRIPTION

The command **account** prints statistics derived from the experiments performed during a desired time.

Statistics are only available if accounting is switched on. You can do this as follows:

- Click **Options** => **Preferences** [set].
- Click **Acquisition** in the left part of the dialog box.
- Check the item **Enable data-acquisition protocol**.
- Click **OK**.

#### INPUT FOLDERS

<tshome>/prog/curdir/acqhistory - acquisition accounting files

#### SEE ALSO

(set, hist)

### 12.2 **crpon, crpoff, crplock, crpobs**

---

#### NAME

**crpon** - Switch the cryo preamplifier on for the lock and observe channel.

**crpoff** - Switch the cryo preamplifier off for the lock and observe channel.

**crpobs** - Switch the cryo preamplifier on for the observe channel.

**crplock** - Switch the cryo preamplifier on for the lock channel.

#### DESCRIPTION

The **crp\*** commands listed above control the internal preamplifier of a cryoprobe. Cryo probes operate at a reduced coil and preamplifier temperature which improves the signal to noise with a factor of 4. They are available as Dual ( $^{13}\text{C}$  observe), Triple resonance (TCI  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ) and also on Quadruple Resonance (QCI) probes.

The command **crpon** switches from the external (HPPR) preamplifier to the internal cryo preamplifier. This happens for both the observe and the lock channel.

The command **crpoff** switches from the internal cryo preamplifier to the external (HPPR) preamplifier. This happens for both the observe and the lock channel.

The command **crplock** switches from the external (HPPR) preamplifier to the internal cryo preamplifier. This happens for the lock channel only.

The command **crpobs** switches from the external (HPPR) preamplifier to the internal cryo preamplifier. This happens for the observe channel only.



---

**Please note that the internal cryo amplifier is also cooled down, like the coil and internal electronics of the Cryo Probe.**

---

### SEE ALSO

[edprobe](#) [► 144]

## 12.3 delpar, delgp, delsh

---

### NAME

**delpar** - Delete parameter sets.

**delgp** - Delete **gradient programs**.

**delsh** - Delete shim files.

### SYNTAX

delpar [<name>]

delgp and delsh have the same syntax as delpar

### DESCRIPTION

The **del\*** commands without argument open a dialog box with a list of the available entries. They are equivalent to the respective edit commands **rpar**, **edgp** and **rsh**. From the dialog box, you can select entries and click **Delete** to delete them. Alternatively, you can use the **del\*** command with one argument, for example:

**delpar myparset**

Deletes the parameter set **myparset**.



---

Note that only user defined entries can be removed.

---

### INPUT FOLDERS

- <tshome>/exp/stan/nmr/par - Bruker and user defined parameter sets.
- <tshome>/exp/stan/nmr/lists/gp - Bruker and user defined gradient programs.
- <tshome>/exp/stan/nmr/lists/bsms - shim files.

### USAGE IN AU PROGRAMS

- DELPAR(name).
- No AU macros are available for the other **del\*** commands.

### SEE ALSO

[edlist](#), [dellist](#) [► 170], (delau, delpul, delcpd, delpy, delmac)

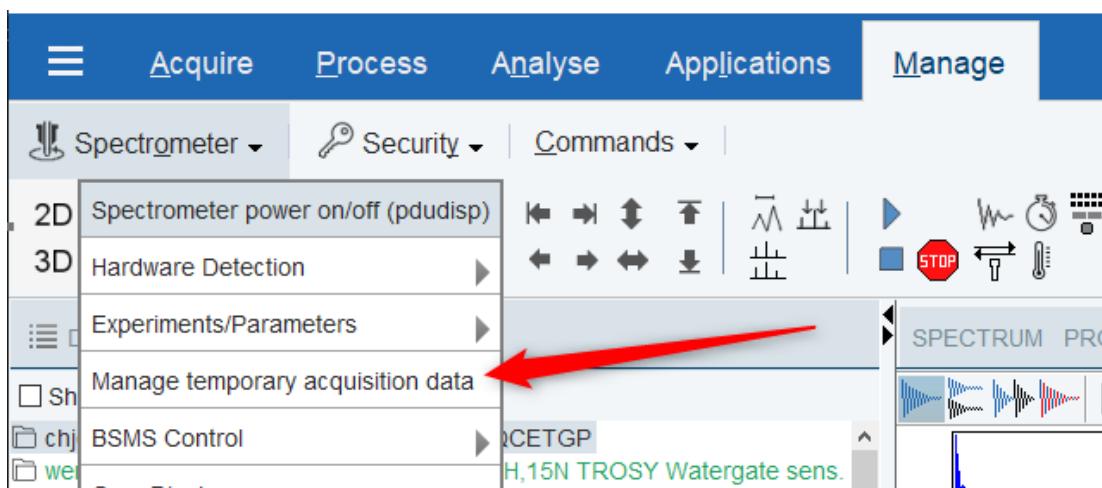
## 12.4 deletetmpfiles

### NAME

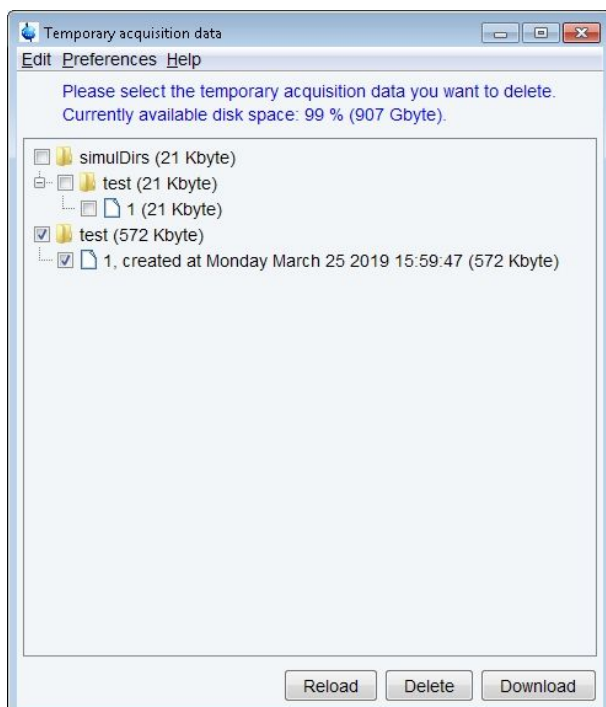
**deletetmpfiles** - Delete temporary acquisition data files

### DESCRIPTION

On a spectrometer, by default, all data stored temporarily on the EPU during an acquisition are deleted after completion of the experiment. This automatic deletion routine can be modified by clicking **Manage | Spectrometer | Manage temporary acquisition data** (or entering the command **deletetmpfiles**).

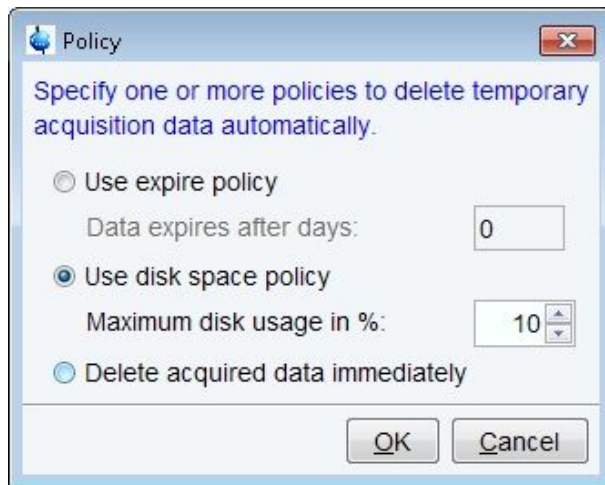


The file tree in the main window displays only the data of those experiment numbers which were created by the same user which currently uses TopSpin:



Any temporary acquisition data of other users are not shown, i.e. also cannot be modified by the current user.

The dialog appearing via the menu **Preferences | Edit temporary acquisition data preferences** was slightly reorganized:



It is not possible anymore to define an expire policy and a disk space policy at the same time, the user has to choose between those options.

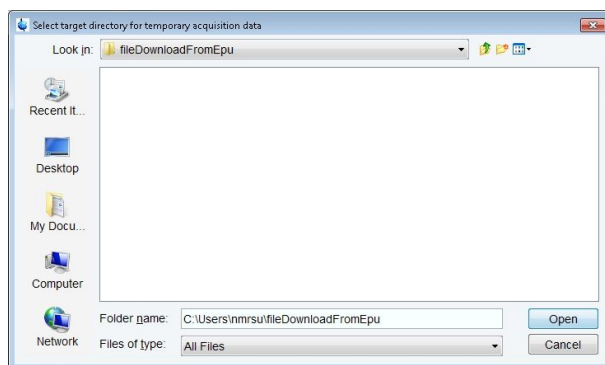
The default setting is **Delete acquired data immediately**.

The functionalities of the **Reload**- and the **Delete**-Button in the main window basically remain unchanged except for the user restrictions for the data displayed, as mentioned above.

Furthermore the main window of the **Temporary acquisition data** - dialogue shows a **Download**-Button.

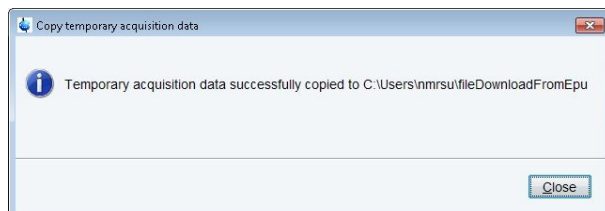
Via this button, the user can copy the experiment directories which were selected in the file tree from the EPU into an arbitrary directory on the workstation.

Clicking **Download** opens a common file dialogue (shown below for a Windows - workstation) where the user can choose or create a target directory on the workstation:



Clicking **Cancel** aborts the copy process.

Clicking **Open** starts the copy process and yields a message in case of success:



**Notice:** Data copied from EPU to workstation are still present on the EPU afterwards. They have to be explicitly deleted by either clicking the **Delete** - button or by changing the deletion policy.

## 12.5 exprof

### NAME

**exprof** - Display excitation profile of selective experiment.

### DESCRIPTION

The command **exprof** displays the excitation profile of a selective experiment. The experiment must have been completely setup for acquisition, before **exprof** is executed.

The command **exprof** opens the dialog shown in the next figure.

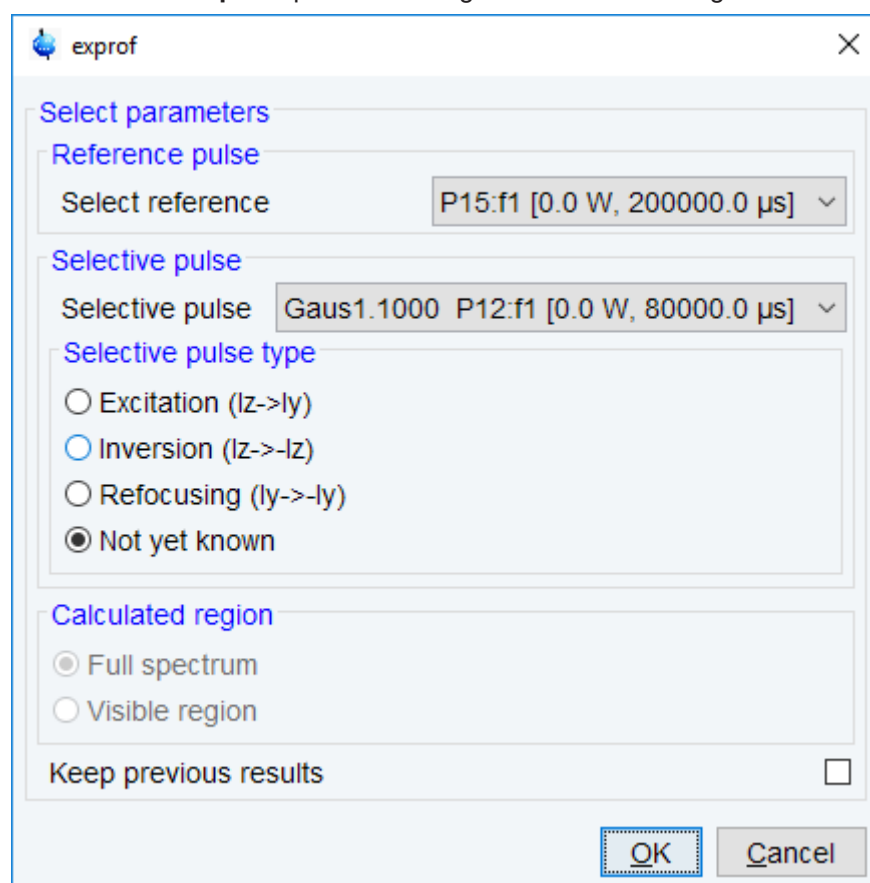


Figure 12.1: exprof

The dialog offers the following options:

- **Reference Pulse**

The 90° hard pulse in the same channel as the selective pulse.

- **Selective Pulse**

The selective pulse to be examined. If your pulse program contains only one selective pulse, and it follows the Bruker style guide (P1=90°, etc.) **exprof** automatically selects the correct reference pulse.

- **Selective Pulse Type**

The rotation type is a selective pulse which allows the excitation of a reduced defined frequency range of the spectrum. Automatically set to the value stored in the shape file. If the shape file does not contain a rotation type, it is set to „not yet known“ and must be selected in the dialog. Shapes created with TopSpin 1.3 or older, or with external programs do not contain the rotation type.

- **Calculated Region** (greyed if no spectrum exists)

The profile can be calculated for the entire spectrum or for the currently displayed region. It always consist of 1000 points.

- **Keep Previous Results**

If enabled, the result of previous **exprof** command(s) is kept, allowing simultaneous display of multiple profiles.

If your pulse program contains only one selective pulse and the waveform contains rotation type, you don't have to set anything in the **exprof** dialog. Just click **OK**, to confirm the dialog.

The command **exprof** requires that the *NMRSim* program, delivered on the TopSpin DVD, is installed.

For further Information please see the Shape Tool manual and the Pulse Programming Manual under **Help | Manuals**.

### OUTPUT PARAMETERS

- PULPROG - pulse program used for the acquisition
- SHAPE - array of shaped pulse parameters

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/
  - *acqu* - acquisition parameters
- <tshome>/exp/stan/nmr/lists/wave/\*
  - Shape files

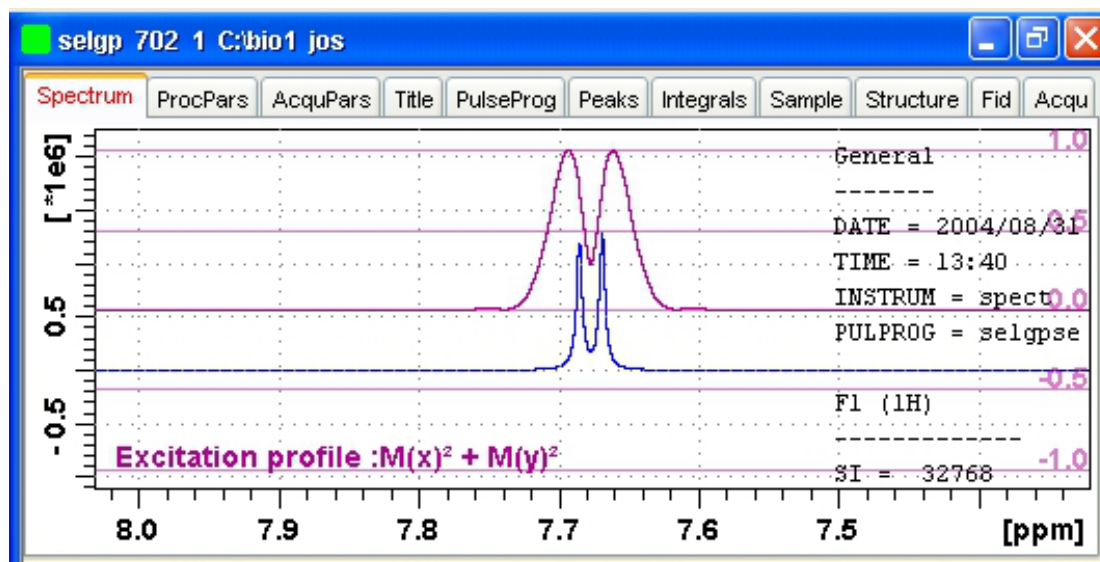


Figure 12.2: selgp

### SEE ALSO

(nmrsim)

## 12.6 getlim1d, getlcosy, getlxhco, getljres, getlinv

### NAME

**getlim1d** - Calc. 1D spectral width according to integral ranges.

**getlcosy** - Calc. 2D cosy spectral width from 1D int. ranges.

**getlxhco** - Calc. 2D xhco spectral width from 1D int. ranges.

**getljres** - Calc. 2D jres spectral width from 1D int. ranges.

**getlinv** - Calc. 2D inverse spectral width from 1D int. ranges.

### DESCRIPTION

The **getl\*** commands listed above calculate and set the optimum spectral width for the specified experiment types. The optimum spectral width is determined from one or two associated 1D datasets, which are defined as the so called second and third dataset. Before the actual experiment is performed, the second (and if necessary the third) dataset must be acquired, Fourier transformed and baseline corrected. The latter processing step implicitly determines the integral ranges. The **getl\*** commands determine the spectral width such that it includes all integral ranges, in other words, all signals.

**getl\*** commands are typically used in automation. They are called from AU programs like **au\_getl1d**, **au\_getlcosy**, **au\_getlinv** and **au\_getlxhco**. These, in turn, are called by IconNMR where the preparation and the actual experiment are defined as a so-called composite 2D experiment (see IconNMR Online help for more information).

**getlim1d** determines the optimum spectral width on a 1D preparation experiment and then sets the parameter SW on the current 1D dataset accordingly.

**getlcosy** determines the optimum spectral width on one 1D preparation experiment. Then it sets the F2-SW and F1-SW on the current 2D COSY dataset accordingly.

**getlxhco** determines the optimum spectral width for F2 and F1 on two different 1D preparation experiments (typically 1H and X). Then it sets the F2-SW and F1-SW on the current 2D XH correlation dataset accordingly.

**getljres** determines the optimum spectral width on one 1D preparation experiment. Then it sets F2-SW on the current 2D J-resolved dataset in accordingly.

**getlinv** determines the spectral width on one 1D preparation experiment. Then it sets F2-SW on the current 2D INVERSE dataset accordingly.



Note that F2-SW refers to the acquisition parameter SW in the F2 direction and F1-SW refers to the same parameter in the F1 direction.

The first 1D preparation experiment is defined as the so called second dataset. The second 1D preparation experiment is defined as the so called third dataset.

### OUTPUT PARAMETERS

- SW - spectral width in ppm

### INPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>
  - *intrng* - integral regions
  - *curdat2* - definition of second and third dataset

### OUTPUT FILES

- <dir>/data/<user>/nmr/<name>/<expno>/

- *acqu* - acquisition parameters
- *acqu2* - F1 acquisition parameters of a 2D dataset

### USAGE IN AU PROGRAMS

- GETLIM  
executes the command **getlim1d**
- GETLCOSY
- GETLXHCO
- GETLJRES
- GETLINV

## 12.7 **hpdisp**

---

### NAME

**hpdisp** - Pulse program display showing signals going to spectrometer hardware, inclusive exact timing, phase and amplitude.

### DESCRIPTION

The command **hpdisp** opens a new window with a display of all hardware events on selected channels.

**hpdisp** presents the results of the pulse program simulation using the same software which sends the commands to hardware in a real experiment.



Please note that displaying each event going to the spectrometer hardware may lead to a very large number of displayed entries, even for simple pulse programs (see the next figure).

---

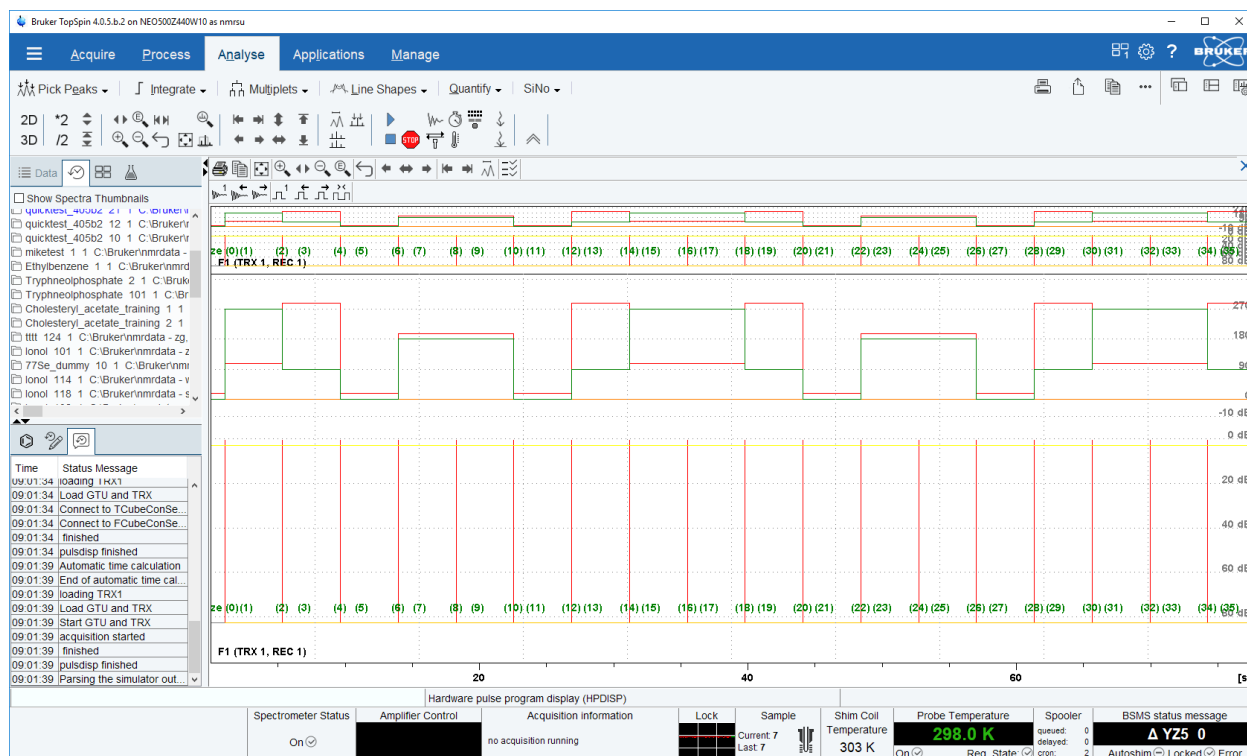


Figure 12.3: hpdisp

E.g. simple 1D experiment using adiabatic pulses for decoupling may generate millions of spectrometer events.

## SEE ALSO

[spdisp](#) [ 227]

## 12.8 spdisp

### NAME

**spdisp** - Symbolic (graphical) pulse program display.

### DESCRIPTION

The command **spdisp** opens a new window with a symbolic pulse program display.

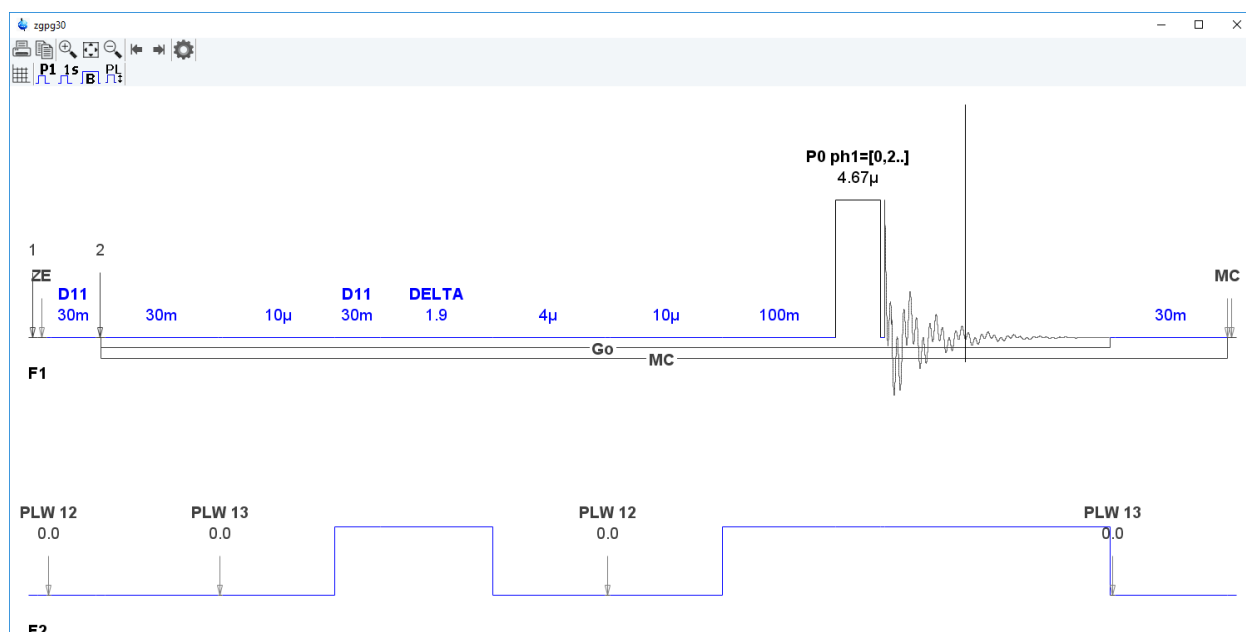


Figure 12.4: *spdisp*

It takes one argument and can be used as follows:

- **spdisp**  
Displays the pulse program defined by the acquisition parameter PULPROG.
- **spdisp <name>**  
Displays the pulse program <name>.

**spdisp** starts the pulse program display part of *NmrSim*. The functionality of this program is described in the *NMRSim* manual. This can be opened by clicking **Help | Manuals | Analysis and Simulation | NMRSim Experiment Simulation**.

**spdisp** can only start if the following conditions are met:

- The Bruker AU programs have been installed (with **expinstall**).
- The *NMRSim* program is installed (from the TopSpin DVD).

## SEE ALSO

(nmrsim)

## 12.9 stdisp

### NAME

**stdisp** - *ShapeTool* for handling RF shapes and gradients.

### DESCRIPTION

The command **stdisp** opens the *ShapeTool* window where you can create, manipulate and analyse RF shapes and gradients (see the next figure).

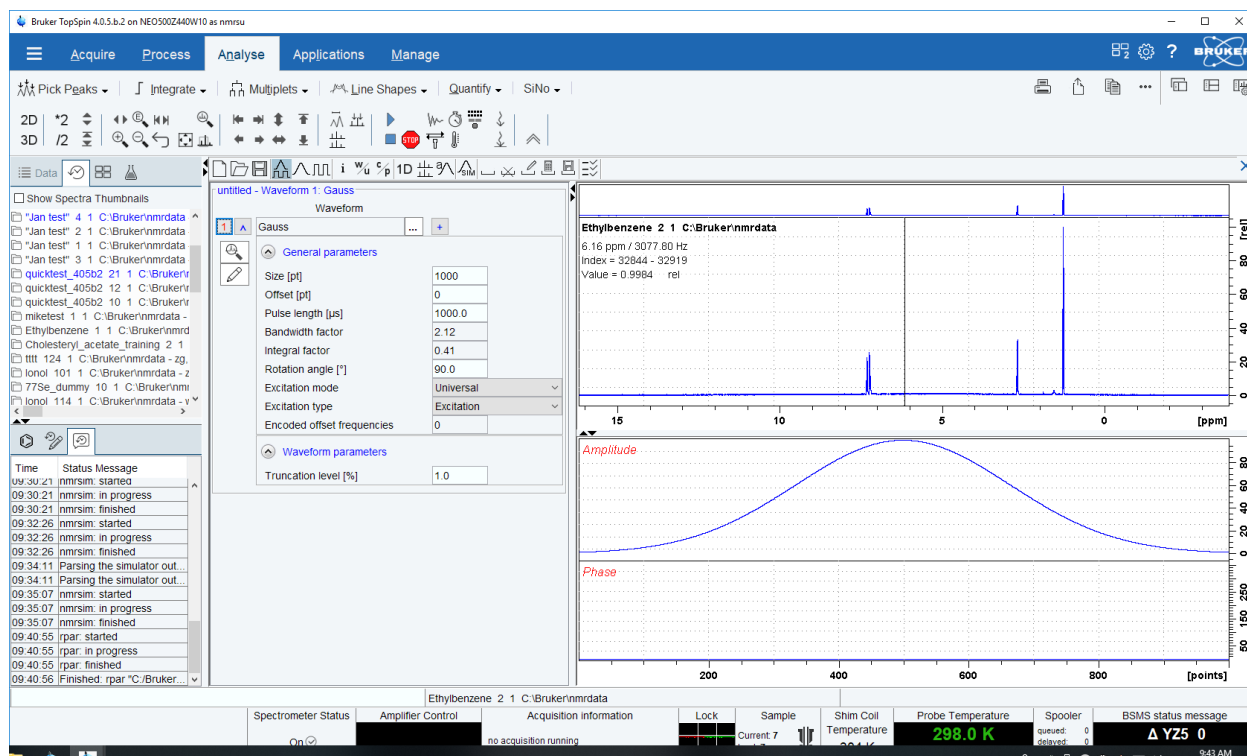


Figure 12.5: stdisp

The functions of the buttons are available as tooltips. A detailed description of **stdisp** can be found under **Help | Manuals | Acquisition Application Manuals | Shapetool**.

## SEE ALSO

[st](#) [ 229]

## 12.10 st

### NAME

**st** - Generate, manipulate and analyze RF shapes and gradients

### DESCRIPTION

The command **st** allows you to generate, manipulate and analyze RF shapes and gradients. It is described in a separate manual which can be opened as follows:

click **Help | Manuals | Acquisition - Application Manuals | ShapeTool**

## SEE ALSO

[stdisp](#) [ 228]

## 12.11 wvm

### NAME

**wvm** – WaveMaker (Software solution for pulse shaping)

### DESCRIPTION

WaveMaker is a software solution for pulse shaping that is based on wave form definitions within the pulse programs. This avoids any need to modify the PROSOL tables when new or non-standard shaped pulses and decoupling or mixing wave forms are required. It also adds flexibility to and improves portability of many standard and user developed experiments and pulse programs. Porting the WaveMaker based pulse programs to NMR systems of different field strength is straightforward and typically requires no further adjustments and PROSOL updates.

For detailed information please have a look at the WaveMaker – Pulse Shaping Software (User Manual). This can be opened by clicking **Help | Manuals | Acquisition - Application Manuals | WaveMaker**.

# 13 Contact

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