

Diffusion

NMR User Manual

Version 2.0

BRUKER

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Introduction

1

This manual is planned for use by the engineer in the installation of the diffusion accessory, and for the user in performing existing experiments and for the setup of new experiments.

Due to the similarity of the imaging and diffusion hard and software, this manual overlaps the AVANCE imaging manual in parts. Therefore the reference to “imaging” will often appear, but can be used interchangeably with “diffusion”.

This manual is only a guide and may not include all the information you would like. If you have any suggestions, please send them to:

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Installation

2

Installation of the Diffusion Software

2.1

The diffusion software package described in this manual, can be used with XWIN-NMR 2.6 on. The package is not available on the XWIN-NMR 2.6 CD-ROM, to install it please refer to **"Installation of the Diffusion Package" on page 45**. From XWIN-NMR 3.0 on the diffusion package will be part of the xwin-nmr CD-ROM and can be installed according to the procedure described below.

The command **expinstall** is used to install the pulse and automation programs for diffusion experiments. The diffusion package is part of the micro imaging package.

Type:**expinstall**

Enter:Password for nmroot

Select:Installation for Micro Imaging Systems

The pulse and au programs are then copied to the appropriate directories and the au programs for imaging are compiled.

The software preparation is now complete, you may now start with the experiments if your imaging hardware is installed and tested. For the installation of software updates, please refer to **"Installation of the Diffusion Package" on page 45**.

Installation of the Diffusion Hardware

2.2

Different hardware configurations for the imaging and diffusion accessories are available. Therefore check your hardware configuration and install the accessory as described in the **"Appendix: Imaging and Diffusion Hardware" on page 71**.

Once you are satisfied with the hardware configuration return and perform the steps in the following section on tests and adjustments.

Installation of a Diffusion Probe

2.3

Install your probe following the procedures described in **"Appendix: Probeheads and Gradients" on page 59**.

Define your Probe in the Probehead File

2.3.1

/XWINNMRHOME/exp/stan/nmr/lists/probeheads

XWINNMR versions before xwinmr3.0:

Type **edhead** in XWINNMR, this editor allows you to define or modify your probe-head list. It is a good practice to remove probes not available on the system from the lists. The file may appear afterward as follows:

5 mm 1H	[01]
diff30	[02]

Here the diffusion probe was called "diff30" to identify a probe of type diff30. There are no restrictions on the choice of the name, it is only important point to specify a different number (CURPROBE) for each probe.

XWINNMR3.0:

Type **edhead** XWINNMR.

Select **New Probe** in the **Probe** pull down menu.

Select **MIC** as **Probe Type** for diffusion or micro imaging probe.

Fill in the **Part Number** and the **Serial Number**, these are mandatory. The other parameters should be filled as far as they are known.

The number appearing in the last column is the identification for your probe.

Define your Diffusion Probe as the Actual One

2.3.2

Type **edhead** in XWINNMR to select your probe. This must be done before adjusting the preemphasis and calibrating the gradient strength. This step is also required each time you switch back from another probe to get access to the proper gradient calibration. See also **"Requirements for Running "diff" on page 46.**

Match the Gradient Amplifier and the Gradient System

2.3.3

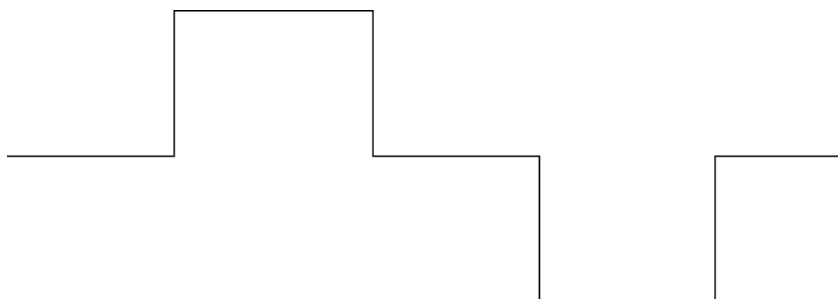
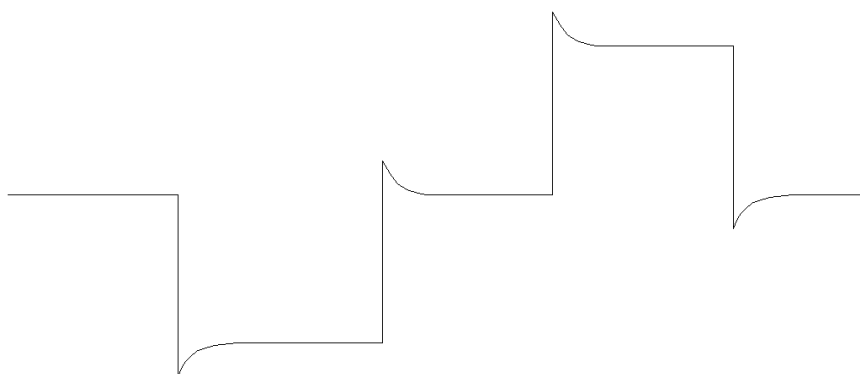
Adjust the loop parameters for your gradient system at the gradient amplifier. For the standard B-AFPA 40 amplifier this is described in **"Installation of the Gradient Amplifiers B-AFPA-40" on page 78.** Usually the values shown in **"B-AFPA-40 Dip Switch Setting" on page 78** are sufficient.

Preemphasis Adjustment

2.3.4

The shape of an FID or an echo, acquired with only a short delay after gradient pulses, may be distorted by eddy currents caused by gradient switching. The influence of the eddy currents can be decreased by modifying the shape of the gradient pulses. Three exponential functions, with different amplitude and different time constants, are available to accomplish this.

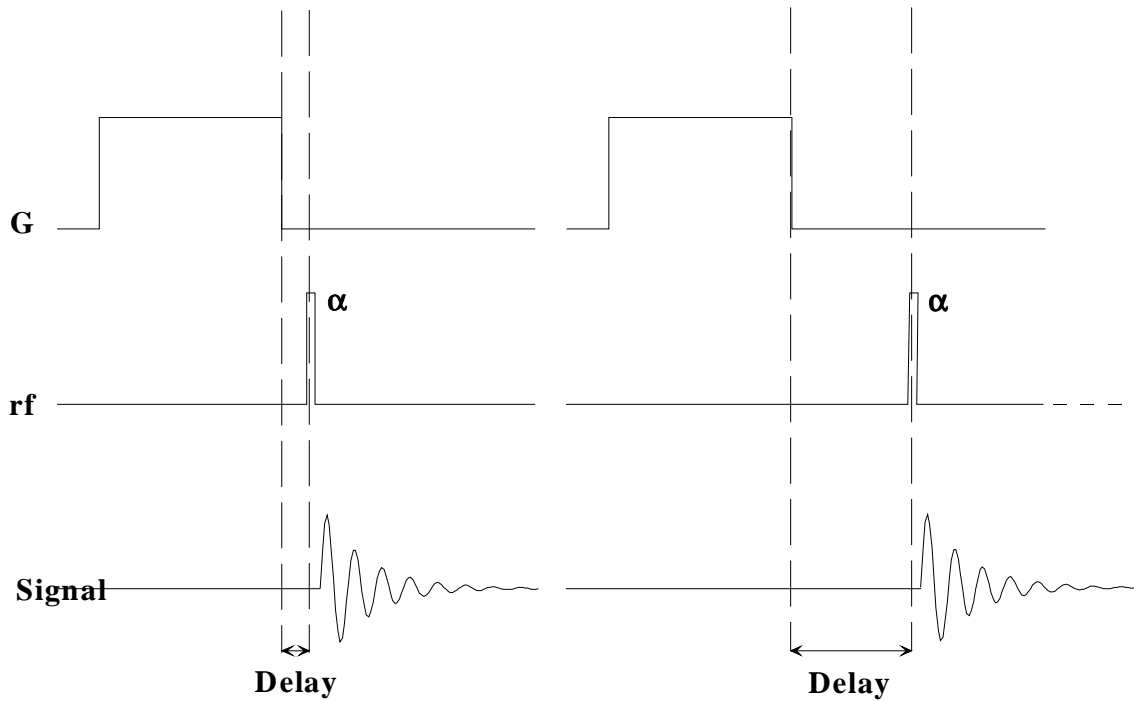
The figure below shows an example of two gradient pulses, one positive the other negative. In order to get this desired gradient behavior in the presence of eddy currents, the current pulse shapes have to be modified as indicated in the section **"Gradient Pulses with Preemphasis (overemphasized)" on page 9.** Usually the required values are much smaller than the one shown there.

Figure 2.1. *Desired Gradient Pulse Shape*Figure 2.2. *Gradient Pulses with Preemphasis (overemphasized)*

The amplitudes and time constants are set in a control window and are stored for individual gradient systems. This is described in the following section.

The preemphasis parameters are *adjusted* by observing fids at varying times after a gradient pulse. Typical time variations after gradient switching, are in the range between 100 μ s and 1 sec, depending on the type of gradient system.

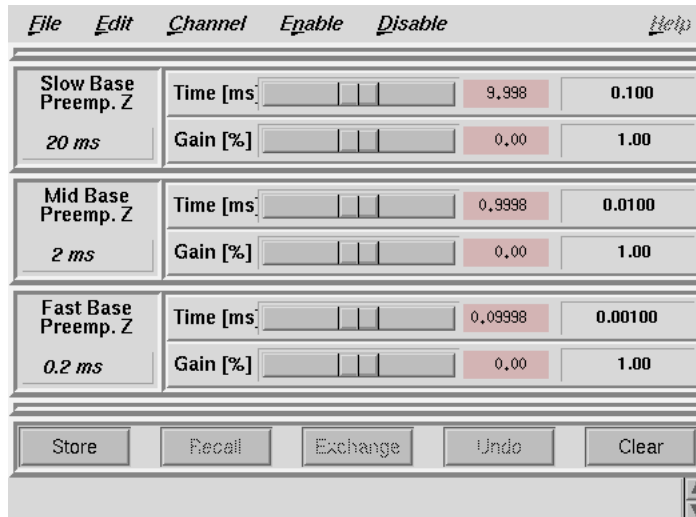
Figure 2.3. Preemphasis Adjustment Program



Menu for the Preemphasis Parameters

The parameters for preemphasis adjustment are shown in the following menu. The menu is activated by the command **setpre**.

Figure 2.4. Preemphasis Control.



Three time bases out of a choice of four can be specified for the time constants of the exponential functions. The precise values of the time constants and the amplitudes are adjusted under slider control in the Time and Gain bars. Values can also

be typed in directly after selecting the corresponding field with the mouse. Each value change will be directly loaded in the preemphasis unit.

When **setpre** is first started it reads the parameters out of the preemphasis unit, e. g. the BGU2, and displays the parameters for Z-gradient channel. The channel can be changed using the channel pull-down menu.

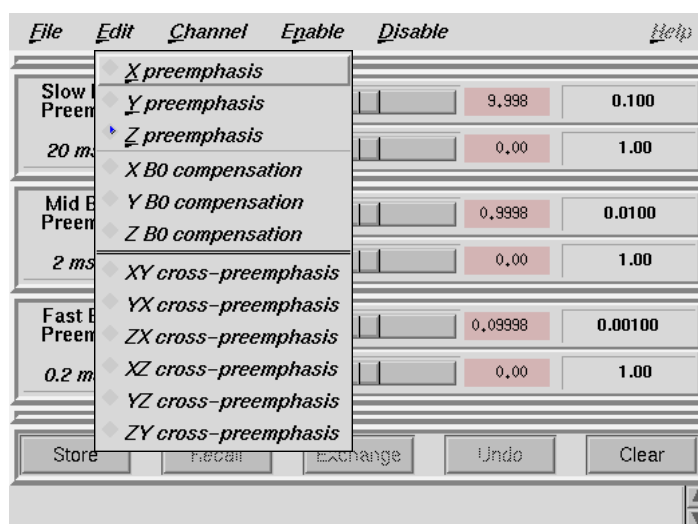
When you do the preemphasis adjustment for the first time, start by loading one of the default files:

/XWINNMRHOME/exp/stan/nmr/parx/preemp/diff25

or:

/XWINNMRHOME/exp/stan/nmr/parx/preemp/diff30.

Figure 2.5. Channel Pulldown Menu



As shown in the picture above, this menu also allows you to select the corresponding B0 compensation channels. Selecting this option is only useful, if the corresponding hardware is available. See **"B0 Shift Compensation" on page 16** for details. Cross-preemphasis is usually not needed in the diffusion and micro imaging environment.

After all of the parameters have been adjusted, they should be saved for use with the gradient system. This can be done just by selecting "Write default", which will create the file:

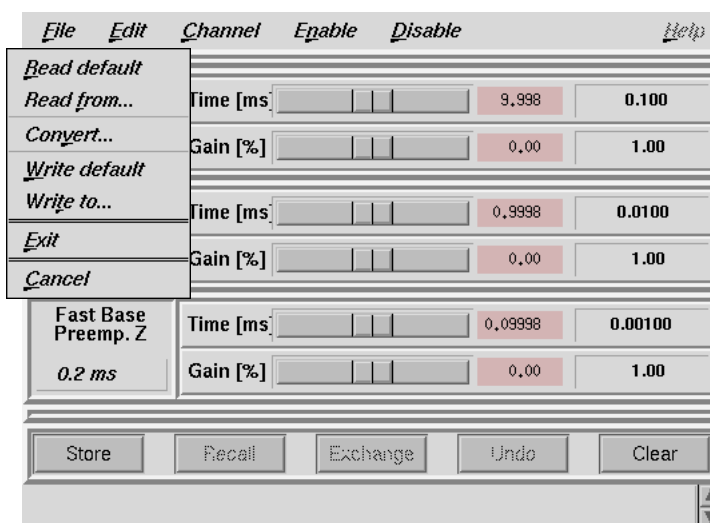
/XWINNMRHOME/exp/stan/nmr/parx/preemphasis/CURPROBE/default

Where CURPROBE is the current probehead which was previously defined by **edhead**. The command "Read default" reads in the same file and loads the parameters automatically to the preemphasis unit.

If preemphasis files created by older versions of **setpre** are to be used, they can be read in using the "Convert" command, which searches for files in the directory:

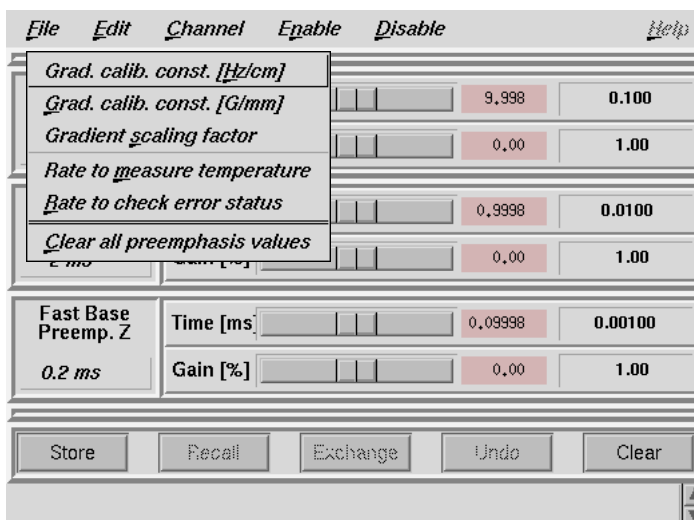
/XWINNMRHOME/exp/stan/nmr/lists/preemp/

Figure 2.6. Preemphasis File Handling.



The “Edit” pulldown menu shown in **“Setpre Edit Menu” on page 12** allows you to set the gradient calibration constant, either in units of Gauss/mm or of Hz/cm. These numbers are assumed for 100% current. The relative calibration can be set here, for 3-axis gradient systems.

Figure 2.7. Setpre Edit Menu



Preemphasis Adjustment

- Insert a water sample into the probehead and shim.
- Set the parameters O1, TD, SWH, RG for a nice looking fid.
- Create a new directory with the **edc** command.
- Open the preemphasis menu using the **setpre** command.

- Run the automation program **diffpreemp** to set the preemphasis pulse program parameters. Use a gradient pulse length of 5 ms, whereas a result of 8 fids will be acquired and displayed sequentially. The gradient pulse amplitude must be initially set to zero. The default delays after the gradient pulses for the 8 fids are shown in the table below.

- Type "**gs**" to start the acquisition and adjust the rf excitation pulse low enough to avoid saturation effects on the 8 fids. All 8 fids must be identical as shown in "**Eight fids Without Gradient Switching**" on page 14. The O1 frequency should be: off resonance.

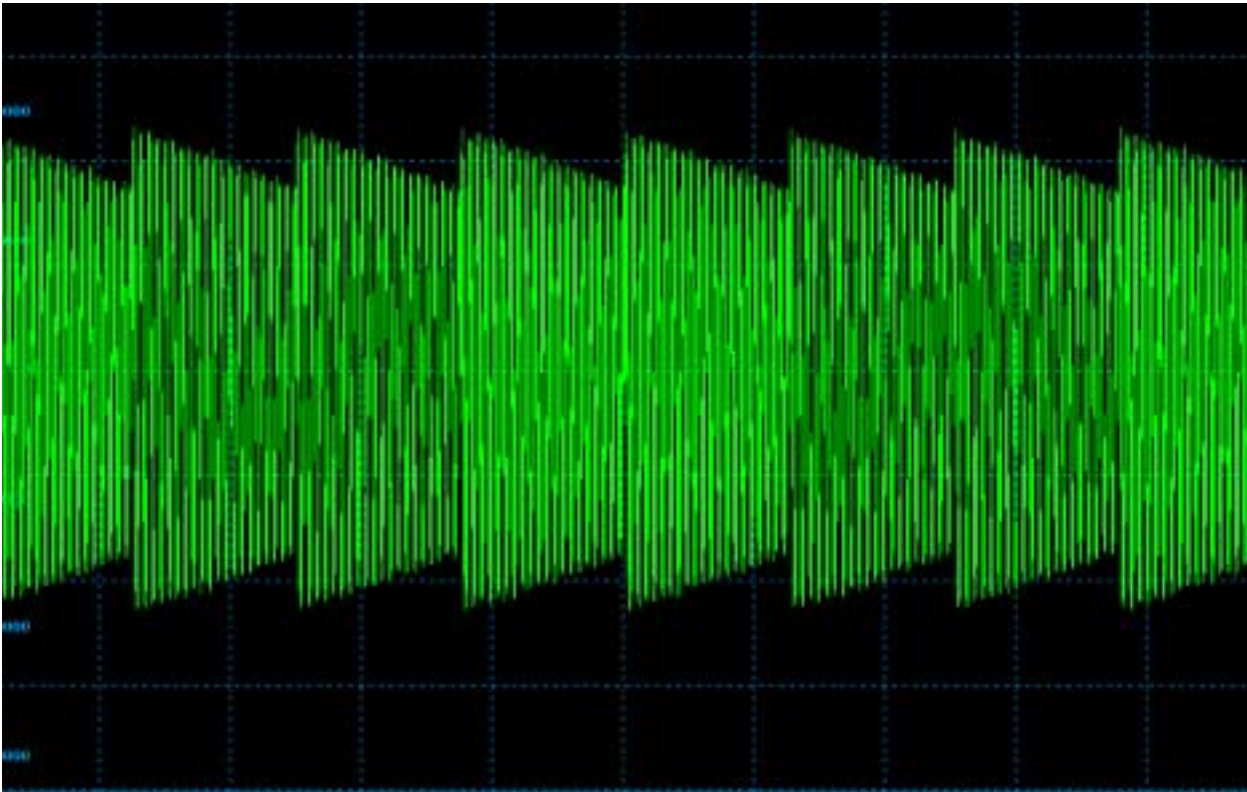
Depending on the type of the gradient system and the amplifier used, the fids may be very unstable. In this case use the blanking option in **diffpreemp**. This will cause the blanking being switched on after the delay. This has the side effect, that the preemphasis is cut off at the time the blanking is activated. On most gradient systems, where the preemphasis values are close to zero, this should not matter. Sometimes it is preferable to do a rough adjustment first without blanking and then switch on the blanking.

⇒ **Note: Residual preemphasis currents may switch the blanking unit to protection (Green LED off). Reset the unit manually, switch off the blanking in diffpreemp, or increase the first delay of the delay list until the blanking unit can handle it.**

Table 2.1. Default Delays Produced by *impreemp*

Delay After Gradient Pulse
200 μ s
400 μ s
900 μ s
2 ms
4 ms
9 ms
20 ms
200 ms

Figure 2.8. *Eight fids Without Gradient Switching*

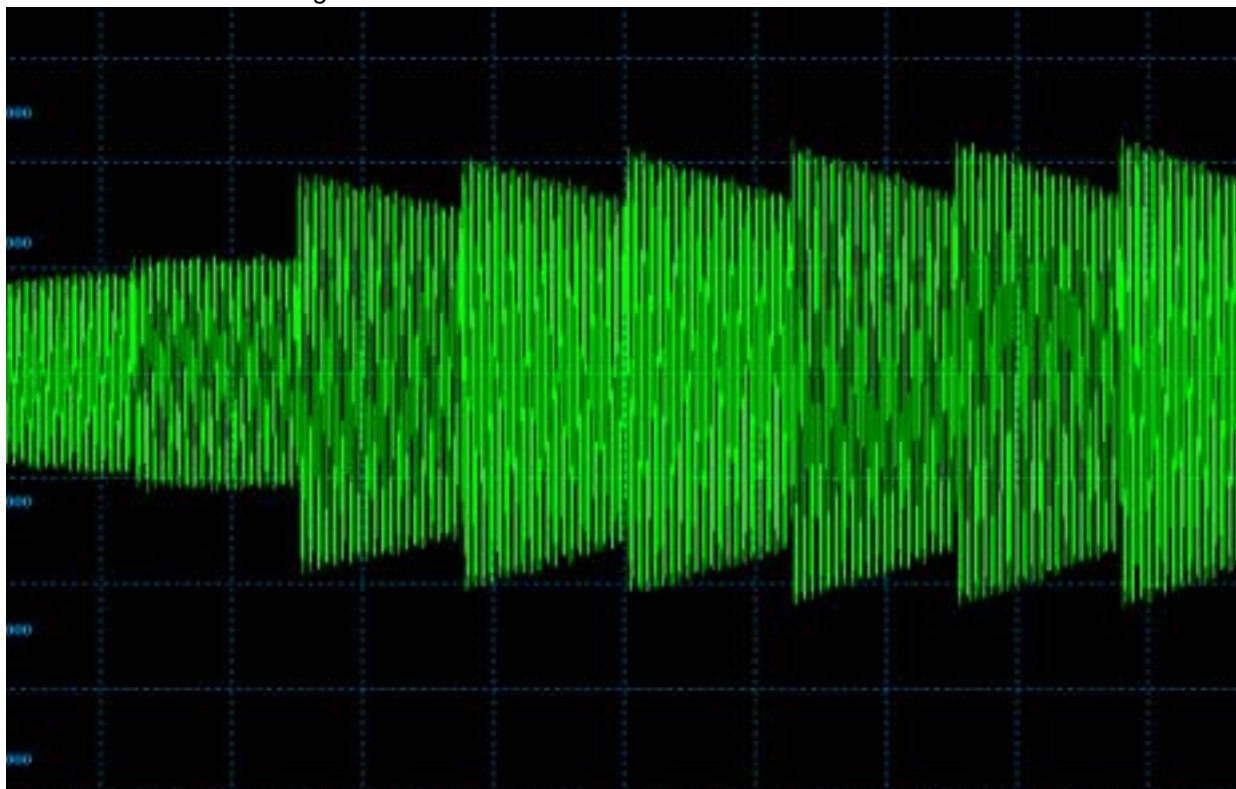


- Stop the acquisition and run “**diffpreemp**” once again. Start with 20% for the gradient amplitude and later increase the amplitude.

The screen should now look like ***"Fids After Gradient Pulses."*** on page 15.

➡ **Note:** *If you don't see any effect of the gradients and while using the blanking option, residual preemphasis currents may have switched the blanking unit to protection (Green LED off). Reset the unit manually, switch off the blanking in diffpreemp, or increase the first delay of the delay list until the blanking unit can handle it.*

Figure 2.9. Fids After Gradient Pulses.

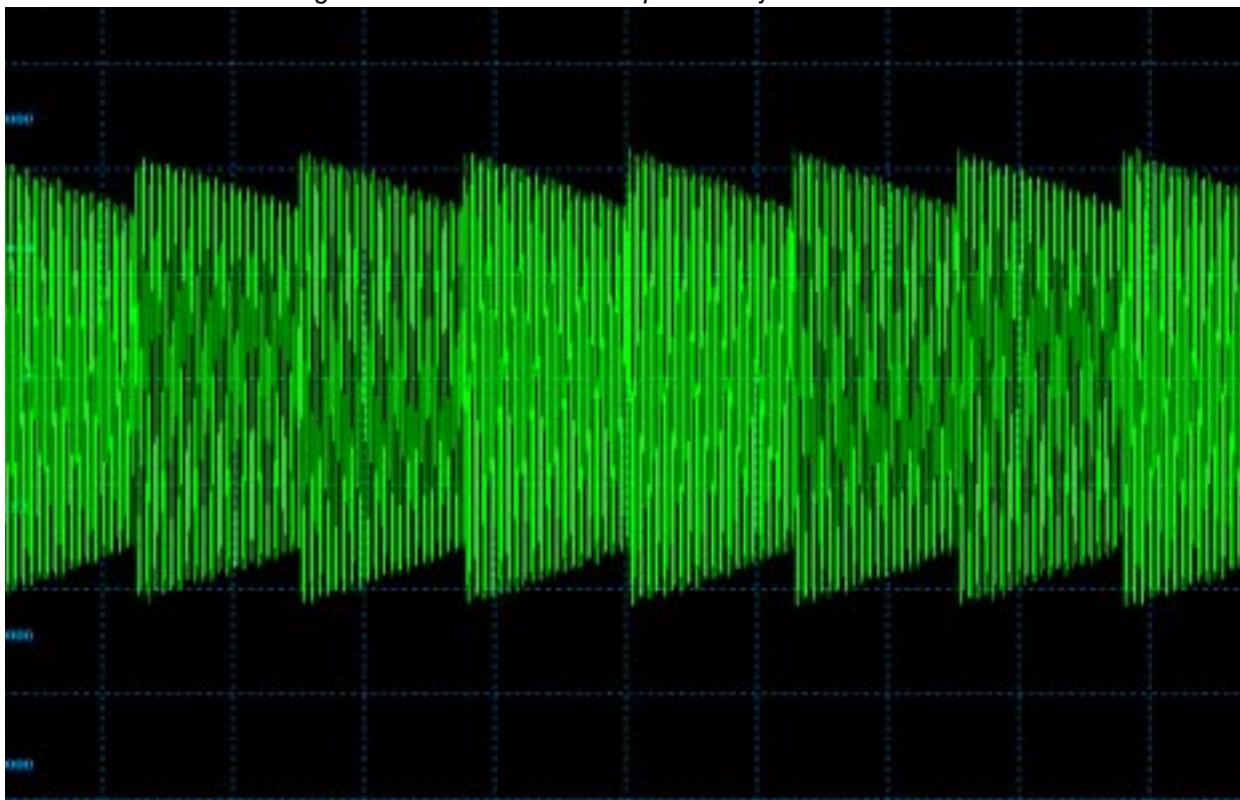


- Modify the gradient pulse shape by changing the time and gain parameters in the setpre menu until all fids are identical. The fid on the right side is used as a reference, since the delay between gradient switching and start of data acquisition is the longest for this fid. It is assumed that all eddy currents are gone with the last fid.

During the adjustment it is recommended that you start with the long time constants and continue with the middle and short time constants afterwards. This procedure corrects the shape of the fids from right to the left.

After the correction, the fids should look like those in **"Fids After Preemphasis Adjustment."** on page 16 below.

Figure 2.10. Fids After Preemphasis Adjustment.



- Save the adjustment parameters using the command in the “**File**” pull down menu.
- Stop the acquisition, run **diffpreemp** once again in order to increase the gradient amplitude or to repeat the procedure for the Y and Z gradients.

B0 Shift Compensation

2.3.5

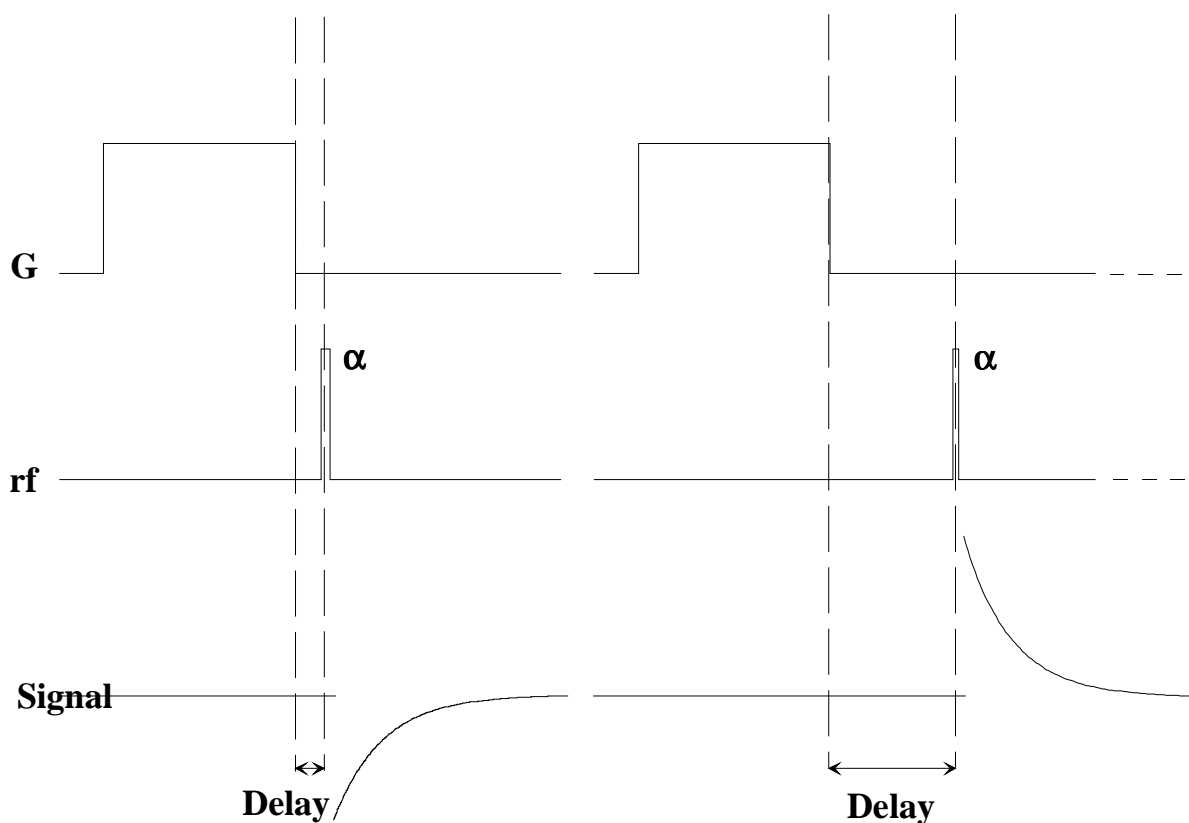
The shape of an FID or an echo, acquired with only a short delay after gradient pulses, may be distorted by shifts of the B₀ field caused by gradient switching. Such field shifts can be lessened by applying compensation pulses to the sweep coil of the magnet. In order to do this, three exponential functions with amplitude and time constants are available.

The amplitudes and time constants are set in a control window and are stored for individual gradient systems. This procedure is as follows:

The B₀ shift compensation is adjusted by observing fids *on resonance* at different times after a gradient pulse. Typical time values after gradient switching are in the range between 100 μs and 1 sec, depending on the type of gradient system. The pulse program is the same as in the case of the preemphasis adjustment.

⇒ **Note:** *The preemphasis adjustment must always be completed before the B₀ shift adjustment (Refer to the section "Preemphasis Adjustment" on page 8).*

Figure 2.11. B0 Shift Adjustment Program



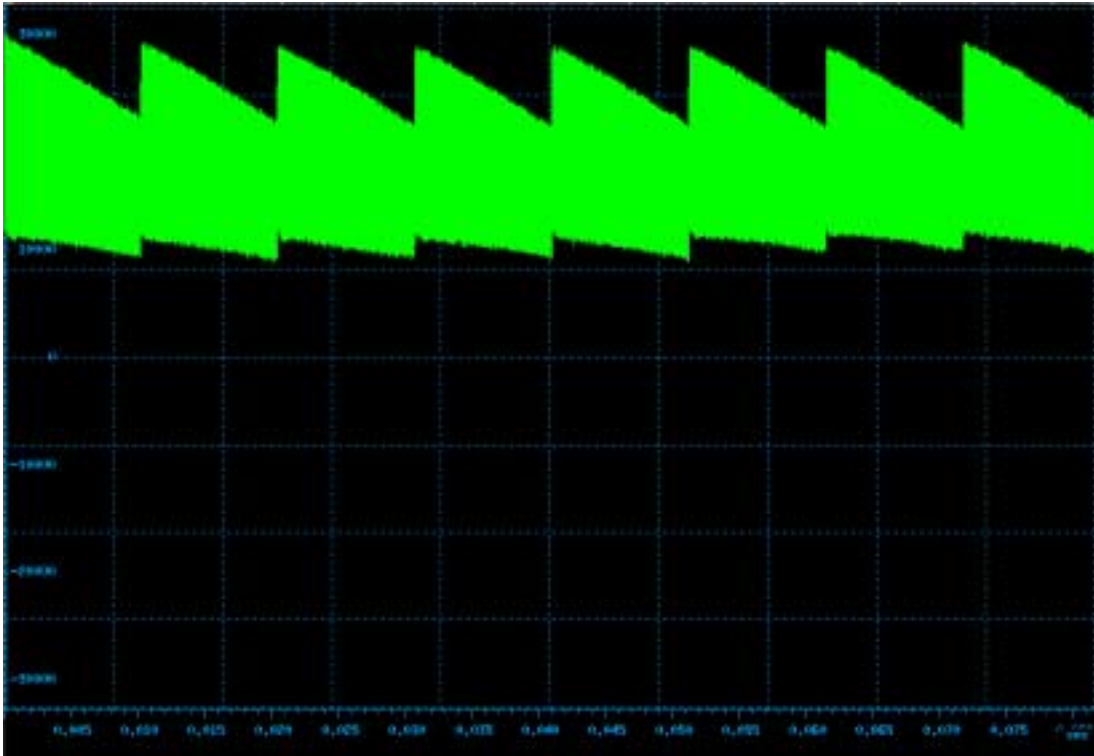
⇒ **Note:** The hardware for the B0 shift compensation consists of an additional amplifier and a switching box. They must be installed as described in the appendix "Installation of the B0 Shift Compensation Unit" on page 84.

B0 Shift Adjustment

- Select the same data set which was used for the preemphasis adjustment.
- Open the preemphasis menu using the **"setpre"** command.
- Run the automation program **"diffpreemp"** to set the pulse program parameters, which will result in eight fids being acquired and displayed sequentially. The gradient pulse amplitude must first be set to zero.
- Type **"gs"** to start the acquisition, and adjust the rf excitation pulse low enough to prevent a saturation effect on the 8 fids. All 8 fids must look the same as shown in the following figure. The O1 frequency must be *on resonance*.

⇒ **On instruments equipped with RX22 receivers it is essential to set O1 and O2 to exactly the same value.**

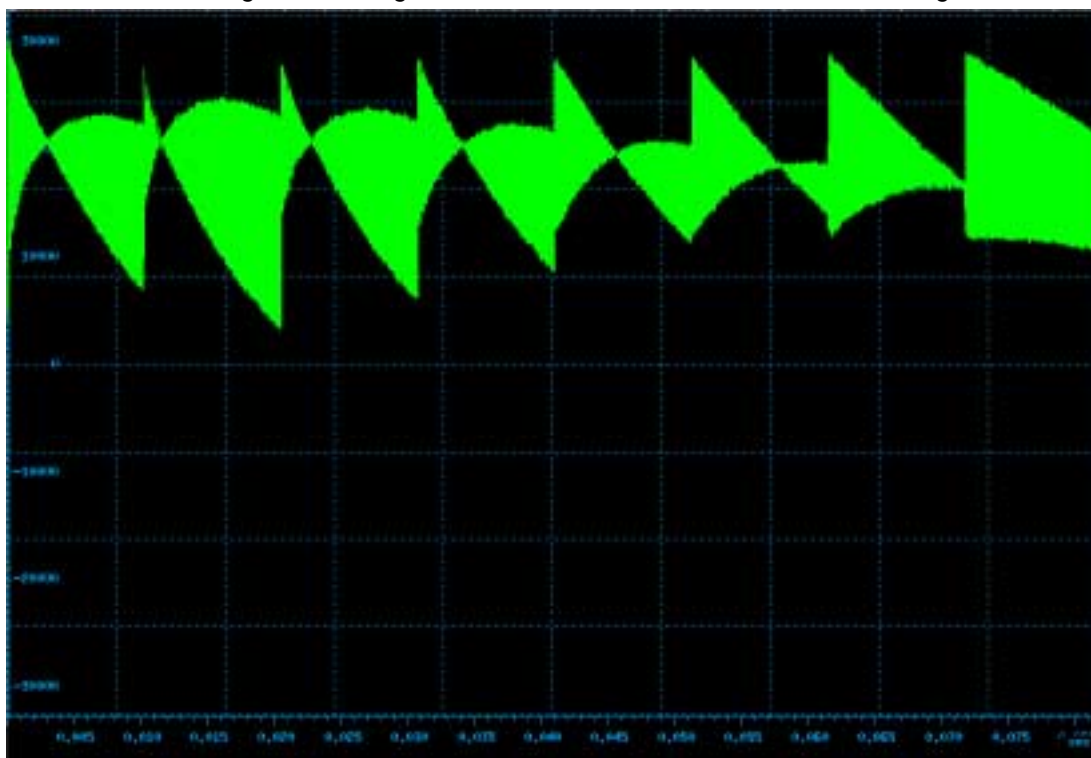
Figure 2.12. Eight fids on Resonance Without Gradient Switching.



- Stop the acquisition and run “**diffpremp**” once again. Start with 20% for the gradient amplitude and later increase the amplitude.

The screen should now look like the figure: **“Eight fids on Resonance With Gradient Switching.” on page 19.** The frequency shift should be clearly visible.

Figure 2.13. Eight fids on Resonance With Gradient Switching.



- Select "x,y or z B0 Mod", depending on which gradient you are currently using, in the setpre menu and modify the correction pulse shape by changing the time and gain parameters until all fids are identical. The fid on the right side is used as a reference, since the delay between gradient switching and the start of data acquisition is the longest for this fid. It is assumed, that for the last fid, the B0 shift is gone.

It is recommended that you start with the long time constants and continue with the middle and short time constants afterwards. This procedure corrects the shape of the fids from right to left.

After the correction the fids should look like those in the figure **"Eight Unshuffled Fids After B0 Adjustment."** on page 20.

Figure 2.14. Eight Unshuffled Fids After B0 Adjustment.



- Save the adjustment parameters using the command in the “File” pull-down menu.
- Stop the acquisition and run **diffpreemp** once again in order to increase the gradient amplitude or to repeat the procedure for the other gradients.

Gradient Calibration

2.3.6

A number of imaging and diffusion probeheads are available with gradient systems of different sensitivities (G/cm/A or mT/m/A), as described in the **"Gradient Calibration values" on page 68**. In order to provide images with the correct field of view (FOV), correct slice thickness (SLTH) and slice position or correct gradient pulses for diffusion experiments, the program needs information about the gradient sensitivity and the maximum current supplied by the gradient amplifiers. Other parameters needed for correctly scaled images are the relative gradient sensitivities between the X, Y and Z-gradients, caused by differences in design and production. This information must be stored during the installation procedure in the preemphasis file, see **"Menu for the Preemphasis Parameters" on page 10**.

⇒ **Note:** Gradient calibration values must no longer be entered into the file `gradient_calib` but into the preemphasis file, which is accomplished by `setpre`. The file `gradient_calib` is then derived automatically from that information.

The reproducibility of the gradient amplifiers and the gradient systems now allows you to use standard values. See **"Gradient calibration values for B-AFPA40" on page 68** for numbers. Fine tuning can be done using diffusion measurements.

The reproducibility of the gradient amplifiers and the gradient systems now allows you to use standard values. See "**Gradient calibration values for B-AFPA40**" **on page 68** for numbers. Fine tuning can be done using diffusion measurements.

The only way calibrate such gradients exactly is to measure the diffusion coefficient of a well known sample carefully and compare the results with the literature values. Some values are listed in **"Useful values of diffusion coefficients" on page 68**, more can be found in the "Bruker Almanac"

Usually one will use a water sample for this calibration, the best is to use the Bruker standard sample called "Doped Water", which is 1% H₂O in D₂O with 0.1g/l GdCl₃. For the proton diffusion coefficient of this sample the values of D₂O can be used, because the sample is practically D₂O, H₂O is only used as a tracer.

If this is not available, one can use normal demineralized water. The water must be doped, using e. g. 1g/l CuSO₄. In this case of course the H₂O diffusion coefficient applies.

➡ **Note: Diffusion coefficients of liquid samples are strongly temperature dependent.**

Two important points have to be taken into account:

1. Calibrate the temperature using an NMR temperature standard, e. g. one of the Bruker "Temperature Calibration" samples. See **"Temperature calibration curve for Ethylenglycol" on page 69** and **"Temperature calibration curve for Methanol" on page 69**.
2. Don't use the air flow temperature control of the probe, disconnect the air flow and switch off the heater. Use the gradient cooling water to control the temperature.

The procedure is as follows:

Measure the diffusion coefficient using the the actual calibration.

Calculate the corrected gradient calibration constant:

$$GCC_{new} = \text{SQRT}\{D\} / D_{Literature} \} GCC_{old}$$

Store the new constant using **setpre**.

If this procedure is used for a 3 axis gradient system, it is a little bit more complicated:

Measure the diffusion coefficient using the the actual calibration independently in all 3 gradient directions.

First correct relative gradient scaling factors, here called S_x, S_y, S_z:

$$S_{xnew} = \text{SQRT}\{\min(D_x, D_y, D_z) / D_x\} S_{xold}$$

$$S_{ynew} = \text{SQRT}\{\min(D_x, D_y, D_z) / D_y\} S_{yold}$$

$$S_{znew} = \text{SQRT}\{\min(D_x, D_y, D_z) / D_z\} S_{zold}$$

Calculate the corrected gradient calibration constant:

$$GCC_{new} = \text{SQRT}\{D\} / D_{Literature} \} GCC_{old}$$

Store the new values of S_x, S_y, S_z and GCC using **setpre**.

Diffusion Experiments

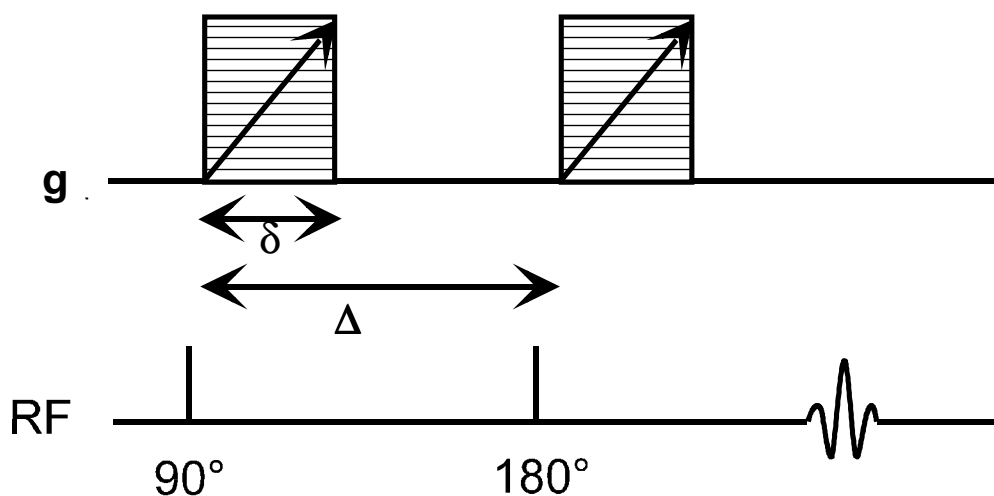
3

Basics

3.1

Diffusion experiments are usually based on two standard types of pulse sequences, the spin echo diffusion sequence¹ (PGSE) and the stimulated echo sequence² (PGSTE). All other published sequences can be understood as modifications of these two sequences. For samples with $T_1 = T_2$ the PGSE sequence is usually the preferred one; for samples with $T_1 \gg T_2$ the PGSTE sequence is often used, as during most of the diffusion time the magnetization can be stored in the Z direction. For the PGSE sequence, the maximum diffusion time is limited by T_2 ; for the PGSTE sequence the maximum diffusion time is limited by T_1 .

Figure 3.1. PGSE Pulse Sequence (diff_se)



We currently support 3 sequences, a PGSE sequence called diff_se, a PGSTE sequence called diff_ste and a bipolar PGSTE, the so called “13 interval sequence”³, here called diff_stepb. All the sequences use a constant gradient pulse duration δ , a constant diffusion time Δ and variable gradient amplitude g . The gradient amplitude is varied using constant increments.

1. E. O. Stejskal and J. E. Tanner, J. Chem. Phys. **42** (1965)
2. J. E. Tanner, J. Chem. Phys. **52**(1970)
3. R. M. Cotts, M. R. Hoch, T. Sun, and J. T. Markert, JMR **83**, 252-266(1989)

Figure 3.2. PGSTE Pulse Sequence (diff_ste)

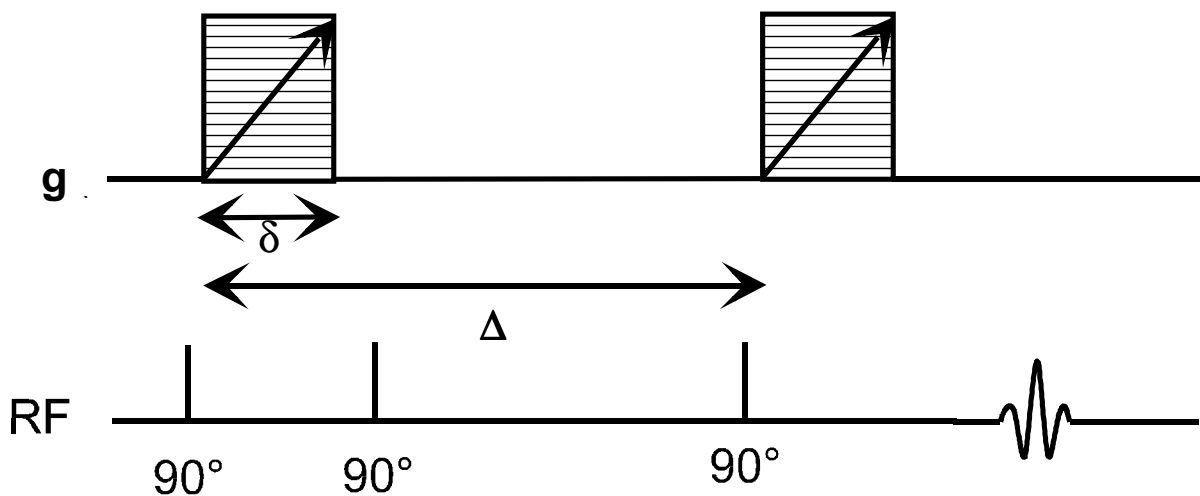
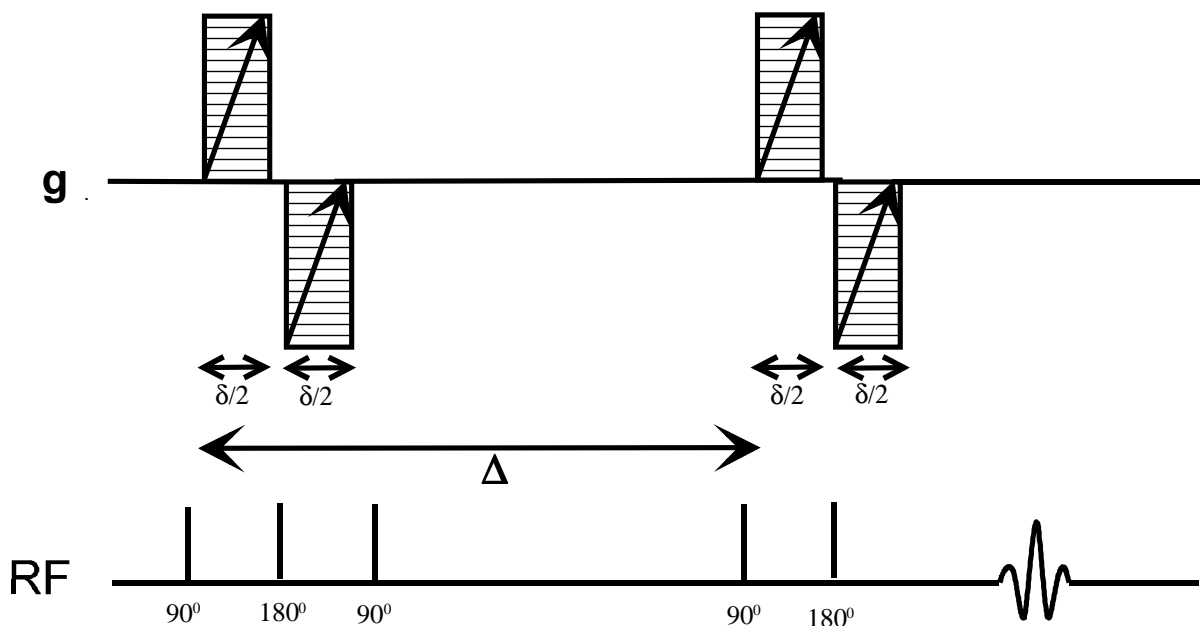


Figure 3.3. 13 Interval PGSTE Pulse Sequence (diff_step)



Setup

3.2

The complete setup described below usually only has to be fully performed once. At any stage parameters can be stored as standard parameters and recalled. The degree of changes depends only on the variety of samples to be measured.

The setup is simplified by using the TclTk scrip **diff**. An example of the use of **diff** is described below, using values suitable for a water sample.

The setup is performed in 3 major steps:

1. The setup of the spectroscopic parameters, i. e. rf pulse length, rf power, spectral width and receiver gain.
2. The setup of the diffusion parameters, gradient pulse length and maximum amplitude, the diffusion time and the receiver gain, which is a function of the echo time.
3. The setup of the 2D measurement parameters, number of gradient steps, number of scans and number of repetitions.

Probehead Exchange

3.2.1

If the probe has to be changed, two important steps have to be performed

1. Select the correct probe using **edhead**
2. Read in the corresponding preemphasis parameters and load them in the preemphasis unit: Run **setpre** and execute **Read default**. See also "**Preemphasis Adjustment**" on page 8.

Spectroscopic Parameters

3.2.2

- Type "**edc**" to define a new data set.
- Type "**rpar diff2D all**". If diff2D is not available, use standard2D
The command **rpar** is only needed if you start from an arbitrary parameter set.
- Type "**edasp**" to set the correct nucleus.
The command **edasp** is only needed if you start from an arbitrary parameter set.
- Set P11 to the required power level for the selected nucleus and rf insert.
- Set P1 to the corresponding 90° pulse.
- Set P2 to the corresponding 180° pulse.
- Set SW or SW_h suitable for your sample.

⇒ **Note: If you don't use the lock, don't forget to set **LOCNUC=off** before starting diff. This will automatically disable the lock blanking in the pulse program. For details see "Lock" on page 47**

Diffusion Parameter Setup Program

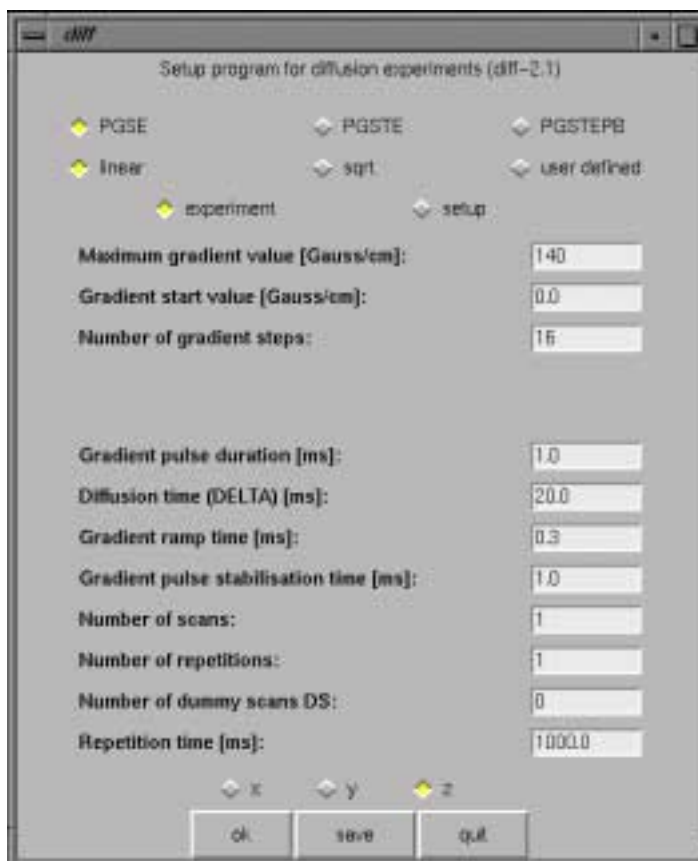
3.2.3

-Type "**diff**" to start the TclTk script. A window as displayed in "**TclTk Window diff in "Experiment Mode"**" on page 26 will show up. The window can be kept open as long as you work on the current dataset.

⇒ **Note: The TclTk script "diff" will only run if called from 2D dataset!**

➡ **Note:** The TclTk script “diff” always works on the parameters of the dataset from which it was started. Before changing the dataset, close the window by pressing the “OK” or “quit” button!

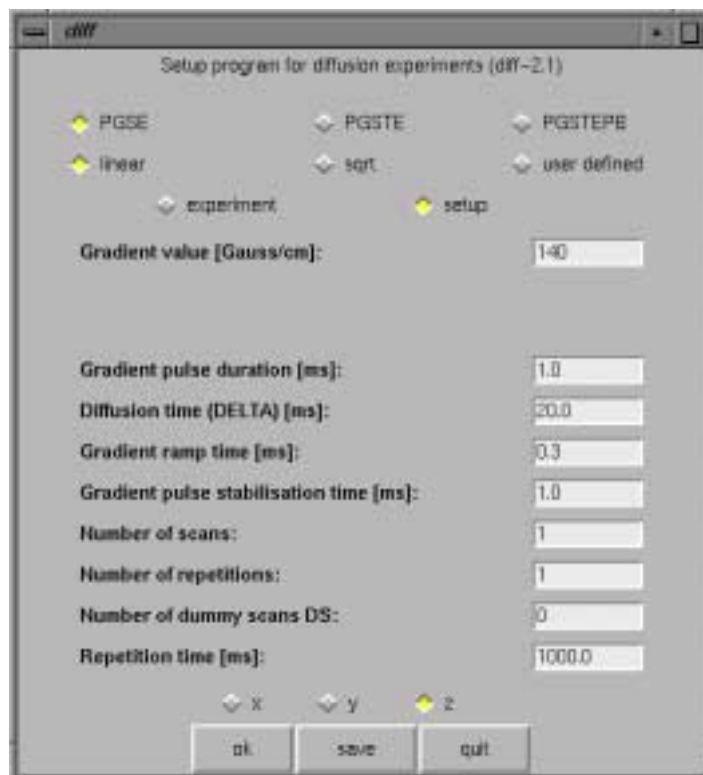
Figure 3.4. TclTk Window **diff** in “Experiment Mode”



Select the experiment you want to perform by clicking on the corresponding button. The descriptions in this section refers to the PGSE experiment.

The TclTk script **diff** always comes up in the experiment mode. To continue the setup click the “**setup**” button.

The window will then change, as shown in [“TclTk Window diff in “Setup Mode”” on page 27.](#)

Figure 3.5. TcITk Window **diff** in “Setup Mode”

Adjust the parameters according to your sample properties. A detailed description of the parameters shown in ["TcITk Window diff in "Experiment Mode" on page 26](#) and ["TcITk Window diff in "Setup Mode" on page 27](#) are given in ["Parameter Description \(physical meaning\)" on page 42](#) and in ["TcITk Script "diff" on page 45](#)

To change the values:

- Click on the entry field.
- Delete the numbers and type in the new number you want.
- Type "return" to activate the relations.

Depending on the parameter hierarchy, the parameters will be checked and e. g. set to the minimum possible value, derived from the other related parameters.

After adjusting all of the parameters you have to save these to the dataset:

- Click "save" to store the parameters.

or: - Click "ok" to store the parameters and to exit the script.

Clicking on "quit" will exit without saving the dataset parameters.

➡ **Note: The first time you click “ok” or “save”, the AU program “diff_t1pars”, which runs in background, will be compiled automatically and the corresponding message will be displayed!**

The setup of the most important parameters the “maximum gradient Value”, the “gradient pulse duration” δ and the “diffusion time” Δ is, in general, an iterative procedure. The adjustment of the receiver gain is dependent on these parameters.

Adjustment of the Gradient Strength

3.2.4

- Set the diffusion time Δ and the gradient pulse duration δ to reasonable start values. Typical start values for water are:

$$\Delta = 20 \text{ ms}$$

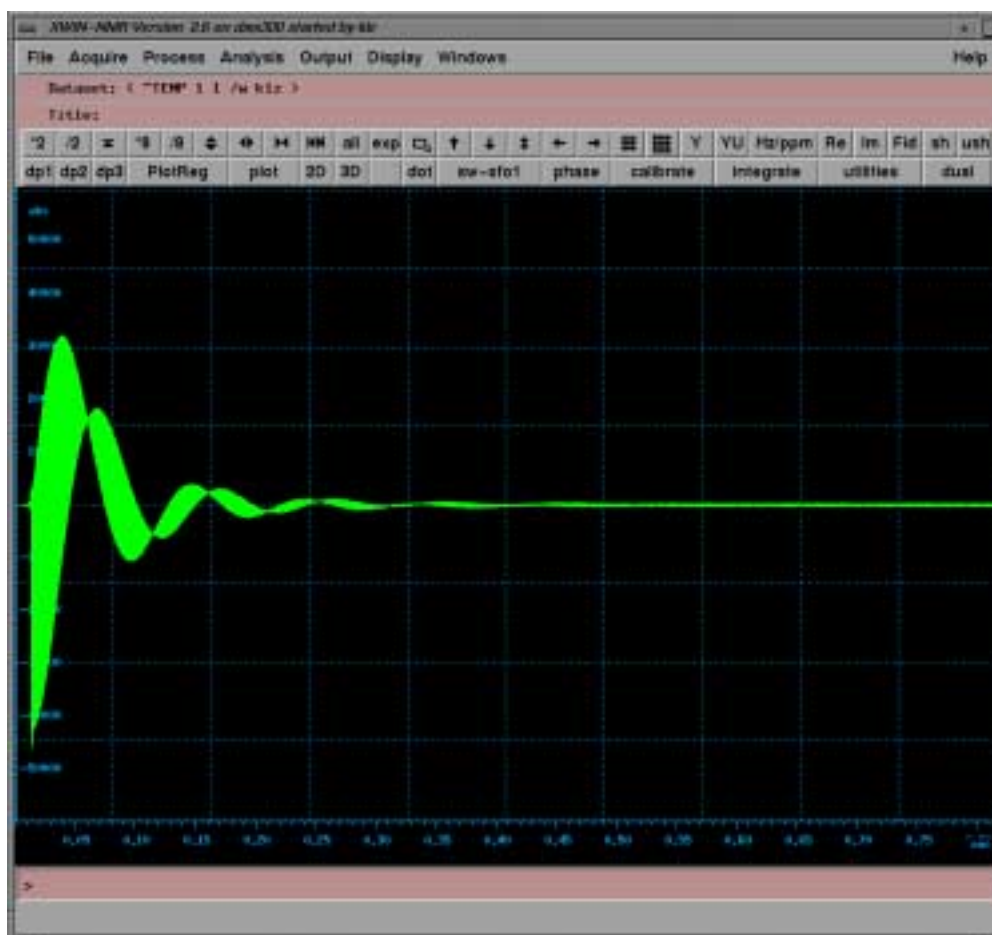
$$\delta = 1 \text{ ms}$$

- Set the maximum gradient strength to zero to adjust the receiver gain.

- Click “save”

- Switch to the acquisition window and run GS or ZG. Look at the echo **"Echo Signal in Time Domain Triggered at the Echo Top" on page 29** and adjust the RG. To look at the spectrum you have to issue the command “rser 1” to get a temporary 1D dataset, where you can perform FT and all other 1D processing.

Figure 3.6. Echo Signal in Time Domain Triggered at the Echo Top

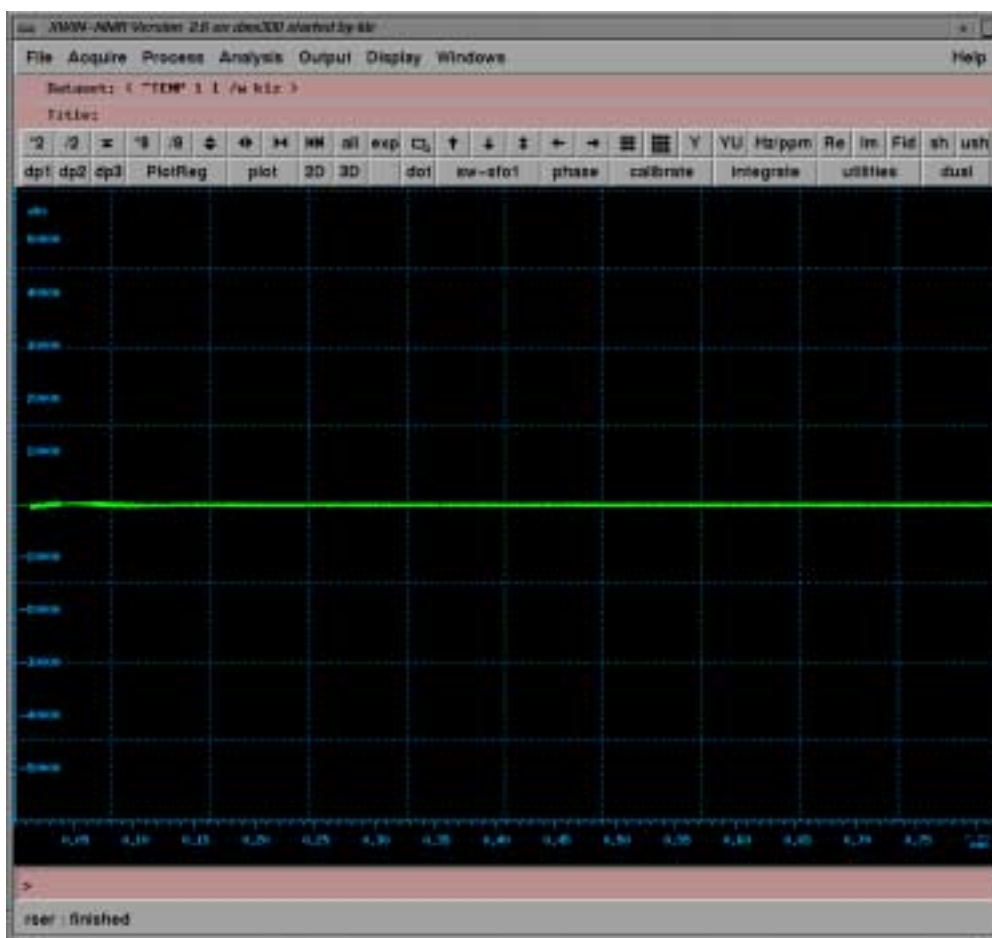


If the signal amplitude seems to be too small, go back to **"Adjustment of the Gradient Strength" on page 28** and reduce the diffusion time. The diffusion in this experiment is limited by T_2 .

- Set the maximum gradient strength to a random value. For water and the parameters shown above use 150 G/cm.
- Click "save".
- Look at the signal amplitude **"Attenuated Echo Signal" on page 30**. In order to provide for a good fit of the data, a signal attenuation of about a factor of 10 is recommended.

If the signal is too big, increase the gradient strength, if it is too small decrease it.

Figure 3.7. Attenuated Echo Signal



Adjustment of the Gradient Pulse Duration

3.2.5

The gradient pulse duration can usually be safely varied between 0.5 ms and 5 ms for the maximum current. Please refer to **"Duty Cycles for Diffusion Gradient Systems" on page 59** for maximum pulse duration and duty cycles.

If you have reached the maximum gradient strength during the **"Adjustment of the Gradient Strength" on page 28** and are still not satisfied with the signal attenuation, increase the gradient pulse duration within the limits described above and go back to the **"Adjustment of the Gradient Strength" on page 28**.

Adjustment of the Diffusion Time

3.2.6

The diffusion time can be varied in the limits given by the other delays in the pulse sequence and the T_2 -relaxation. The minimum possible value is mostly controlled by the gradient pulse duration and the gradient pulse stabilization time. The minimum value is automatically calculated by the **diff** script, it will show up as soon as you enter 0 for the diffusion time.

If you have reached the maximum gradient strength during the **"Adjustment of the Gradient Strength" on page 28** and the maximum gradient pulse duration during the **"Adjustment of the Gradient Pulse Duration" on page 30** and are

still not satisfied with the signal attenuation, increase the diffusion time and go back to the **"Adjustment of the Gradient Strength" on page 28.**

The diffusion time is not only important for the signal attenuation, it is a very important parameter concerning restricted diffusion.

Running the Experiment

3.3

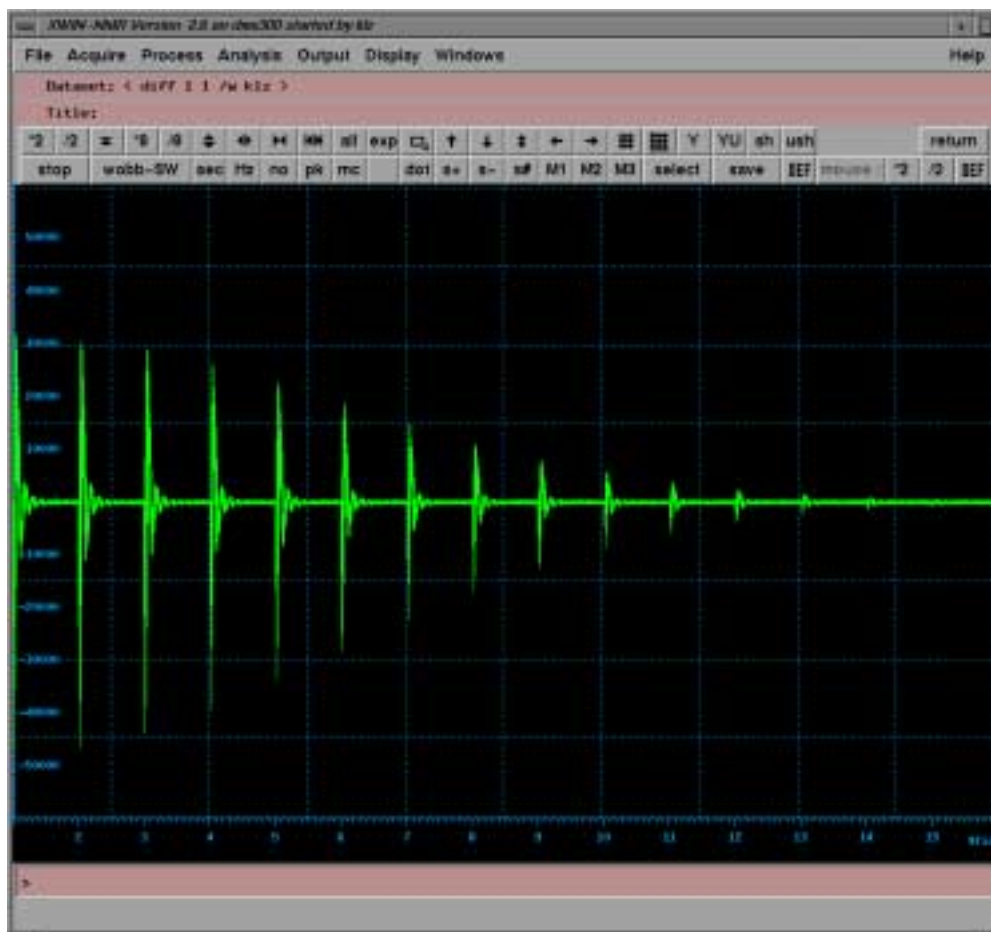
To run the experiment switch to the "experiment mode" by clicking on the **experiment** button. The window will change to the **"TclTk Window diff in "Experiment Mode" on page 26.** Here you have to adjust the **number of gradient steps**, the **number of scans**, the **number of repetitions** and the **number of dummy scans**.

Click **save** or **ok**, to store the parameters.

Type **zg**.

After the acquisition is finished you can display the data as shown in **"Echo Decay Due to Growing Diffusion Gradients." on page 31**

Figure 3.8. Echo Decay Due to Growing Diffusion Gradients.



Type **"edp"**.

Select **"PH_mod"** **"mc"** in the F2 column.

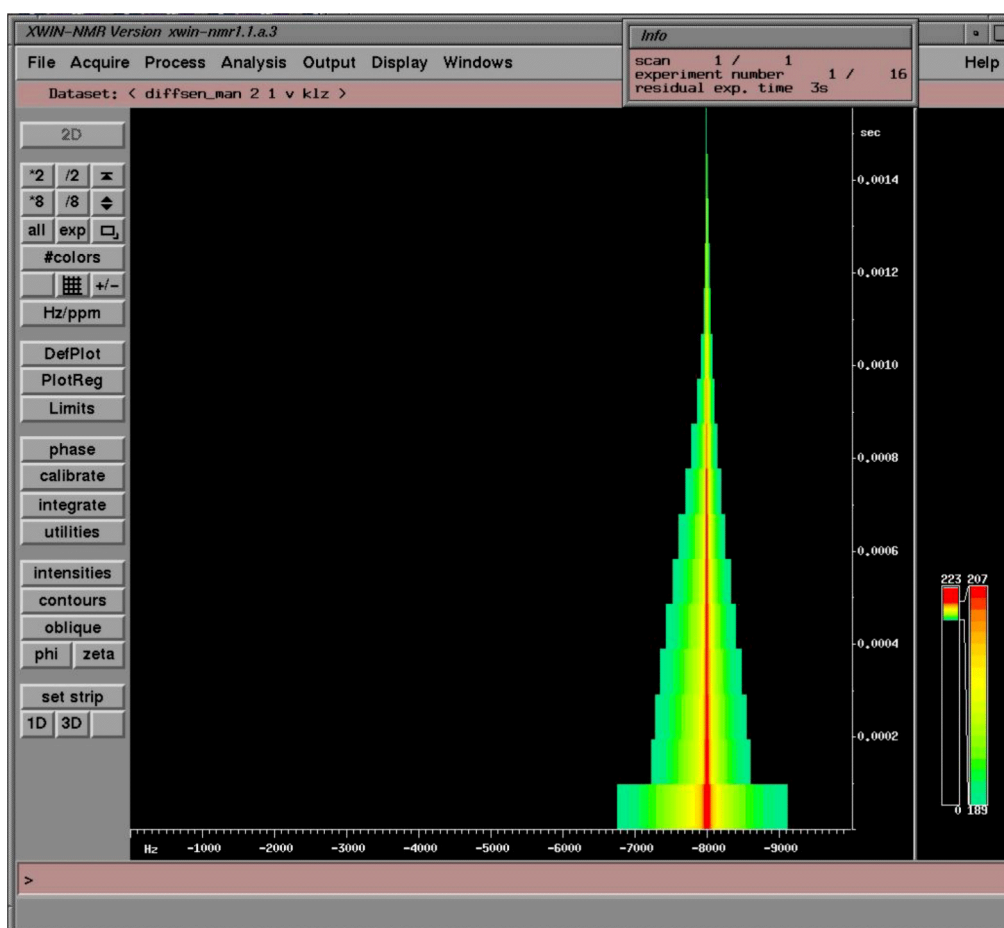
Select **"WDW"** **"no"** in the F2 column.

The sizes are set by the au program, the other parameters are not, because they are determined by the user.

Exit **"edp"** by typing save.

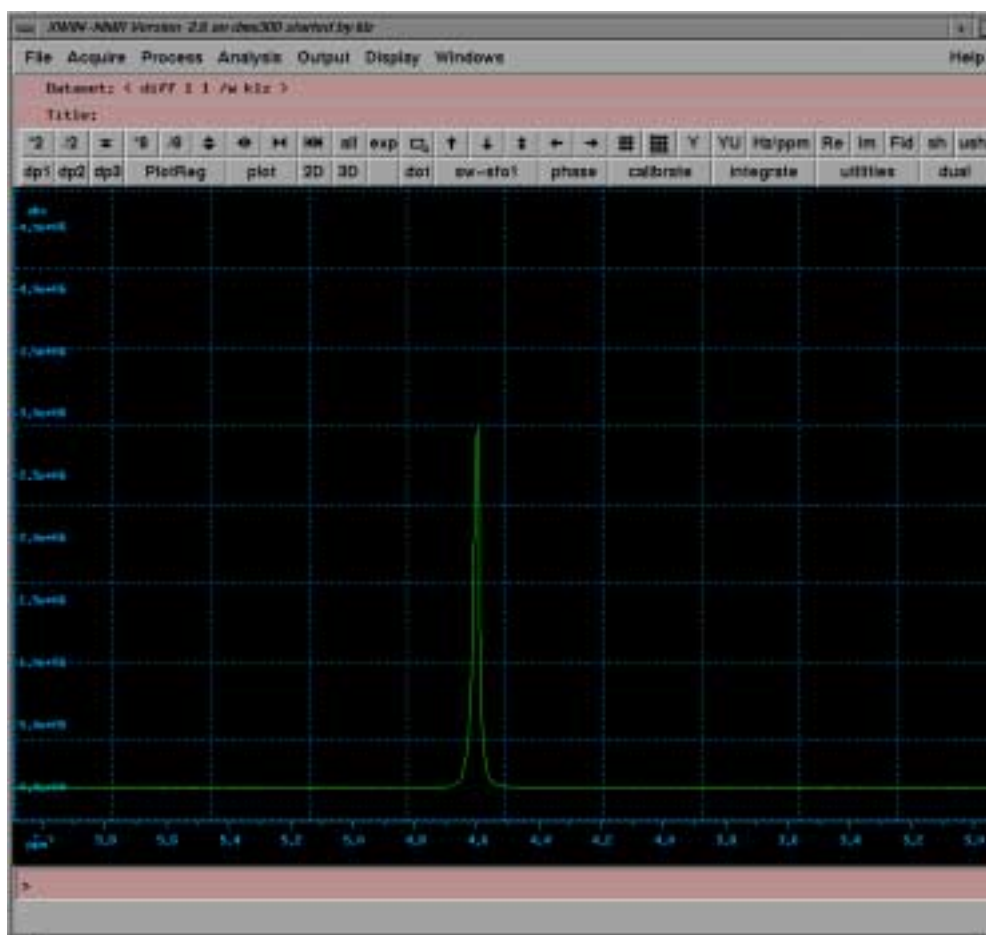
Type **"xf2"**

Figure 3.9. Echo Decay After xf2



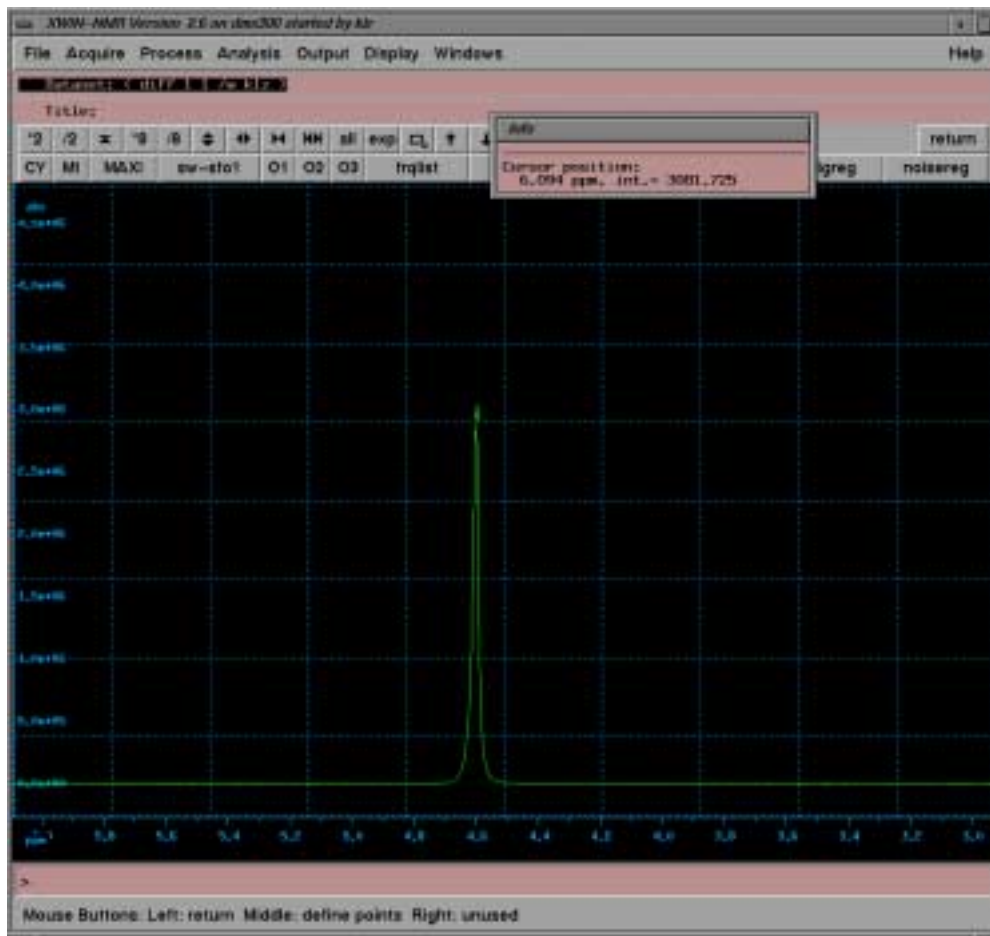
- Switch to the **"T1/T2"** submenu in the **"Analysis"** menu
- Type **"rspc"** or select it in the **"processing menu"**.

Figure 3.10. Selected Spectrum from the 2D Dataset.



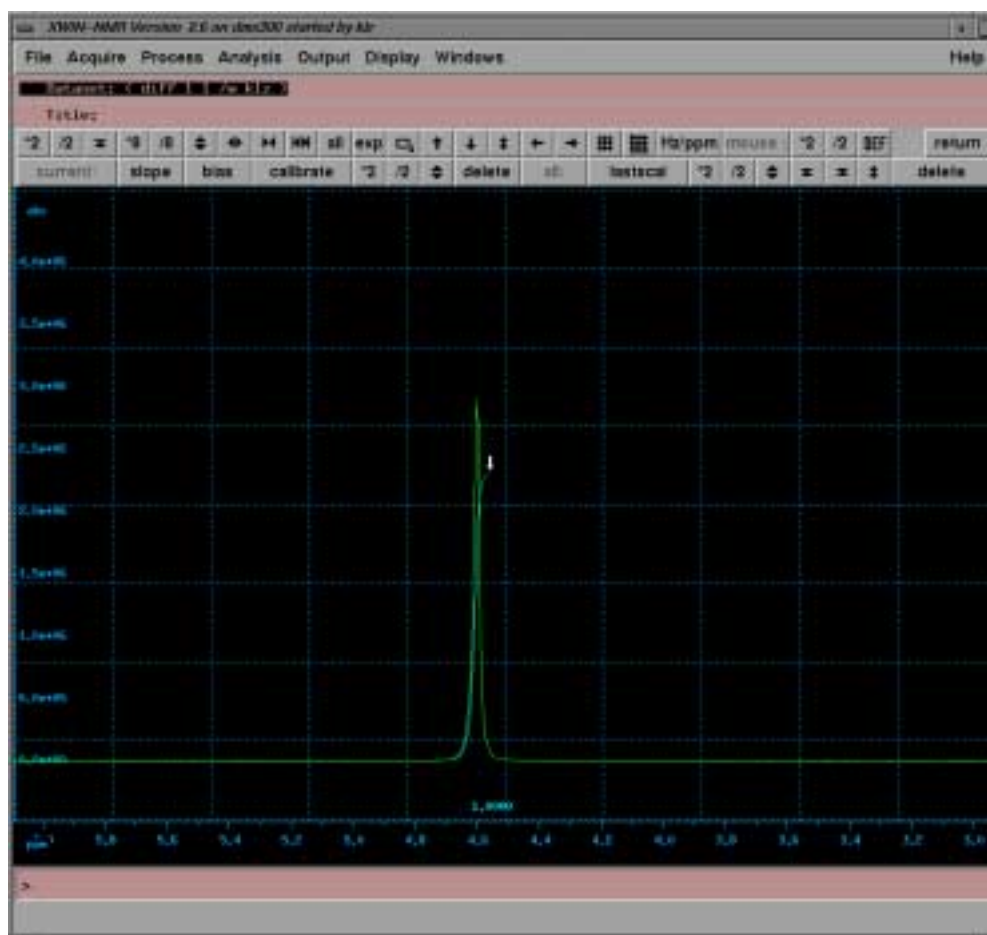
- Select the “utilities” submenu to define the peak.
- Select “defpoints” and the peak by pressing the middle mouse button.

Figure 3.11. Spectrum with Selected Peak.



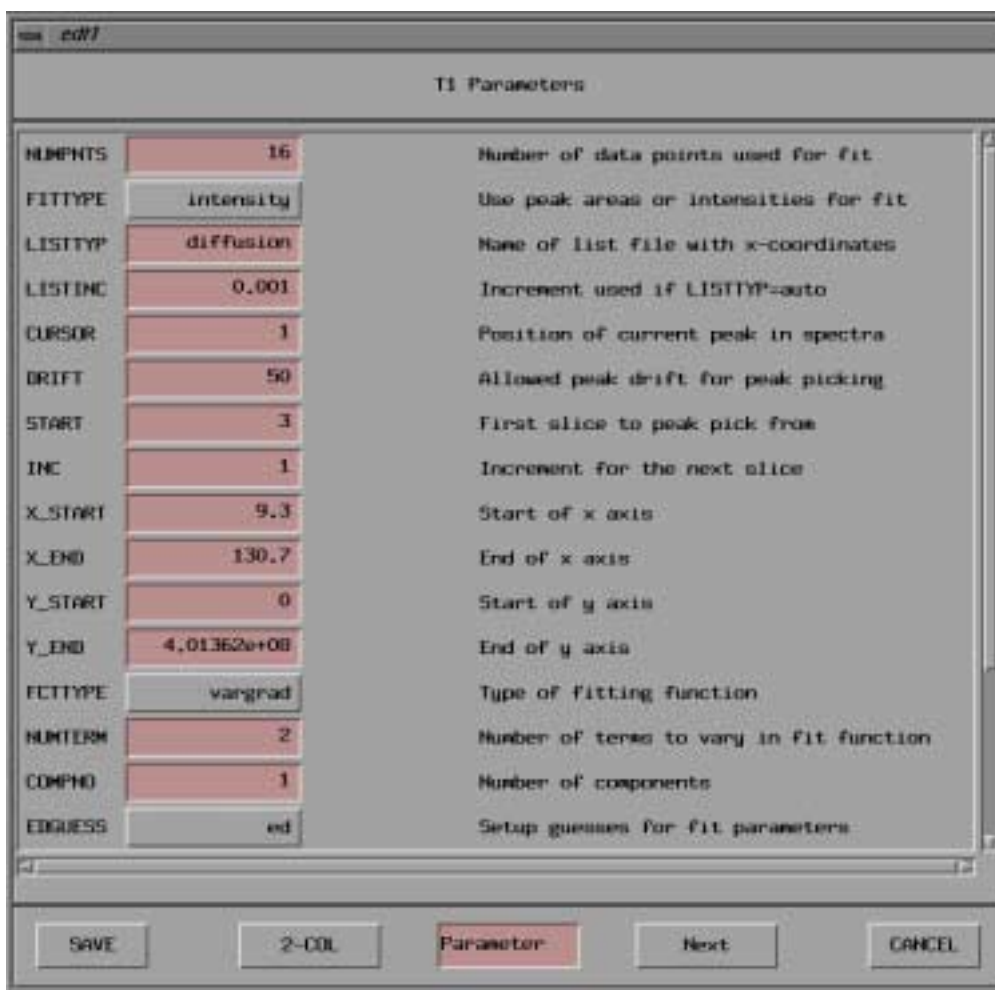
- Exit **“defpoints”** by pressing the left mouse button and then return.
- Select **“integrate”**
- Define the integral.

Figure 3.12. Spectrum with Selected Integral



- Return using **“write & return”**
- Switch back to the **“T1/T2”** submenu in the **“Analysis”** pull-down menu
- Type **“edt1”** or select it from the **“Processing”** menu.

Figure 3.13. The edt1 Menu



All the parameter described here are preset to usually reasonable values, if **diff** was executed on the data set before, see ["Lock" on page 47](#).

- Set "FITTYPE" to "intensity" or "area", depending whether you want to use the peak height of the peak integral. Currently the default setting set by **diff** is intensity.

The parameters from "Cursor" down to "INC" are usually OK. The parameters "NUMTERM" and "EDPARM" are only used in T1/T2 fittings. The parameters "X_START" to "Y_END" are set automatically.

- Set "FCTTYPE" to "vargrad".

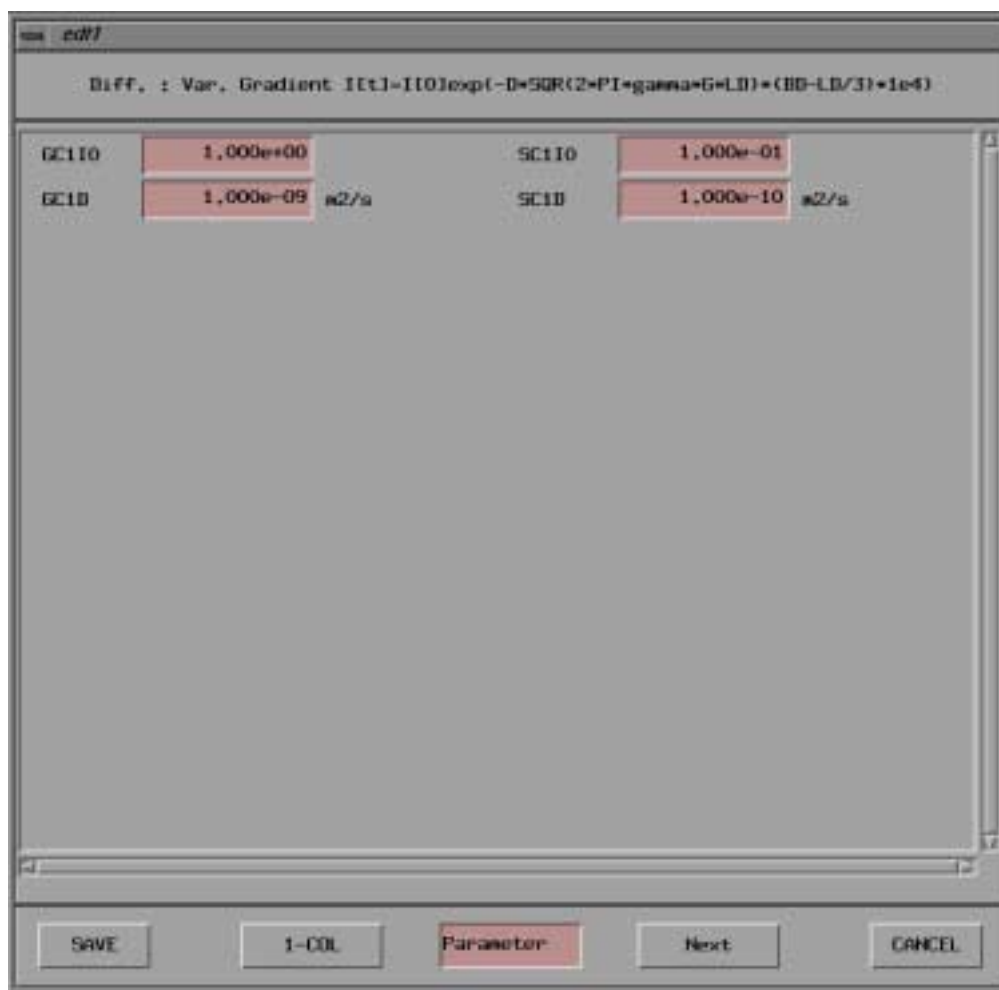
i.e. diffusion experiment with variable gradient but constant deltas.

- Set "COMPNO" to 1

"COMPNO" defines the number of exponents to be fitted. The maximum is 6 for this experiment.

- Press "EDGUESS"

Figure 3.14. EDGUESS Submenu



The top line of this menu shows the formula used here. The numbers in the left column represent the estimates for the amplitudes and the diffusion coefficients. The amplitudes “**GC110, GC210...**” are normalized to one, e.g. the sum of all used amplitudes should be one. In practice you can usually set all amplitudes to one and the fit algorithm will still work. The diffusion coefficients “**GC1D, GC2D.**” are in units of m^2/s , here the estimate should be in the order of magnitude.

The **diff** script presets the values of **GC1D, GC2D** and **GC3D**:

$$\text{GC1D} = 10^{-9} \text{ m}^2/\text{s}$$

$$\text{GC2D} = 10^{-11} \text{ m}^2/\text{s}$$

$$\text{GC3D} = 10^{-13} \text{ m}^2/\text{s}$$

The numbers in the right column represent the initial steps of the fit routine, usually they are set to one tenth of the corresponding value in the left column.

After setting all required values, leave the “**EDGUESS**” submenu by pressing “**SAVE**”.

In the lower part of the “**edt1**” menu you can see the experimental parameters “**GAMMA**”, “**LITDEL**” and “**BIGDEL**”, representing with γ , δ and Δ , respectively.

Diffusion Experiments

These parameters are described in "Lock" on page 47. If `diff` has been run previously, they are preset to the correct values.

Figure 3.15. The `edt1` Menu Lower Part

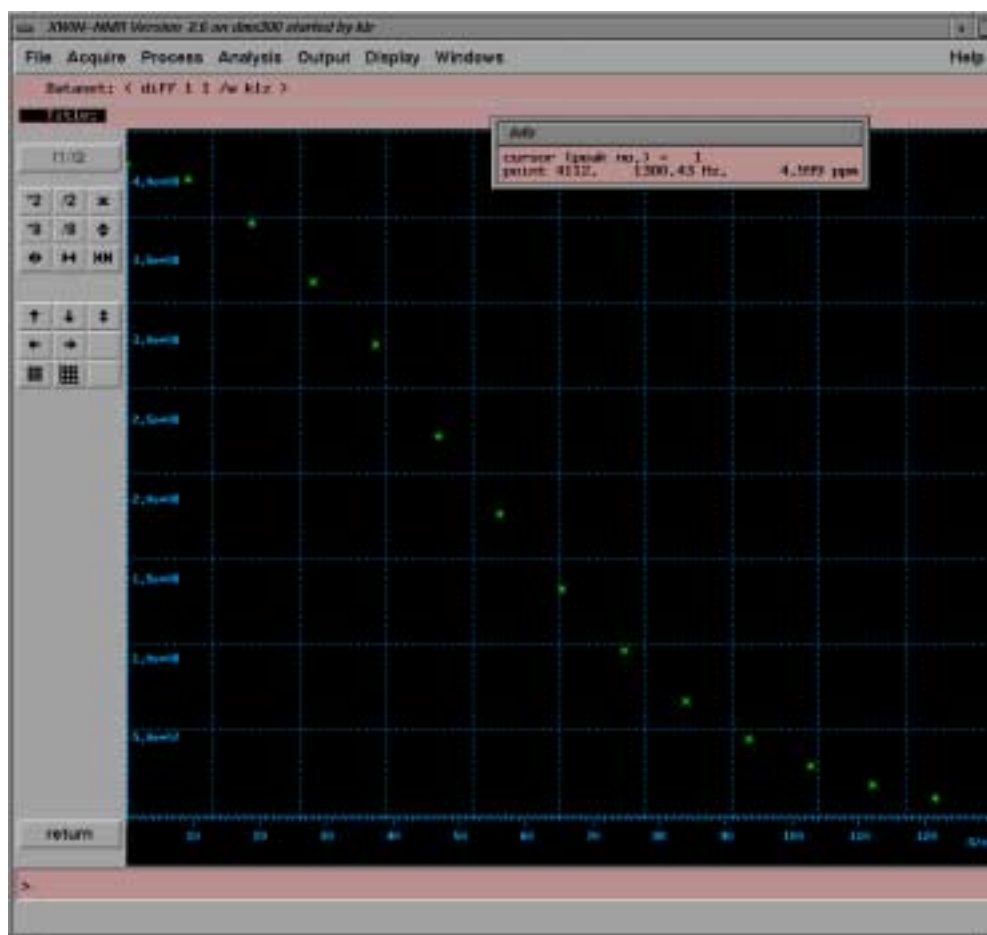
The screenshot shows a window titled 'edt1' with a sub-header 'T1 Parameters'. It contains a list of parameters with their values and descriptions. The parameters are:

Parameter	Value	Unit	Description
DRIFT	50		Allowed peak drift for peak picking
START	3		First slice to peak pick from
INC	1		Increment for the next slice
X_START	9.3		Start of x axis
X_END	130.7		End of x axis
Y_START	0		Start of y axis
Y_END	4.01362e+08		End of y axis
FCTTYPE	vargrad		Type of fitting function
NUMTERM	2		Number of terms to vary in fit function
COMPNO	1		Number of components
EDGUESS	ed		Setup guesses for fit parameters
GAMMA	4.257e+03	Hz/G	gamma
LITDEL	1.0	usec	little delta
BIGDEL	20.0	usec	big delta
EIPARM	ed		Show parameters after fit
CONV	1e-05		Convergence limit for fit algorithm

At the bottom of the window, there are five buttons: 'SAVE', '2-COL', 'Parameter', 'Next', and 'CANCEL'. The 'Parameter' button is highlighted in red.

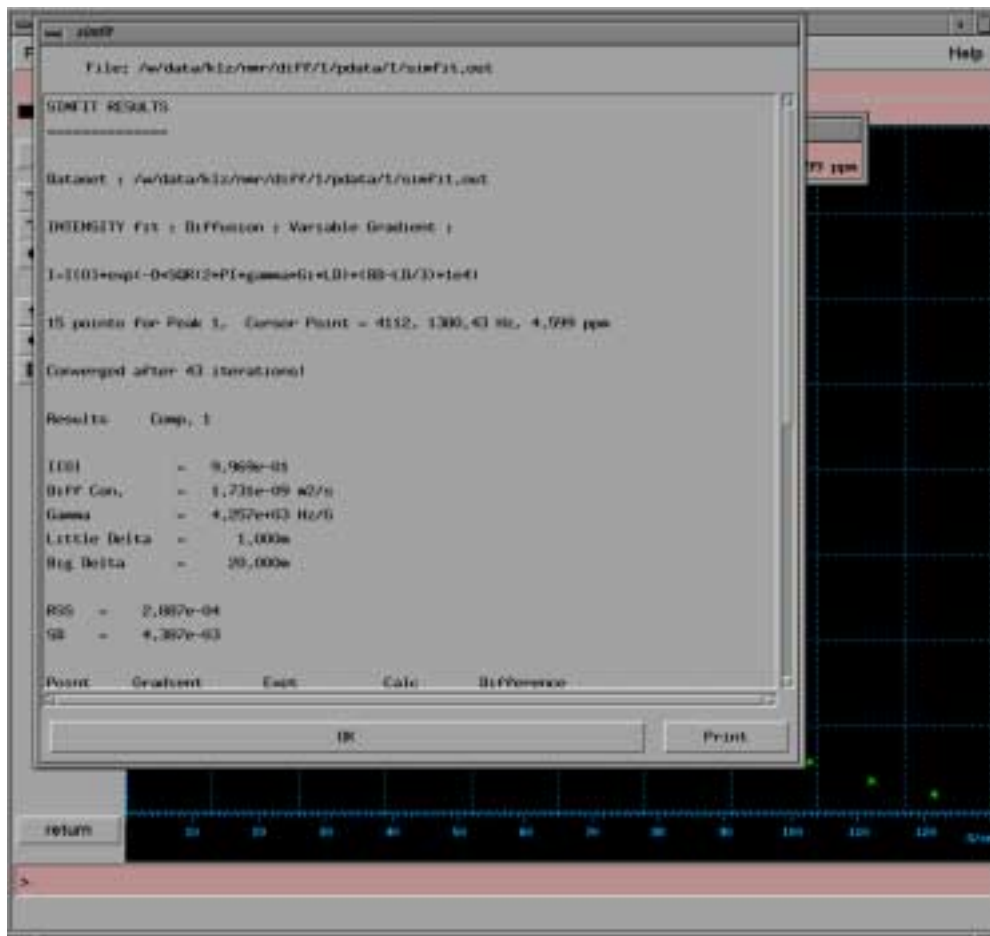
- Exit "`edt1`" by pressing the "save" button
- Type "`pd`" or select it from the "Processing" menu.

Figure 3.16. Simfit



- Type "simfit" or select it from the "Processing" menu.

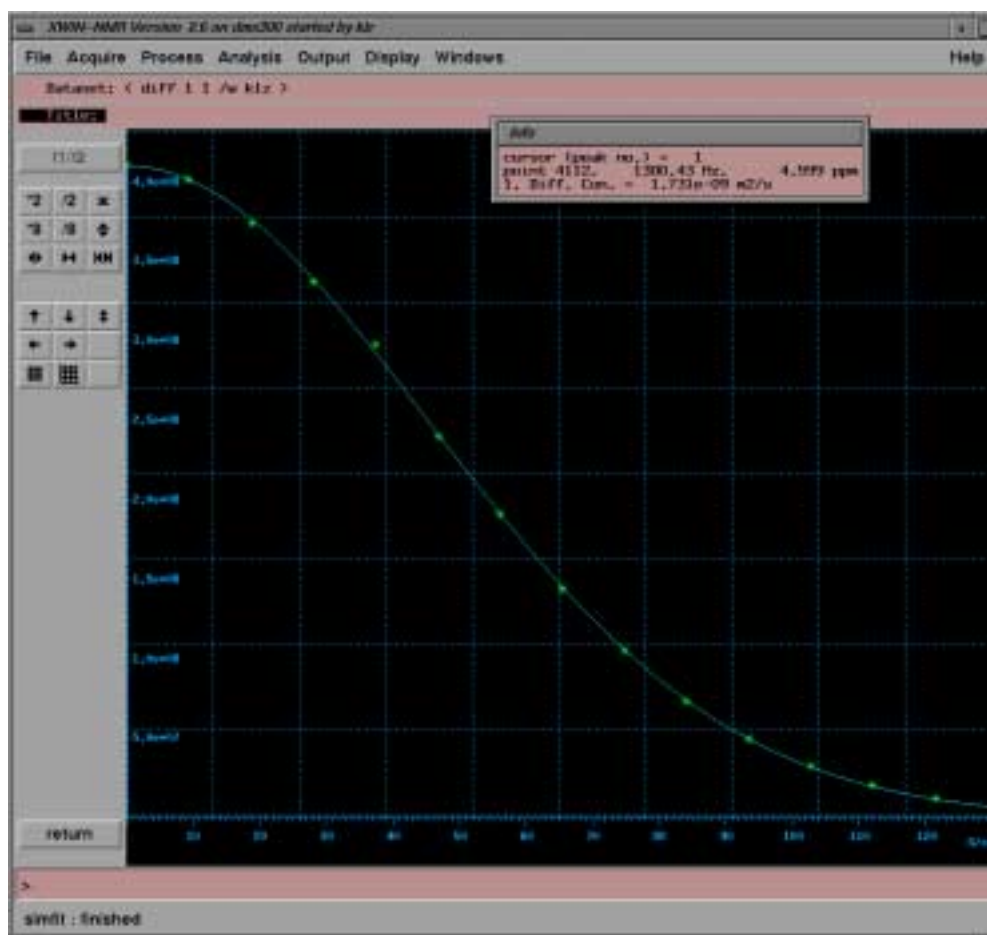
Figure 3.17. Simfit Results



The Simfit result screen is displayed, if “CURPRIN” is set to “\$screen” in the “edo” menu. This printout can, of course, also be sent to a printer, e.g. by setting “CURPRIN” to “\$hpdj550c”. The displayed file is also automatically stored in the processed data directory with the name **simfit.out**.

- Press “ok”

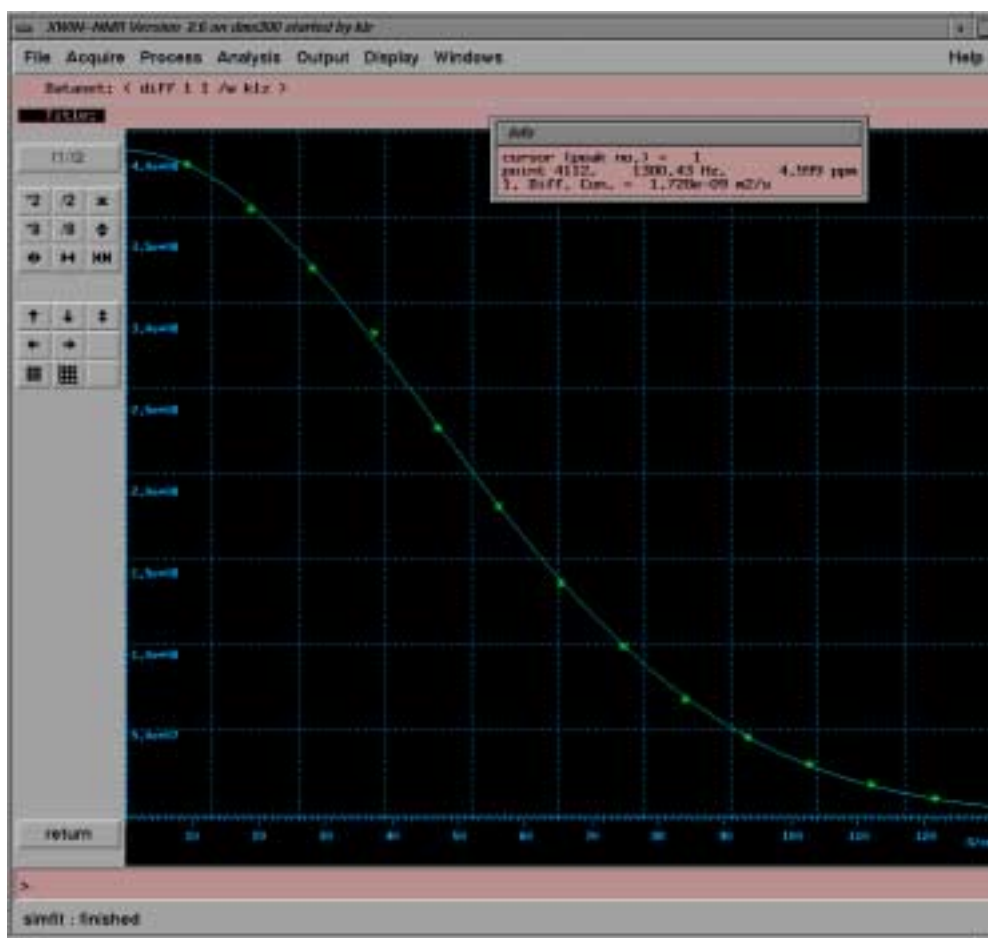
Figure 3.18. Fitted Diffusion Curve



The first point in the figure above is a little off, because of a too fast repetition. This can be easily eliminated as follows:

- Put the cursor into the data window and press the left mouse button.
- Select the point to be eliminated by moving the cursor to it.
- Press the middle mouse button to eliminate the point.
- Double click left mouse button to leave the “elim” function
- Type “simfit” or select it from the “Processing” menu once again.

Figure 3.19. Fitted Diffusion Curve, Second Attempt



Parameter Description (physical meaning)

3.5

Gradient Values in Setup

3.5.1

During the setup sequence there is only one gradient value in use.

Gradient Values in Experiment

3.5.2

The diffusion experiments described here perform a series of increasing gradient values with constant increments. The series starts with **Gradient start value** g_{start} and ends with **Maximum gradient value** g_{max} . The gradient increments g_{incr} depend on the **number of gradient steps** $td1$:

$$g_{\text{incr}} = (g_{\text{max}} - g_{\text{start}}) / (td1 - 1)$$

All delays are expected to be set in units of milliseconds (ms), explicit unit specification as in XWINNMR is not implemented.

Gradient pulse duration δ : Effective length of the gradient pulse, for a trapezoidal gradient the length of one ramp plus the plateau is taken in order to calculate the correct area. In the case of PGSTEGBP, the sum of the two pulses is taken.

Diffusion time Δ : Delay between the centers of the gradient pulses, representing the observed diffusion time. In the sequence used here D is the same as the echo time ($t = TE/2$). In the case of PGSTEGBP, the diffusion time is corrected in order to allow fitting of the data using the standard formula.

Gradient ramp time: In order to provide best gradient performance combined with maximum gradient area, the gradient pulses are trapezoidal. The rising and the falling edge of the trapezoid is defined by the parameter **gradient ramp time**, i. e. the steepness of the ramp is independent of the pulse length. For details of the gradient programming see "**Gradient Programs**" on page 57

Gradient stabilization time: Delay to allow the preemphasis to decay, eddy currents and the amplifier to ring down. After this delay the gradient blanking unit, if installed, will be switched to the blanking mode, i. e. the amplifier is disconnected. The length of this delay depends on numerous system parameters like magnet type, field strength, gradient system type, and on the requirements of spectral resolution. Usually 3 ms is a safe value, delays down to 300 μ s have been used for broader resonance lines.

Number of scans NS: This parameter describes the number of scans done for a certain gradient amplitude, performing a 4-phase cycle. Therefore **NS** should be a multiple of 4. If less accumulations are required, smaller numbers are also possible.

Number of repetitions: This parameter describes the number of repetitions for the whole experiment. If multiple scans are necessary, it is usually best to use a combination of e. g. **NS** = 4 and any number of repetitions. There are two advantages of splitting the total number of scans in this way:

1. The quality of the experiment can be observed during the run and, as soon as the S/N ratio is found to be sufficient, the experiment can be terminated using the XWINNMR **halt** command.
2. The average power applied to the gradient system is more evenly distributed over the experiment time. Therefore, the heat development in the gradient system will be lower compared to an experiment with a high **NS** value, and the **number of repetitions** = 1.

Higher numbers of **NS** are only recommended for experiments with short repetition times, as each repetition costs more time, as a dummy loop is performed for each repetition and additional time is required for data storage.

⇒ **Note: Take care of the gradient duty cycle (see "Duty Cycles for Diffusion Gradient Systems" on page 59) specially in experiments with short repetition times.**

The Number of dummy scans sets the XWINNMR DS parameter (this is contrary to older diff versions).

Diffusion Experiments

The Number of dummy gradient pulses: This parameter defines the number of gradient pulses applied before the actual start of each scan, using the same timing as in the real experiment. Usually this parameter will be set to 0, only in extreme cases it might be necessary in order to bring the gradient amplifier to thermal equilibrium before the scan.

The Repetition time represents the overall duration of one scan, not including dummy scans and data handling.

Appendix: Diffusion

This section describes the various programs and parameter sets related to the diffusion experiments described previously.

⇒ **Note:** *In contrast to the earlier versions of the diffusion package, the same fixed gradient matrix as in high resolution spectroscopy is now used (see "Gradient orientation matrix cag par" on page 57), which allows standard parameter handling.*

TclTk Script "diff"

A.1

The TclTk script **diff** is successor to the AU programs used in earlier versions of the diffusion package. The major advantage for the user is, that they only have to touch the parameters they want to change and are not forced to answer unwanted questions.

General Operation

A.1.1

The TclTk script **diff** is called from XWINNMR. When the script is executed it reads a set of **acqu** parameters from the current data set. After execution the script allows the user to change parameters at any time. Any changes affect only parameters within **diff**, as long as the **ok** or **save** button have not been used. At the time you press **ok** or **save**, the TclTk script **diff** will update the parameters in the dataset from which it was started. It will not recognize a change of the dataset in foreground.

In addition to **acqu** parameters, e.g. delays, loopcounter, pulsprogram name and so on, **diff** also sets some default T1 parameters used to fit the diffusion constant, which simplify the processing.

Installation of the Diffusion Package

A.1.2

1. If the diffusion package is on the XWINNMR CDROM, follow the standard installation procedure (see "Installation of the Diffusion Software" on page 7).
2. If you receive the installation or update package from another source, e.g. the Bruker FTP server, the general procedure on UNIX system is as follows:
 - Put the file `diff-$version.tar.gz` into e. g. your home directory \$HOME

- Perform the following commands on UNIX shell level:

```
gunzip $HOME/diff-$version.tar.gz
```

```
cd $XWINNMRHOME
```

```
tar xvf $HOME/diff-$version.tar
```

- Run **expinstall** as described in **"Installation of the Diffusion Software" on page 7**

3. If you receive the installation or update package from another source, e.g. the Bruker FTP server, the general procedure on Windows-NT system is as follows:

- Put the file diff-\$version.zip into e. g. C:\TEMP

- Unzip it to \$XWINNMRHOME e. g. C:\Bruker\XWINNM

- Run **expinstall** as described in **"Installation of the Diffusion Software" on page 7**

Requirements for Running "diff"

A.1.3

1. XWINNMR 2.6 or newer is required.

2. The file

```
$XWINNMRHOME/exp/stan/nmr/parx/preemp/$CURPROBE/default
```

must be present. The parameter CURPROBE is defined by the XWINNMR command:

```
edhead
```

If the preemphasis file is not yet installed use **setpre** to create it (see **"Installation of a Diffusion Probe" on page 7**).

Relations Between "diff" and "acqu" Parameters

A.1.4

This chapter describes the relationship between the parameters in **diff** and the **acqu** file. Parameters in **diff** sometimes directly represent **acqu** parameters, other times rather indirectly. The table below shows these relationships.

Changing a parameter in **diff** will cause all the relationships to be checked. The hierarchy between the relations tries to follow a "common sense" concept, e. g. the echo time and the repetition time will be kept the same as long as the other parameters allow this. The two examples below represent how this works:

1. If you increase the gradient pulse duration, the diffusion time will be kept the same until d9 is less than 5 μ s. Keeping this diffusion time the same would violate the diffusion time relationship, i. e. d9 would be negative, therefore the diffusion time would now grow with the gradient pulse duration.

2. Afterwards, if you decrease the gradient pulse duration the diffusion time would be kept as it was before you started decreasing the pulse duration.

This type of hierarchy will satisfy most practical experimental cases. The easiest way to get used to this concept is to play with different settings to get a feeling of how it works.

Table 0.1. *diff Parameters Versus acqu Parameters for PGSE Experiment*

diff Parameter	XWINNMR Parameter	Modified Parameter
Maximum gradient value x-gradient: y-gradient: z-gradient:	gpx2*gradient_calib ^a gpy2*gradient_calib gpz2*gradient_calib	gpx1, gpx2, gpx3 gpy1, gpy2, gpy3 gpz1, gpz2, gpz3
Gradient start value	gpz0*gradient_calib	gpz0
Number of gradient steps	td1	td1
Gradient pulse duration ^b	p17+ p18	p18
Diffusion time (DELTA)	d2 + P18 + d11 + P17 +2*p1 + 20us + d9	d9
Gradient ramp time	p17	p17
Gradient pulse stabilisation time	d2	d2
Number of scans	ns	ns
Number of repetitions	l1	l1
Number of dummy scans ^c	ds	ds
Number of dummy gradient pulses	l13	l13
Repetition time	2*(d2 + p18 + d11 + p17 + p1 + 20us + d9) + aq + d1	d1

a. gradient_calib: Gradient calibration constant, in units of Gauss/cm, divided by 100, because XWINNMR constants are in percent

b. All delays in diff are in units of ms

c. Dummy scans are performed explicitly in the pulse program, DS is always set to zero. See e. g. **"PGSE Pulse Program diff se.gp" on page 49**

The *diff* script reads the acqu parameter **LOCNUC**. If **LOCNUC** is *off*, *diff* sets the loop counter **L12** to *zero*. This causes the *lock hold* feature of the BSMS not to be used. Otherwise **L12** is set to *one* and the *lock hold* is used. This was implemented to avoid unwanted effects of the *lock hold* in unlocked operation.

T1 Parameters Set by diff

The T1 package of XWINNMR is used to fit the diffusion coefficients. Diff sets the following values of the t1pars file, which can usually be accessed by the *edt1* command in *XWINNMR*, see "*Processing*" on page 32 for details. The parameter storage is accomplished through the au program *diff_t1pars*, which is automatically called by *diff* during *save* or *ok*.

Table 0.2. T1Parameters Set by diff

Parameter Name	Parameter Value
BIGDEL	Diffusion time
LITDEL	Gradient pulse duration
GAMM	Gamma value of selected nucleus
FCTTYPE	10 (i. e. variable gradient)
FITTYPE	Intensity or area ^a
LISTTYPE	difflist ^b
COMPNO	1
DRIFT	50
GUESSES	Some normally usefull start-values for the GUESSES are set

- a. Currently the default value is fixed to intensity, can be modified in *edt1*. The default value can be changed by modifying the line „xau diff_t1pars“ in the *diff* script
- b. This causes the T1 routine to search the *vdlist* in the data directory under the name “difflist”

DOSY parameters

In order to allow dosy processing for data acquired after a *diff* setup, the following DOSY parameters are stored automatically. These parameters can be edited us-

ing the **eddosy** command in xwinmr. Due to the same reason the file name of the *vdlist* file was changed from **diffusion** to **difflist**.

Parameter Name	Parameter Value
Gdist	Diffusion time
Glen	Gradient pulse duration
Gamma	Gamma value of selected nucleus
Nexp	1 (Number of exponentials)

Pulse Programs

A.2

Diff sets the name for the pulse program (PULPROG) to **diff_se.gp** for the **PGSE** experiment, to **diff_ste.gp** for the **PGSTE** and to **diff_stebp.gp** for the **PGSTE** experiment with bipolar gradient pulses, refer to the program codes below.

All these programs have been modified since the last version. First the so called gp syntax is used now, no separate gradient program is needed. Dummy scans are now handled as in standard HR pulse programs. Also the standard include file Grad.incl is now used.

PGSE Pulse Program *diff_se.gp*

A.2.1

```

;diff_se.gp
;2D Steiskal Tanner sequence
;forAVANCE KLZ 29.01.98
;new version using gp syntax 13.12.99 KLZ
;now standard include files and lock commands only on l12 03.08.00 KLZ
;dummy gradient pulses included l13 05.10.00 KLZ

#include <Grad.incl>
#include <Avance.incl>

ze
10u
5m pl1:f1 ;set rf power level

if (l12) {
    start, d1 LOCKH_OFF
        d11 UNBLKGRAMP LOCKH_ON;unblank gradient amplifier

```

```

} else {
    start, d1
        d11 UNBLKGRAMP
}
if (I3) {
    dummy,p17:gp1*diff_ramp;    trapezoidal gradient pulse
        p18:gp2*diff_ramp    ;trapezoidal gradient pulse
        p17:gp3*diff_ramp    ;trapezoidal gradient pulse
        d2                    ;gradient stabilisation time
        d9 BLKGRAMP          ;tau
        d11 UNBLKGRAMP      ;unblank gradient amplifier
    lo to dummy times I13
}

p1:f1 ph1                    ;p1 :90 degree pulse
p17:gp1*diff_ramp            ;trapezoidal gradient pulse
p18:gp2*diff_ramp            ;trapezoidal gradient pulse
p17:gp3*diff_ramp            ;trapezoidal gradient pulse
d2                            ;gradient stabilisation time
d9 BLKGRAMP                  ;tau
d11 UNBLKGRAMP              ;unblank gradient amplifier
p2:f1 ph2                    ;180 degree pulse
p17:gp1*diff_ramp            ;trapezoidal gradient pulse
p18:gp2*diff_ramp            ;trapezoidal gradient pulse
p17:gp3*diff_ramp            ;trapezoidal gradient pulse
d2                            ;gradient stabilisation time
d10 BLKGRAMP                ;tau

go=start ph31
100u wr #0 if #0 zd igrad diff_ramp
lo to start times td1 ;td1 = number of gradientsteps
if (I12) {
    1s rf #0 LOCKH_OFF        ;reset file pointer
} else {
    1s rf #0                  ;reset file pointer
}
lo to start times I1        ;I1 = Number of repetitions
exit

```

```
ph1=0 ;2
ph2=0 1 2 3
ph3=0
ph31=0 2
```

PGSTE Pulse Program diff_ste.gp

A.2.2

```
;diff_ste.gp
;2D stimulated echo sequence
;new version using gp syntax 14.12.99 KLZ
;now standard include files and lock commands only on I12 03.08.00 KLZ
;dummy gradient pulses included I13 05.10.00 KLZ

#include <Grad.incl>
#include <Avance.incl>
ze
10u
5m pl1:f1 ;set rf power level

if (I12) {
    start, d1 LOCKH_OFF
        d11 UNBLKGRAMP LOCKH_ON ;unblank gradient amplifier
} else {
    start, d1
        d11 UNBLKGRAMP
}

if (I3) {
    dummy,p17:gp1*diff_ramp ;trapezoidal gradient pulse
    p18:gp2*diff_ramp ;trapezoidal gradient pulse
    p17:gp3*diff_ramp ;trapezoidal gradient pulse
    d2 ;gradient stabilisation time
    d9 BLKGRAMP ;tau
    if (I11) {d11 UNBLKGRAMP ;unblank gradient amplifier
        p17:gp4 ;trapezoidal gradient pulse
        p19:gp5 ;trapezoidal gradient pulse
        p17:gp6 ;trapezoidal gradient pulse
        d2
```

```

    }
    if (I12) {
        d5 BLKGRAMP LOCKH_OFF ;long tau
        d11 UNBLKGRAMP LOCKH_ON ;unblank
    } else {
        d5 BLKGRAMP ;long tau
        d11 UNBLKGRAMP ;unblank
    }
    lo to dummy times I13
}

p1:f1 ph1 ;90 degree pulse
p17:gp1*diff_ramp ;trapezoidal gradient pulse
p18:gp2*diff_ramp ;trapezoidal gradient pulse
p17:gp3*diff_ramp ;trapezoidal gradient pulse
d2 ;gradient stabilisation time
d9 BLKGRAMP ;tau
p1:f1 ph2 ;90 degree pulse
if (I11) {
    d11 UNBLKGRAMP ;unblank gradient amplifier
    p17:gp4 ;trapezoidal gradient pulse
    p19:gp5 ;trapezoidal gradient pulse
    p17:gp6 ;trapezoidal gradient pulse
    d2
}
if (I12) {
    d5 BLKGRAMP LOCKH_OFF ;long tau
    d11 UNBLKGRAMP LOCKH_ON ;unblank gradient amplifier
} else {
    d5 BLKGRAMP ;long tau
    d11 UNBLKGRAMP ;unblank gradient amplifier
}

p1:f1 ph3 ;90 degree pulse
p17:gp1*diff_ramp ;trapezoidal gradient pulse
p18:gp2*diff_ramp ;trapezoidal gradient pulse
p17:gp3*diff_ramp ;trapezoidal gradient pulse
d2 ;gradient stabilisation time
d10 ph0 BLKGRAMP ;tau
go=start ph31

```

```

100u wr #0 if #0 zd igrad diff_ramp
lo to start times td1                ;td1 = number of gradientsteps
if (l12) {
    1s rf #0 LOCKH_OFF                ;reset file pointer
} else {
    1s rf #0                          ;reset file pointer
}
lo to start times l1                  ;l1 = Number of repetitions
exit

```

```

ph0=0
ph1=0 0 2 2 1 1 3 3 2 2 0 0 3 3 1 1
ph2=0 2 0 2 1 3 1 3 2 0 2 0 3 1 3 1
ph3=0 0 0 0 1 1 1 1 2 2 2 2 3 3 3 3
ph31=0 2 2 0 1 3 3 1 2 0 0 2 3 1 1 3

```

```

;diff_stebp.gp
;2D stimulated echo sequence
;new version using gp syntax 14.12.99 KLZ
;now standard include files and lock commands only on I12 03.08.00 KLZ
;dummy gradient pulses included I13 05.10.00 KLZ
;gradient pulse position symetrized 26.10.00 KLZ

#include <Grad.incl>
#include <Avance.incl>
ze
10u
5m p1:f1 ;set rf power level

if (I12) {
    start, d1 LOCKH_OFF
        d11 UNBLKGRAMP LOCKH_ON;unblank gradient amplifier
} else {
    start, d1
        d11 UNBLKGRAMP
}
if (I3) {
    dummy,d2 ;gradient stabilisation time
        d9 ;tau
        p17:gp1*diff_ramp ;trapezoidal gradient pulse
        p20:gp8*diff_ramp ;trapezoidal gradient pulse
        p17:gp9*diff_ramp ;trapezoidal gradient pulse
        d2 ;gradient stabilisation time
        d9 ;tau
        d2 ;gradient stabilisation time
        d9 ;tau
        p17:gp10*diff_ramp;trapezoidal gradient pulse
        p20:gp11*diff_ramp;trapezoidal gradient pulse
        p17:gp12*diff_ramp;trapezoidal gradient pulse
        d2 ;gradient stabilisation time
        d9 BLKGRAMP ;tau

```

```

if (I11) {
    d11 UNBLKGRAMP      ;unblank gradient amplifier
    p17:gp4             trapezoidal gradient pulse
    p19:gp5             ;trapezoidal gradient pulse
    p17:gp6             ;trapezoidal gradient pulse
    d2

if (I12) {
    d5 BLKGRAMP LOCKH_OFF      ;long tau
    d11 UNBLKGRAMP LOCKH_ON   ;unblank
} else {
    d5 BLKGRAMP              ;long tau
    d11 UNBLKGRAMP          ;unblank gradient amplifier
}
}
lo to dummy times I13
}

p1:f1 ph1                ;90 degree pulse
d2                       ;gradient stabilisation time
d9                       ;tau
p17:gp7*diff_ramp        ;trapezoidal gradient pulse
p20:gp8*diff_ramp        ;trapezoidal gradient pulse
p17:gp9*diff_ramp        ;trapezoidal gradient pulse
d2                       ;gradient stabilisation time
d9                       ;tau
p2:f1 ph4
d2                       ;gradient stabilisation time
d9                       ;tau
p17:gp10*diff_ramp       ;trapezoidal gradient pulse
p20:gp11*diff_ramp       ;trapezoidal gradient pulse
p17:gp12*diff_ramp       ;trapezoidal gradient pulse
d2                       ;gradient stabilisation time
d9 BLKGRAMP              ;tau
p1:f1 ph2
if (I11) {d11 UNBLKGRAMP  ;unblank gradient amplifier
    p17:gp4             ;trapezoidal gradient pulse
    p19:gp5             ;trapezoidal gradient pulse
    p17:gp6             ;trapezoidal gradient pulse
    d2
if (I12) {

```

```

        d5 BLKGRAMP LOCKH_OFF      ;long tau
        d11 UNBLKGRAMP LOCKH_ON   ;unblank gradient
    } else {
        d5 BLKGRAMP                ;long tau
        d11 UNBLKGRAMP            ;unblank gradient amplifier
    }

    p1:f1 ph3    ;90 degree pulse
    d2                ;gradient stabilisation time
    d9                ;tau
    p17:gp7*diff_ramp ;trapezoidal gradient pulse
    p20:gp8*diff_ramp ;trapezoidal gradient pulse
    p17:gp9*diff_ramp ;trapezoidal gradient pulse
    d2                ;gradient stabilisation time
    d9                ;tau
    p2:f1 ph4
    d2                ;gradient stabilisation time
    d9                ;tau
    p17:gp10*diff_ramp ;trapezoidal gradient pulse
    p20:gp11*diff_ramp ;trapezoidal gradient pulse
    p17:gp12*diff_ramp ;trapezoidal gradient pulse
    d2                ;gradient stabilisation time
    d10 ph0 BLKGRAMP ;tau
    go=start ph31
    100u wr #0 if #0 zd igrad diff_ramp
    lo to start times td1                ;td1 = number of gradientsteps
    if (l12) {
        1s rf #0 LOCKH_OFF                ;reset file pointer
    } else {
        1s rf #0                            ;reset file pointer
    }
    lo to start times l1                ;l1 = Number of repetitions
    exit

    ph0=0
    ph1=0 0 2 2 1 1 3 3 2 2 0 0 3 3 1 1
    ph2=0 2 0 2 1 3 1 3 2 0 2 0 3 1 3 1
    ph3=0 0 0 0 1 1 1 1 2 2 2 2 3 3 3 3

```


ph4=0
ph31=0 2 2 0 1 3 3 1 2 0 0 2 3 1 1 3

Gradient Programs

A.3

In contrast to the older diffusion package, this version does not use the gradient rotation functionality of XWINNMR. Because of this, more compatibility with the high resolution spectroscopy standards are reached. The cag_par file is therefore fixed, see "**Gradient orientation matrix cag par**" on page 57. Nevertheless, **diff** creates this to ensure the contents of this file are correct.

As mentioned already in "**Pulse Programs**" on page 49, separate gradient programs are no longer used. The trapezoidal gradient shape is achieved by applying 3 shaped gradients, back to back, called ramp_up, on and ramp_down. This construct allows to change the gradient pulse length without changing the steepness of the ramp.

Gradient orientation matrix cag_par

A.3.1

1.0
1.0
1.0
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0

Appendix: Probeheads and Gradients

Duty Cycles for Diffusion Gradient Systems

B.1

Usually it is difficult to give a general duty cycle definition for a gradient system, or the practical use of such a definition would be difficult for the user. Therefore in this section a duty cycle definition suitable for diffusion experiments is given. Two numbers are important, the average power, P_{ave} , and the maximum current, I_{max} . The two are related by the on off ratio, $r_{on/off}$. All calculations are done assuming an experiment with 2 gradient pulses of duration D_{pulse} . The power is calculated in units of A^2 , the resistance is left out for simplification (assume $R = 1\Omega$):

$$P = I^2$$

$$P_{ave} = I^2 * r_{on/off}$$

$$r_{on/off} = 2 * D_{pulse} / D_{Repetition}$$

There is another important number for the gradient systems, the maximum pulse duration at a certain current, $D_{Pulse,max}(I)$. This is because the average power can only describe the long term behavior, while the gradient system can be burned during one long pulse:

$$D_{Pulse,max}(I) = D_{Pulse,max}(I_{max}) * I_{max}^2 / I^2$$

⇒ **Note: The maximum pulse length calculated by this formula must not be exceeded.**

Transformations of these formula:

1. Calculate the minimum repetition time for a given gradient pulse length and current:

$$D_{Repetition} \geq 2 * D_{pulse} * I^2 / P_{ave,max}$$

2. Calculate the maximum gradient pulse length for a give repetition time and a given current:

$$a) D_{Pulse,max} \leq 1/2 * D_{Repetition} * P_{ave,max} / I^2$$

$$b) D_{Pulse,max} \leq D_{Pulse,max}(I_{max}) * I_{max}^2 / I^2$$

⇒ **Note: Both formulae a) and b) have to be calculated and the smaller of the 2 results has to be taken.**

EXAMPLE:

1. Assuming the maximum allowed current and the maximum allowed pulse-length for a diff25 gradient system, we used the following minimum repetition time would result:

$$I = 40 \text{ A}$$

$$D_{\text{Pulse}} = 5 \text{ ms}$$

$$D_{\text{Repetition}} \geq 1000 \text{ ms}$$

2. Assuming the maximum repetition time and the gradient current are given, for a diff25 gradient system the following maximum gradient duration would result:

$$I = 20 \text{ A}$$

$$D_{\text{Repetition}} = 100 \text{ ms}$$

$$D_{\text{Pulse}} = 2 \text{ ms}$$

This result is due to part a) of formula 2.

3. Assuming the maximum repetition time and the gradient current are given, for a diff25 gradient system the following maximum gradient duration would result:

$$I = 20 \text{ A}$$

$$D_{\text{Repetition}} = 2000 \text{ ms}$$

$$D_{\text{Pulse}} = 20 \text{ ms}$$

This result is due to part b) of formula 2.

➡ **Note: A safe and easy procedure for this is as follows: Use only a gradient pulse length, which would allow for the maximum possible current, and a repetition time, which would allow for the maximum current with the maximum gradient pulse length. You then would only have to go beyond these limits if you have to consider the calculations above again.**

EXAMPLE: If you use the following limits for the example with the diff25, you will be always safe:

$$D_{\text{Repetition}} \geq 1000 \text{ ms}$$

$$D_{\text{Pulse}} \leq 5 \text{ ms}$$

Table B.1. Gradient Duty Cycle

Gradient System	I_{max} (A)	$P_{\text{ave,max}}$ (A ²)	$D_{\text{Pulse,max}}(I_{\text{max}})$ (ms)
diff25	40	16	5
diff30	40	16	5

The Diff25 probehead consists of a probehead body with exchangeable rf coils of different diameters and type, an actively shielded z gradient coil and a gradient coil security box.

Figure B.1. Diff25 probehead, rf inserts and gradient security box



The specifications are shown in the following table.

Table B.2. Diff25 Probehead and Gradient Specifications

Gradients	z
Gradient strength	24 G/cm/A
ID/OD	18/60 mm
Linearity +- 2.1% peak-peak	cylinder diameter 10 mm length 10 mm
Inductance	70 μ H
Resistance	=< 600 m Ω
Rise time, 0-40A, 120V	< 60 μ s
Cooling	water
Maximum current tested	40 A
Exchangeable rf coil types	saddle
Rf-coil diameters	5, 10 mm
Nucleus	1H and/or X

Table B.3. Diffusion Probeheads

H8233	PH MICDIF100WBSAT5/10H	100 WB
H7979	PH MICDIF200WB SAT5/10 H	200 WB
H7750	PH MICDIF300WB SAT5/10 H	300WB
H8029	PH MICDIF400WB SAT5/10 H	400 WB

Handling of the Diff25 Probehead:

➡ **Mounting the rf inserts on the probehead body must be made very carefully, because the inserts are very small and are made of glass. They can break during the exchange. The most important step is the removal of the gradient coil from the probehead body. The gradient must not be tilted, when it is taken off the probehead body!**

1. Removal of the gradient coils from the probehead body

- The gradient is plugged onto the probehead body and screwed down with a ring. Rotate the ring to unscrew the gradient coils.
- Put the probe, together with the gradient system, into the plexi rod, which is delivered with the probe.
- Pull the probe body carefully out of the plexi rod while keeping the gradient system fixed on the plexi rod. This way the gradient system cannot be tilted relative to the probe body. Take care that the water cooling tubes are not disturbed.
- After the probe body is completely out of the plexi rod the gradient system can be pulled out as well.

2. Exchange of rf inserts

- The saddle coil type inserts are fixed with two 3 mm screws. These must be unscrewed before the insert can be pulled off from the probehead body.
- After exchanging the insert make sure that you use the same non-magnetic screws to fix the insert.

3. Mounting of the gradient coils

- Use the procedure described in the removal, but in reverse order. Take care that the cooling tubes are not damaged.

4. Gradient impedance adaptation

- Set the dip switches at the front panel of the B-AFPA-40 amplifiers in order to match the load of the gradient coils as shown in the following table. Contact the Bruker imaging application group, when other gradient amplifiers are used.

Table B.4. B-AFPA-40 Dip Switch Setting

Gradient system	Gradient	C Dip Switch	R Dip Switch	C	R
Diff25	Z	0000 0001	0100 0000	0.22 nF	100 kΩ

5. Gradient security

- Connect the gradient security box between the imaging rack and the gradient coils as shown in the section **"Gradient Current and Cooling Connections" on page 67**.

6. Cooling of the gradients

Water cooling for the gradients is highly recommended. The temperature of the gradient system is displayed at the front panel of the BGU-II. The BGU-II switches the gradients off, when the temperature reaches 56°C.

- Connect the hoses for the gradient cooling as shown in section: **"Installation of the gradient blanking unit" on page 81**, and switch the cooling on.

Table B.5. Values for the gradient cooling

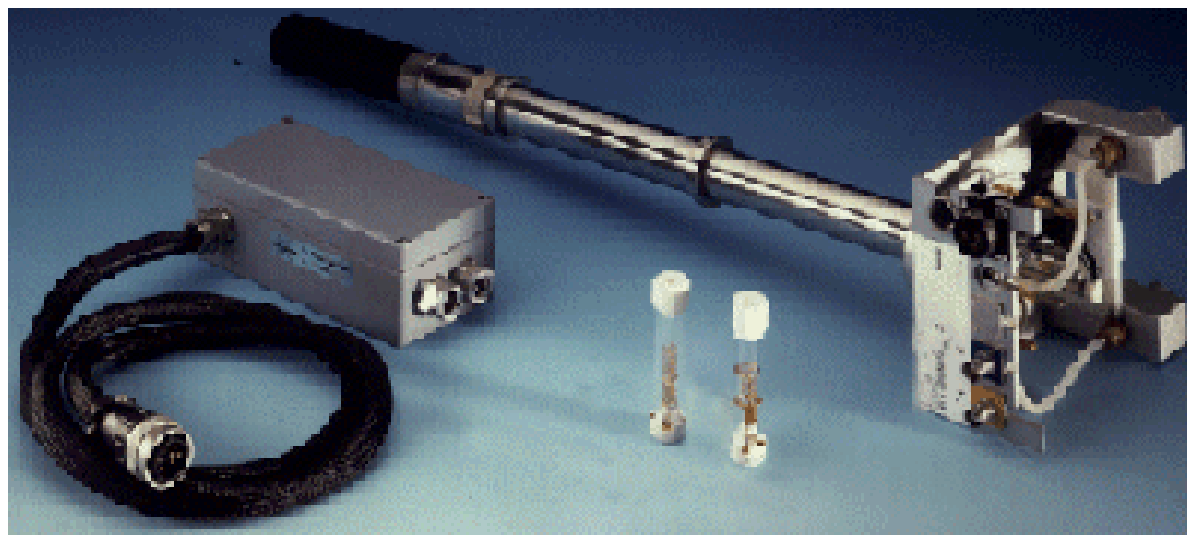
Water pressure	0.3 - 1.0 bar
Water temperature	10 - 20 °C

Note: When the gradients were previously used with water cooling, it is recommended that you remove the water in the gradient system with forced air, before the water hoses are disconnected from the gradient system and from the gradient security box.

7. Experiment start

- Connect the rf cable and start the experiments. Observe the gradient system temperature and modify the cooling conditions of the experiment, if necessary.

Figure B.2. Diff30 Probehead, rf Inserts and Gradient Security Box



The Diff30 probehead consists of a probehead body with exchangeable rf coils of different diameters and type, an actively shielded z gradient coil and a gradient coil security box.

The specifications are shown in the following table:

Table B.6. Diff30 Probehead and Gradient Specifications

Gradients	z
Gradient strength	30 G/cm/A
ID/OD	19/40 mm
Linearity +/- 2.5% peak-peak	15 mm diameter sphere
Inductance	=< 250 μ H
Resistance	=< 650 m Ω
Rise time, 0-40A, 120V	
Cooling	water
Maximum current tested	40 A
Exchangeable rf coil types	solenoid, saddle
Rf-coil diameters	2 - 10 mm
Nucleus	1H and/or X

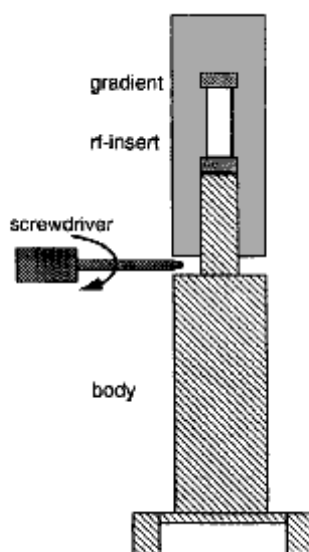
Handling of the Diff30 Probehead:

⇒ **Mounting the rf inserts on the probehead body must be made very carefully, because the inserts are very small and some of them are made of glass. They can break during the exchange. The most important step is the removal of the gradient coil from the probehead body. The gradient must not be tilted, when it is taken off the probehead body!**

1. Removal of the gradient coils from the probehead body

- When the gradients were previously used with water cooling, it is recommended that you remove the water in the gradient system with forced air, before disconnecting the gradient coil system from the probehead body.
- Plug the gradient onto the probehead body and screw it down with the fastening ring. Rotate the ring to disconnect the gradient coils.
- Carefully detach the gradient from the probehead body by using a screwdriver as shown in the figure below. Remove the gradients completely without tilting it, otherwise the glass on the rf insert will break!

Figure B.3. Gradient Coil Removal



2. Exchanging the rf inserts

- The saddle coil type inserts are not fixed with screws. Pull the insert off the probehead body. The solenoid coils are fixed with one or two screws, remove the screws and pull the insert off.
- Mount another insert on the probehead body. Fasten it in the same manner as in the case of the solenoid inserts using the screws.

- Make sure that there is no water droplets from the gradient cooling on the probehead body. Remove potential water drops with a tissue or a fan.

3. Mounting the gradient coils

- Push the gradient coil system carefully over the rf inserts. Do not tilt the gradients, or else the glass of the rf insert will break!

- Screw down the ring to tighten the gradients on the probehead body. The gradient system fixes the glass type rf inserts on the probehead body. **Do not use too much power to fix the ring.**

4. Gradient impedance adaptation

- Set the dip switches at the front panel of the B-AFPA-40 amplifiers in order to match the load of the gradient coils as shown in the following table. Contact the Bruker imaging application group, when other gradient amplifiers are used.

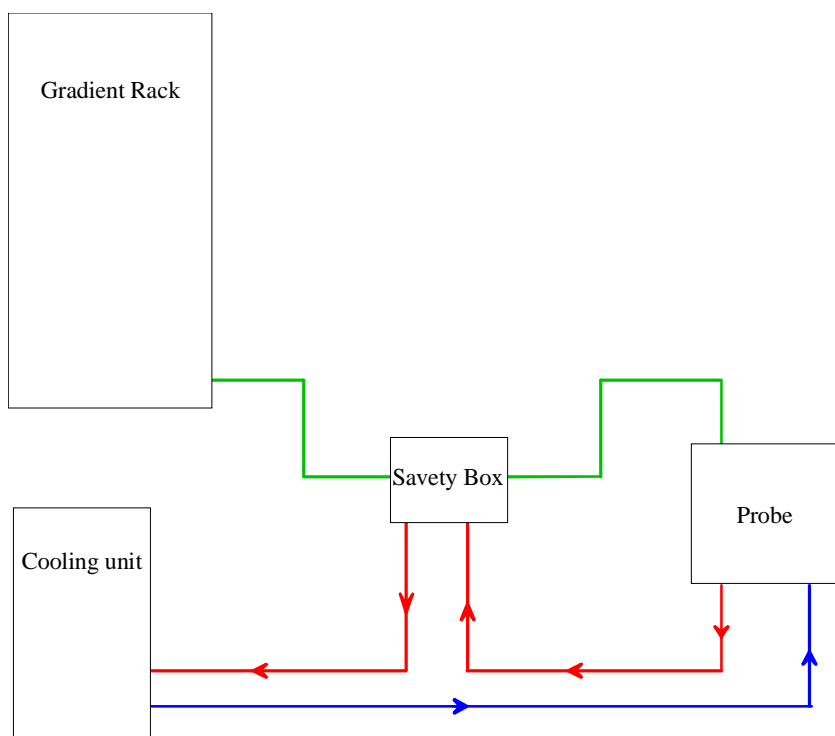
Table B.7. B-AFPA-40 Dip Switch Setting

Gradient system	Gradient	C Dip Switch	R Dip Switch	C	R
Diff30	Z	0000 0001	0100 0000	0.22 nF	100 k Ω

5. Gradient security

- Connect the gradient security box between the imaging rack and the gradient coils as shown below.

Figure B.4. Gradient Current and Cooling Connections



6. Gradient cooling

Water cooling for the gradients is highly recommended for all measurements. The temperature of the gradient system is displayed at the front panel of the BGU-II. The BGU-II switches the gradients off, when the temperature reaches 50°C.

- Connect the hoses for the gradient cooling as shown above and switch the cooling on.

➡ **There are two arrows on the cover of the gradient coil system. They indicate the water flow direction. Make sure, that the hoses are connected in the proper way, so that the cooling water is flowing in the correct direction!**

Table B.8. Values for the Gradient Cooling

Air pressure	ca. 1 bar
Water pressure	0.3 - 1.0 bar
Water temperature	10 - 20 °C

7. Starting the Experiment

- Connect the rf cable and start with the experiments. Observe the gradient system temperature and modify the cooling conditions of the experiment, if necessary.

Gradient Calibration values

B.4

Table B.9. Gradient calibration values for B-AFPA40

Gradient System	Gradient Calibration Constant G/mm
diff25	96
diff30	118

Table B.10. Useful values of diffusion coefficients^a

Sample	Temperatur [C]	D [$10^{-9}\text{m}^2/\text{s}$]
H ₂ O	20	2.031
H ₂ O	25	2.299
D ₂ O	25	1.872

a. Data by courtesy of Dr. M. Holz (Inst. of Phys. Chem., Uni Karlsruhe, FRG)

Figure 0.1. Temperature calibration curve for Ethylenglycol

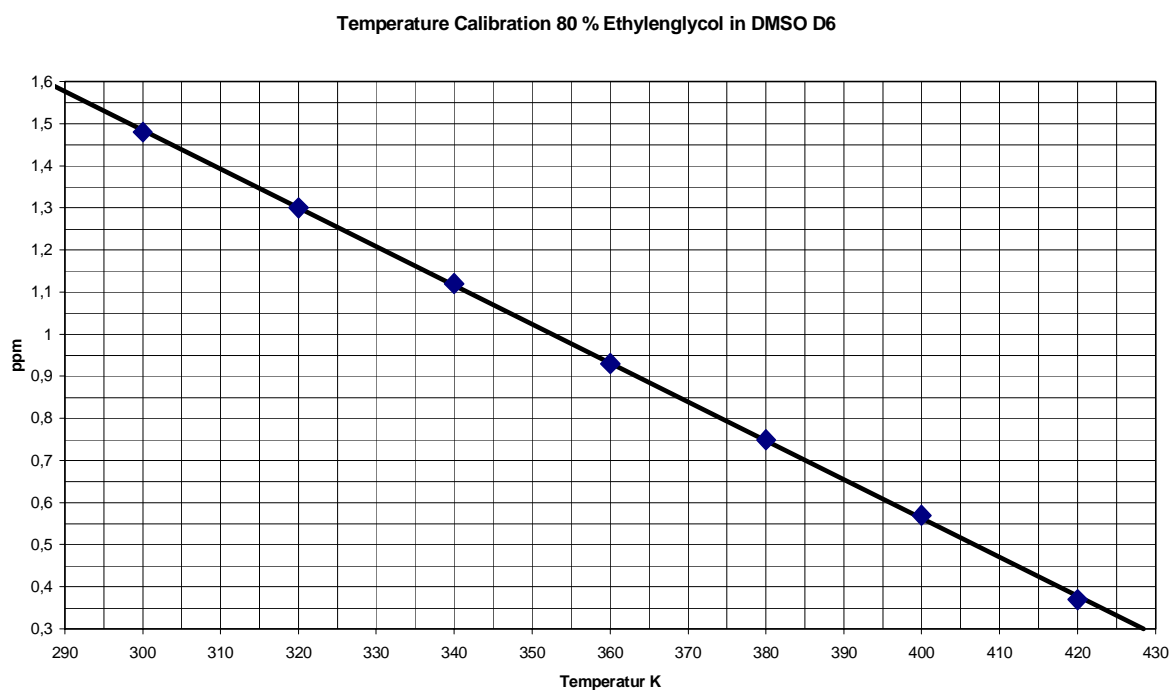
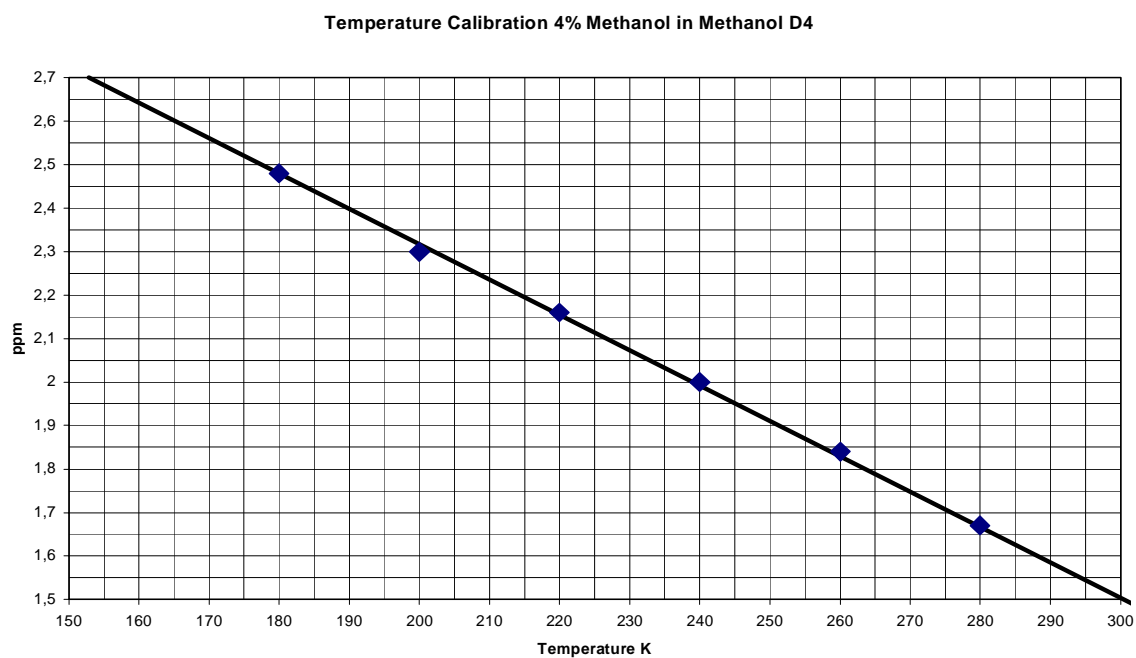


Figure 0.2. Temperature calibration curve for Methanol



Appendix: Imaging and Diffusion Hardware

The imaging accessory consists of the following basic hardware components: The gradient control unit (GCU), the preemphasis and B0 correction unit (BGU-II), three gradient amplifiers (B-AFPA-40) and a gradient water cooling unit. An additional amplifier for the B0 compensation and an amplifier blanking unit are available as options. These parts are identical for all imaging accessories and independent of the NMR frequency. Diffusion systems using z only probe may have only one gradient amplifier and will usually have a blanking unit.

Various probeheads with different 3 axis (xyz) and single axis (z) gradient systems, and a large number of single or double tuned rf-coils with different diameters ranging from approximately 2 mm up to 64 mm are available as well as additional accessories for VIVO experiments and special sample holders.

The following section describes the installation of the hardware.

The handling of the probeheads and gradients is described in the **"Appendix: Probeheads and Gradients" on page 59.**

Imaging hardware part list

C.1

Table C.1. Imaging Accessories

Option No.	Description
BH0354	D*X, COMPLETE MICROIMAG. W/O (NO) PROBE

Table C.2. Imaging Accessory Components

Part number	Description	Qty.
H002165	MICRO IMAGING ACC D.X BASIC NO PROBE	
H2546	AQX GCU BOARD	1
H5577	AQX BUS 5 CONNECTOR BOARD	1
HZ2969	CABLE FLK 64P40	1
W1206288	BAFPA40 FOR BGU2 GRASP	1

Table C.2. Imaging Accessory Components

Part number	Description	Qty.
W1206288	BAFPA40 FOR BGU2 GRASP	1
W1206288	BAFPA40 FOR BGU2 GRASP	1
H5380	BGU2 GRADIENT UNIT XYZ	1
H5517	CABLE COAX RG316 40CM SMB/SMB	2
H5496	CABLE SET MICRO IMAG BGU2	1
Z31247	MAN BGU2 GRAD.UNIT REMOTE CON.	1
H9015	MAN MICROIMAG AVANCE	1
H8087	SINGLE CABINET M AUFSATZ O FAN	1
H10960	PRINTER DESK JET 660C	1y
O001009	GRADIENT WATER COOLING UNIT	1
H5496	CABLE SET MICRO IMAG BGU2	1
HZ2691	CABLE KOAX 150 BNC/TWIN-BNC/SF	3
P1567	CABLE KOAX 2000MM SFT/SFT	3
HZ2690	CABLE KOAX 2P2000 BNC/TWIN	3
HZ0409	CABLE KOAX 2P3000 TWIN BNC/BNC	1
HZ3202	CABLE KOAX 2P5000 BNC/TWIN	1
HZ0969	CABLE RD 6P8700 MIRI AMPL PH	1
HZ04055	CABLE RD 9P4500 BU/BU	1
H5509	CABLE RD 25P2000 SFT/BU MINI-D	3
H5510	CABLE RD 50P8000 BU/BU	1
3000	CABLE RD ST NETZ SCHUKOZU.3122	1
19457	ST ADAP 9P SFT/SFT	1
14110	PNK SCHLAUCH PA HART SW 10X8	20
3033	ST BU 2 G KURZSCHLUSS JUMPER	30
CALIBRATION SAMPLES DEPENDENT ON THE PROBE TYPE		
H3695	GRAD CALIBRATION SAMPLE MICRO	1
H9018	GRAD CALIBRATION SAMPLE MINI	1

Table C.3. Diffusion Accessories

Option No.	Description
BH0380	Diffusion access.cplt. with probe 1H/12 10mm

Table C.4. Diffusion Accessory Components

Part Number	Description	Qty.
H002166	DIFFUSION ACC D.X BASIC NO PROBE	
H2546	AQX GCU BOARD	1
W1206288	BAFPA40 FOR BGU2 GRASP	1
W1208357	BGB40 BLANKING 1 CHANNEL	1
H5530	BGU2 GRADIENT UNIT Z FOR GRASP	1
H5577	AQX BUS 5 CONNECTOR BOARD	1
HZ2969	CABLE FLK 64P40	1
H5517	CABLE COAX RG316 40CM SMB/SMB	2
H5780	CABLE SET DIFFUSION ACC BGU2	1
O001009	GRADIENT WATER COOLING UNIT	1
Z31247	BGU2 GRAD.UNIT REMOTE CON	1
H9153	MAN DIFFUSION ACCESSORY AVANCE	1
H5780	CABLE SET DIFFUSION ACC BGU2	1
HZ03858	CABLE 1P100 ADAPTER SMA/SMB	1
P1567	CABLE KOAX 2000MM SFT/SFT	1
HZ2690	KOAX 2P2000 BNC/TWIN CABLE	1
HZ04096	CABLE KOAX 2P3000 TWIN BNC/BNC	1
HZ04062	CABLE KOAX 2P400 TCU/T3-RCU	1
HZ3202	CABLE KOAX 2P5000 BNC/TWIN	1
HZ1603	CABLE RD 2P7000 GRASP AMPL PH	1
HZ0548	CABLE RD 9P 10000	1
HZ0549	CABLE RD 9P 3500	1
HZ03856	KABELBAUM L HOLD/HOMOSPOIL INV	1

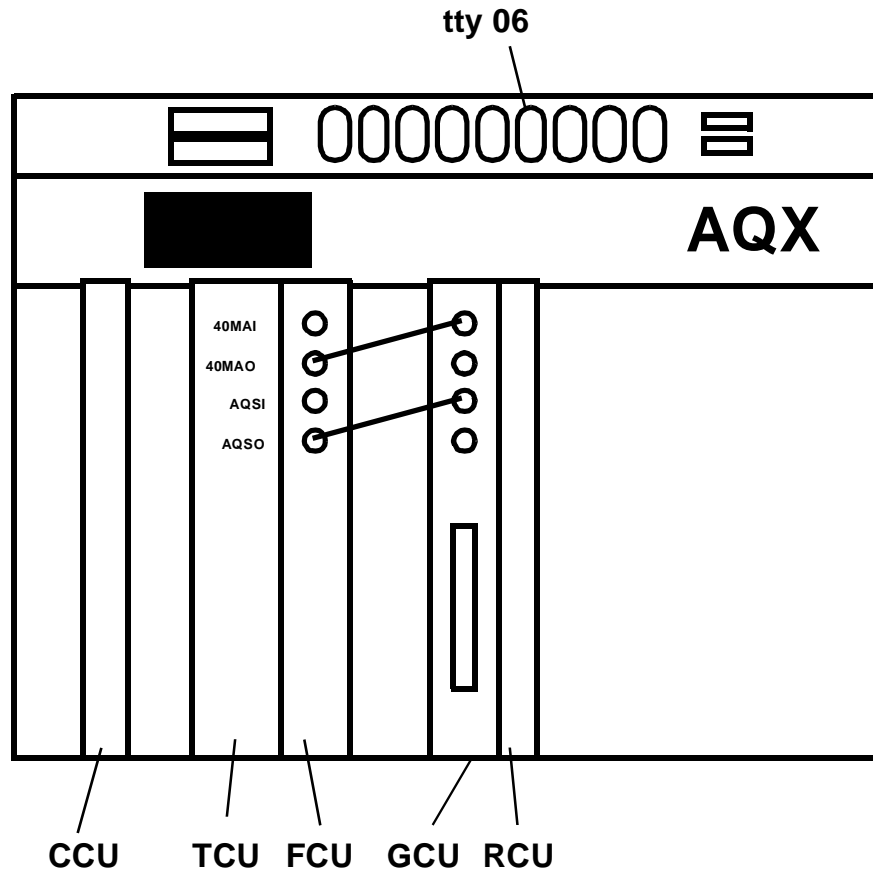
Table C.4. Diffusion Accessory Components

Part Number	Description	Qty.
H5509	CABLE RD 25P2000 SFT/BU MINI-D	1
H5510	CABLE RD 50P8000 BU/BU	1
3000	CABLE RD ST NETZ SCHUKOZU.3122	2
14110	PNK SCHLAUCH PA HART SW 10X8	20
3033	ST BU 2 G KURZSCHLUSS JUMPER	30

Table C.5. Diffusion Probeheads diff25

H8233	PH MICDIF100WBSAT5/10H	100 WB
H7979	PH MICDIF200WB SAT5/10 H	200 WB
H7750	PH MICDIF300WB SAT5/10 H	300WB
H8029	PH MICDIF400WB SAT5/10 H	400 WB

Figure C.1. Installation of the GCU



The GCU is mounted in a slot between the frequency control units (FCU's) and the receiver control unit (RCU) as shown in the figure.

If there is no free slot available between the FCU and RCU, move the RCU to another position using the following steps:

- Mount the AQX Bus Connector board P/N H5577 and the cable P/N HZ2969 on the motherboard.
- Move the bus terminator resistors from the old to the new connector board.
- Take care, that the jumpers are set on the motherboard at the positions of the empty slots.

When the GCU is the last board next to the RCU, the 40 MHz lines 40MAO and AQSO must end in 50 Ohms on the GCU board. Therefore, set the jumpers W1 and W2 on the GCU board and remove the jumpers W2 and W3 on the neighboring FCU board.

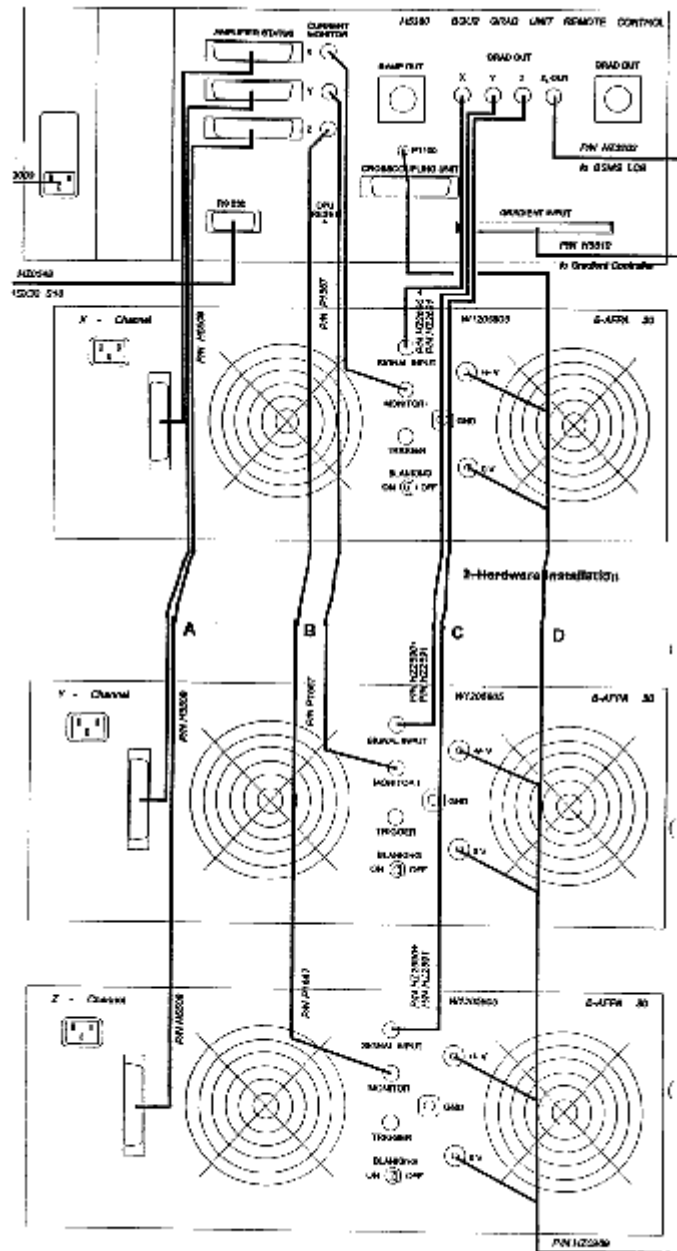
- Insert the GCU board into the free slot of the AQX rack and remove the jumpers on the motherboard.

- Connect the 40 MHz coax cable P/N H5517 between the 40MAO on the FCU board and the 40MAI on the GCU board.
- Connect the coax cable (P/N H5517) between the AQSO on the FCU board and the AQSI on the GCU board.

Wiring of the Imaging Rack

C.4

Figure C.2. Imaging Rack

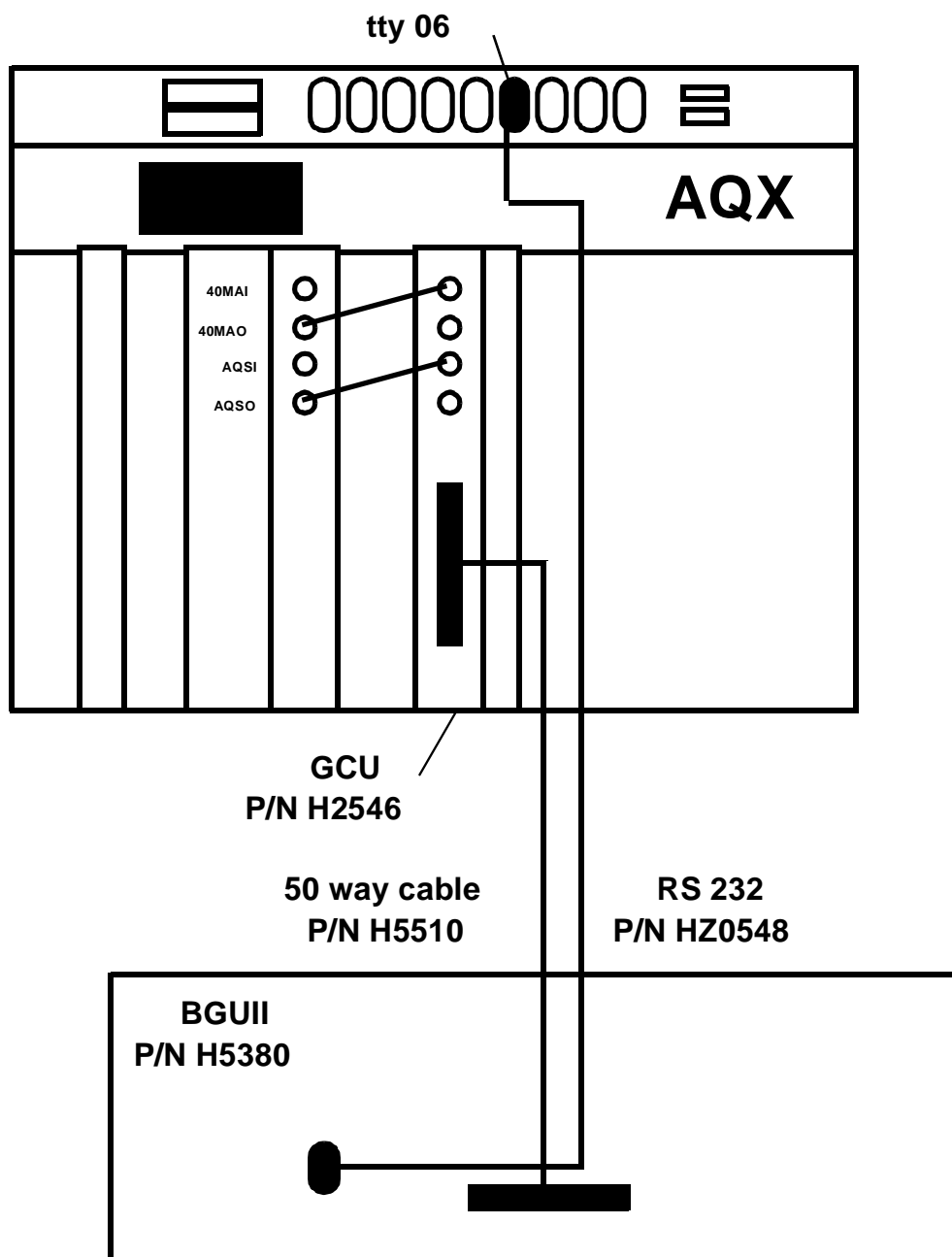


The imaging rack contains the BGU-II and the gradient amplifiers. Check to see if the wiring is correct between the BGU-II and the B-AFPA-40 amplifiers as shown in figure B.3.

Connections Between the GCU and Imaging Rack

C.5

Figure C.3. The AQX and BGU-II



- Connect the RS232 cable P/N HZ0548 between the BGU-II and a free TTY input on the SIB board in the AQX rack. TTY06 is reserved for the BGU-II.

- Connect the 50 way cable P/N H5510 between the GCU and the BGU-II.

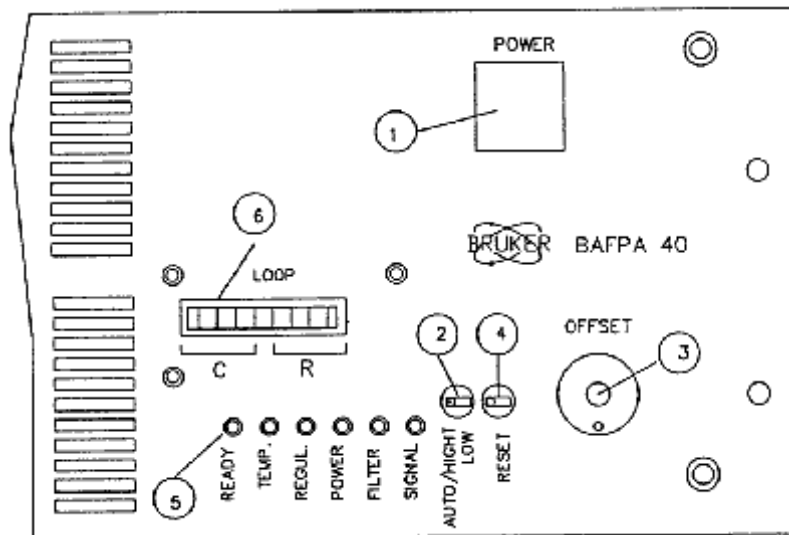
Installation of the Gradient Amplifiers B-AFPA-40

C.6

A number of different gradient coils are used with the imaging accessory. The coils differ in inductance and resistance. In order to optimize the gradient pulse shape and the gradient switching speed, the B-AFPA-40 amplifiers provide the adoption of the load by adjusting RC-combinations on a feedback circuit.

The values for R and C are set by dip switches on the front panel of the amplifiers, marked as label (6) in the figure below.

Figure C.4. B-AFPA-40 Front Panel with Dip Switches (6)



The following table shows the recommended dip switch settings for some gradient coils delivered by Bruker. The values in the table have been determined in the Bruker laboratories, and can be modified by the adjustment procedure, described in the following section. Contact the Bruker imaging application group, when other gradients, not included in the table, are used.

Table C.6. B-AFPA-40 Dip Switch Setting

Gradient system	Gradient	C Dip Switch	R Dip Switch	C	R
Diff25	Z	0000 0001	0100 0000	0.22 nF	100 kΩ
Diff30	Z	0000 0001	0100 0000	0.22 nF	100 kΩ
Micro5	X	0000 1000	0001 0000	1.5 nF	20 kΩ

Table C.6. B-AFPA-40 Dip Switch Setting

Gradient system	Gradient	C Dip Switch	R Dip Switch	C	R
Micro5	Y	0000 0100	0001 0000	1.0 nF	20 k Ω
Micro5	Z	0000 1000	0000 1000	1.5 nF	15 k Ω
Micro2.5	X	0000 1100	0001 0000	2.5 nF	20 k Ω
Micro2.5	Y	0000 1100	0001 0000	2.5 nF	20 k Ω
Micro2.5	Z	0000 1100	0001 0000	2.5 nF	20 k Ω
WBSHold	X	0011 0000	0011 0000	6.9 nF	14.3 k Ω
WBSHold	Y	0001 0100	0000 1000	3.2 nF	15 k Ω
WBSHold	Z	0000 1000	0010 0000	1.5 nF	50 k Ω
Mini0.5	X	0001 1100	0000 1000	4.7 nF	15 k Ω
Mini0.5	Y	0001 0000	0000 1000	2.2 nF	15 k Ω
Mini0.5	Z	0001 0000	0001 0000	2.2 nF	20 k Ω
Mini0.36	X	0000 0001	0100 0000	0.22 nF	100 k Ω
Mini0.36	Y	0000 0001	0100 0000	0.22 nF	100 k Ω
Mini0.36	Z	0001 0000	0001 0000	2.2 nF	20 k Ω

Adjustment Procedure:

⇒ **Do not set all dip switches to zero while the B-AFPA-40 is switched on! Select at least one switch for R and one for C. Otherwise, the gradients and/or the amplifiers can be damaged.**

- Install the probehead for imaging or diffusion applications as described in the **"Imaging hardware part list" on page 71**
- Set the B-AFPA-40 dip switches for the imaging probehead (see the previous table).
- Run the au program **imgrad** in a 1D dataset.
- Check that all gains of the preemphasis parameters are set to zero.
- Start the acquisition with **gs**.
- Observe the gradient shapes on the oscilloscope.

- Modify the dip switches until the best shape is reached (see figure B.5 below).

The best pulse rise behavior is shown in the following figure (b). Incorrect adjustments can cause an overshoot of the pulse (a) or too slow gradient rise times (c).

Figure C.5. Gradient pulse adjustment

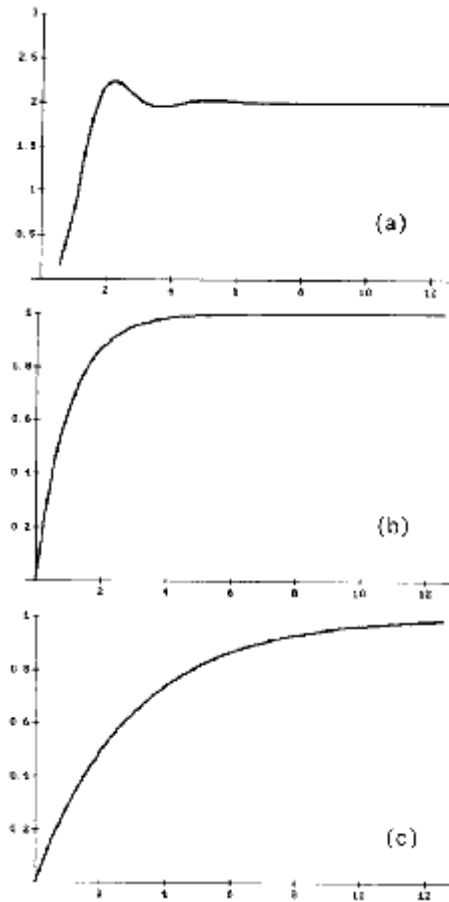
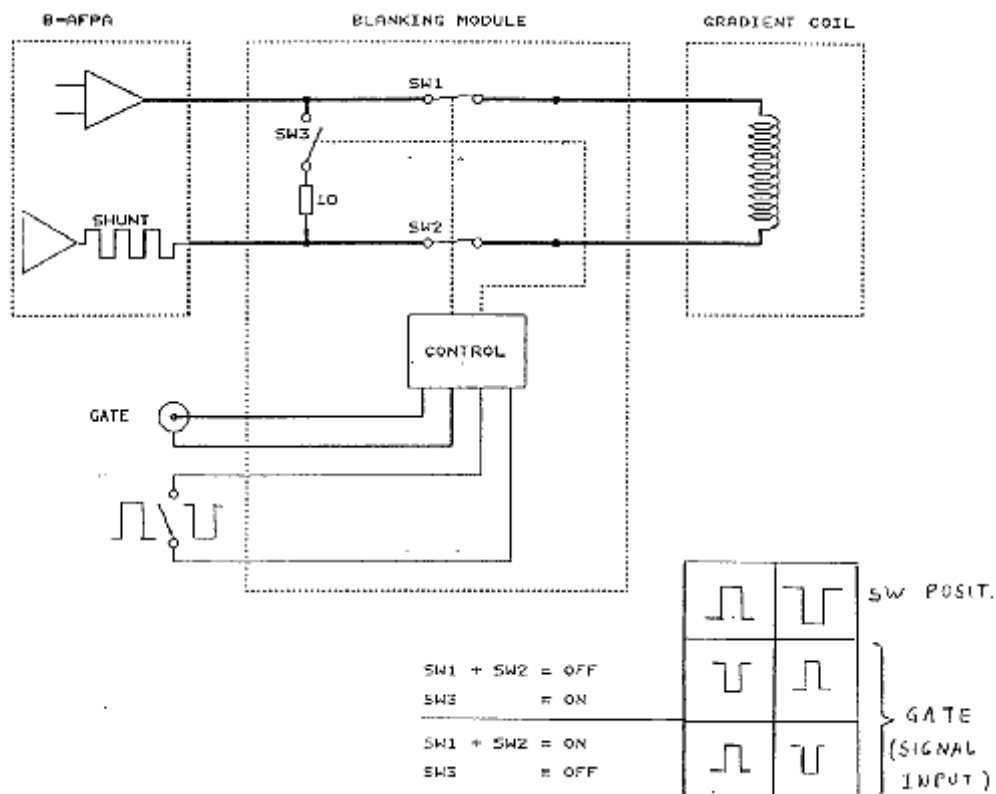


Figure C.6. Gradient Blanking Unit BGB3x40A (W1207793)



The gradient blanking unit is used to disconnect the gradient amplifiers from the gradient coils during the data acquisition e.g. in diffusion experiments with very strong gradient coils. The blanking unit exists with one or three channels. A hardware manual is available using the part number W1207893/01.

- Connect the cables from the B-AFPA-40 current amplifiers to the input of the blanking unit.
- Connect the cable from the gradient coil to the output of the blanking unit.
- Connect the "Blanking Control" cables to the corresponding BNC sockets "Signal Input", see "Blanking Pulses on AVANCE" on page 82.
- Set the selector for positive or negative logic of the gating pulse.

How to use the BGB Blanking Unit.

The blanking unit is controlled by blanking pulses, generated from the spectrometer console during the pulse program. The blanking pulses are created by setting special bits in the NMR control word 0 as shown in the following table.

Table C.7. *Blanking Pulses on AVANCE*

Backpanel I	Pin
Blanking X gradient: c32 or setNMR0 32	C
Blanking Y gradient: c33 or setNMR0 33	H
Blanking Z gradient: c34 or setNMR0 34	M

⇒ **Note:** *On AVANCE instruments all NMR controls are active low. Therefore the blanking pulse selector switch at the blanking unit must be set to active low.*

⇒ **Note:** *The older pulse programs must be modified in order to make use of the blanking feature. The new version of the programs contain these modifications.*

A number of macros are defined in the file **Grad_Blank.incl** for a comfortable handling of the blanking features. The file is listed in the following.

```

;Grad_Blank.incl - file included to handle the gradient blanking unit
#define BLKGRAMP_ALL setnmr0^32 setnmr0^33 setnmr0^34
#define UNBLKGRAMP_ALL setnmr0|32 setnmr0|33 setnmr0|34
#define BLKGRAMP_X setnmr0^32
#define BLKGRAMP_Y setnmr0^33
#define BLKGRAMP_Z setnmr0^34
#define UNBLKGRAMP_X setnmr0|32
#define UNBLKGRAMP_Y setnmr0|33
#define UNBLKGRAMP_Z setnmr0|34

```

An example of an imaging pulse program, where the blanking unit is connected and where no gradient blanking must be applied, is given below. The modifications of the pulse program are the lines which include: `#include <Grad_Blank.incl>` and `UNBLKGRAMP_ALL`.

```

; imgess for Gradient-Echo-Single-Slice
#include <Grad_Blank.incl>
      1s ze           ; zero data NBL blocks
      10u UNBLKGRAMP_ALL
10    d31:ngrad      ; slice gradient on
      d2 fq1:f1      ; gradient stabilization delay

```

p3:sp0 ph1 ; slice selective pulse
and so on...

An example of a diffusion pulse program, where the blanking unit is connected and where gradient blanking is applied, is given in **"PGSE Pulse Program diff se.gp" on page 49**. The modifications of the pulse program are the lines which include: #include <Grad_Blank.incl>, BLKGRAMP_ALL, UNBLKGRAMP_Z and BLKGRAMP_Z.

⇒ **Note: The following will work for the AMX spectrometers. This style is not used on AVANCE spectrometers.**

It is recommended that you use **bit0** from the NMR control word 2 for the blanking of the gradients. The signal is available on pin JJ at the Backpanel connector BPI.

- Connect pin JJ from BPI at the spectrometer console with the one or three signal input BNC connectors at the blanking unit.

- Set the selector switch for positive/negative logic at the front panel of the blanking unit to negative logic (switch down).

- Modify the pulse program as shown in the following example:

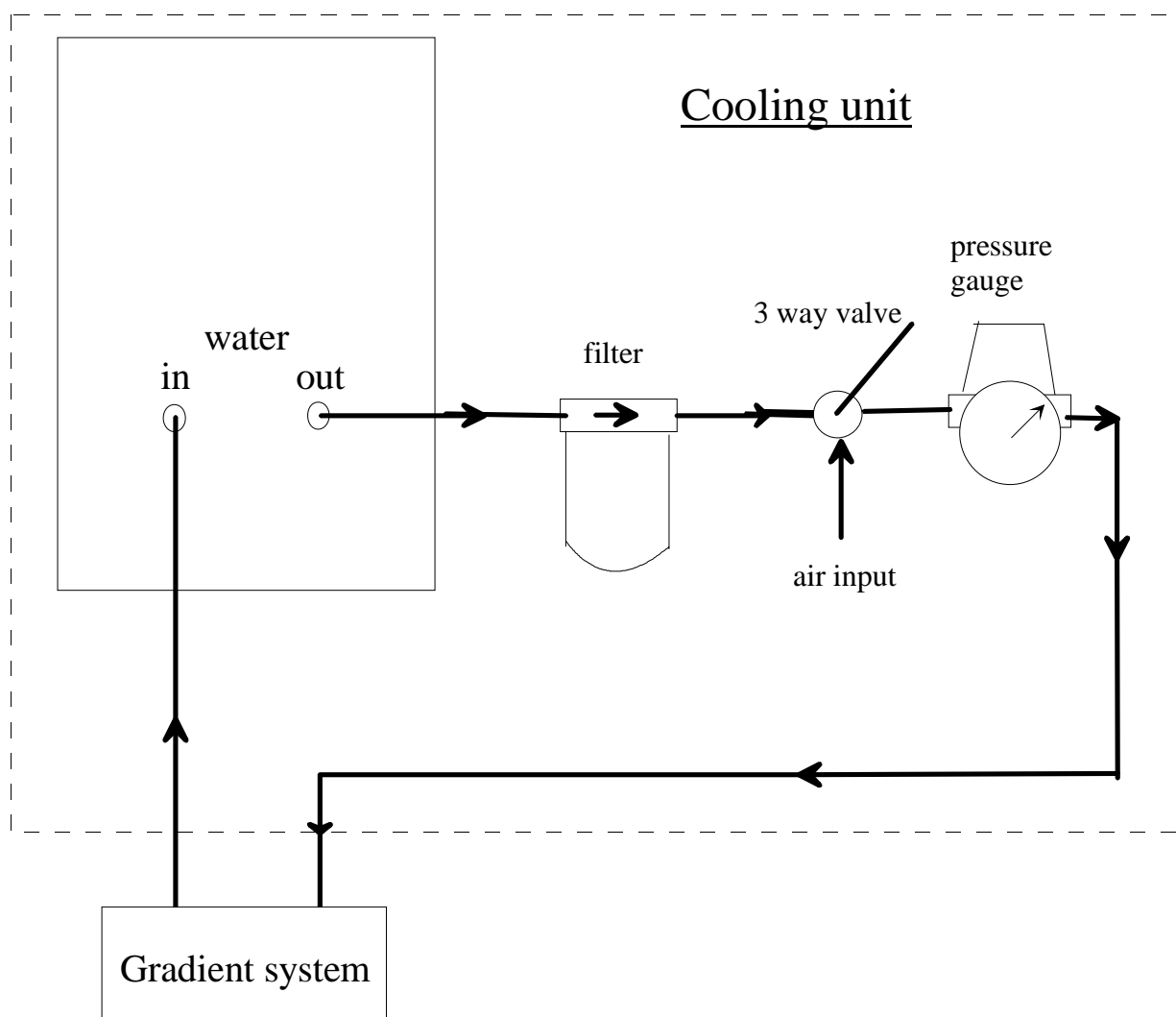
```
;file: imblank
;version 221096 DGR
;pulse sequence to show the use of the BGB3x40A gradient blanking unit.
;use bit0 from nmrctl word 2 on pin JJ from BPI

#define BLKGRAMP_ALL setf2 ^0
#define UNBLKGRAMP_ALL setf2 |0

ze
1s BLKGRAMP_ALL ; blank all gradients
10 d1 ;relaxation delay
5m UNBLKGRAMP_ALL unblank all gradients
10u:ngrad ;dephasing read gradient on
3m ;dephasing delay
10u:ngrad ;gradient off
1m
1m ph3 BLKGRAMP_ALL ;blank all gradients
go=10 ph0
```


All the new gradient coil systems are water cooled for an improved and safer performance. The cooling is accomplished through a closed loop water circuit, driven by a water pump. The temperature of the water output is adjustable. A water filter and a pressure reduction device are added after the output of the water pump housing. A three way valve is added, where one input can be used to press forced air into the cooling circuit. This is used in order to remove the water from the gradient coil, when the gradient system has to be disconnected from the experimental setup. The connections of the individual parts are shown in the following drawing.

Figure C.8. Gradient Cooling Accessory



- ➡ **Note: The water pressure must not exceed 1 bar, normal operation pressure is 0.3 to 0.5 bar.**
- ➡ **Check the water flow from time to time by observing the pressure at the pressure reduction device. When the pressure is zero no water is flowing.**

Another way to check the water flow is simply to disconnect the water hose for a short moment at the output of the gradient system.

The water flow can be blocked, when the filter element is polluted e.g. by algae, which may grow in the water after a while.

The growing of algae can be stopped by adding a water conditioner (Art.9025.1 ROTH), available under part number "69663".

A package of 10 filter elements for replacement is available under part number "H9531".

The recommended concentration is 0.6 ml water conditioner for 4 l of water (0.15 ml/l or 1.5 ml/10l or 1.8 ml/HAAKE-UWK45)

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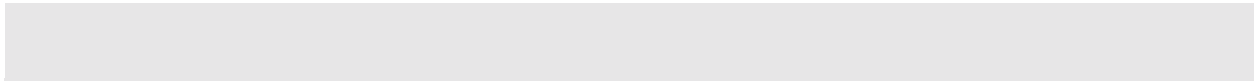
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