topspin

BRUKER

Bruker BioSpin

Shapetool

TopSpin 2.1

Version 2.1.2

NMR Spectroscopy

think forward

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NMR

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Contents

Chapter 1

Introduction

1.1 About this manual

This manual describes the Topspin Shapetool, the program which allows you to create, analyze and manipulate RF- and Gradient Shapes. Shapetool can be used in two different ways:

- The command stdisp opens a graphical interface that allows to view shapes, and to interactively create and manipulate shapes using various parameters.
- The command st <parameters> allows to generate or manipulate shapes from the TOPSPIN command line. The main purpose of this syntax is that the command can easily be included in AU programs to produce shapes automatically.

Chapter 2 of this manual describes the graphical interface, whereas the remaining chapters describe the usage of the st command.

1.2 About Shapes

Shapetool allows you to create, analyze or manipulate two types of shapes, RF shapes and gradients. An RF shape consists of phase and amplitude values, whereas a gradient only consists of amplitude values. Once created or changed, a shape is stored in a text file in JCAMP-DX format suitable to be displayed with stdisp or executed by TOPSPIN acquisition commands.

For RF shapes all files are read from or stored in the directory:

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

For gradients all files are read from or stored in the directory:

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

1.3 Conventions

Font conventions

stdisp - commands to be entered on the command line are underlined

Analysis - commands to be clicked are in times bold italic

Alignment - Dialog window fields are in times bold

`intrng` - filenames are in courier

name - any name which is not a filename is in times italic

Chapter 2

Interactive Shapetool

To start the interactive Shapetool interface:

+ Click ***Spectrometer*** ' ***Shape Tool***

or enter stdisp on the command line.

The Shape Tool window will appear (see Fig. 2.1.). This consists of a toolbar, a command line and a split pane with a data section at the right and a parameter section at the left.

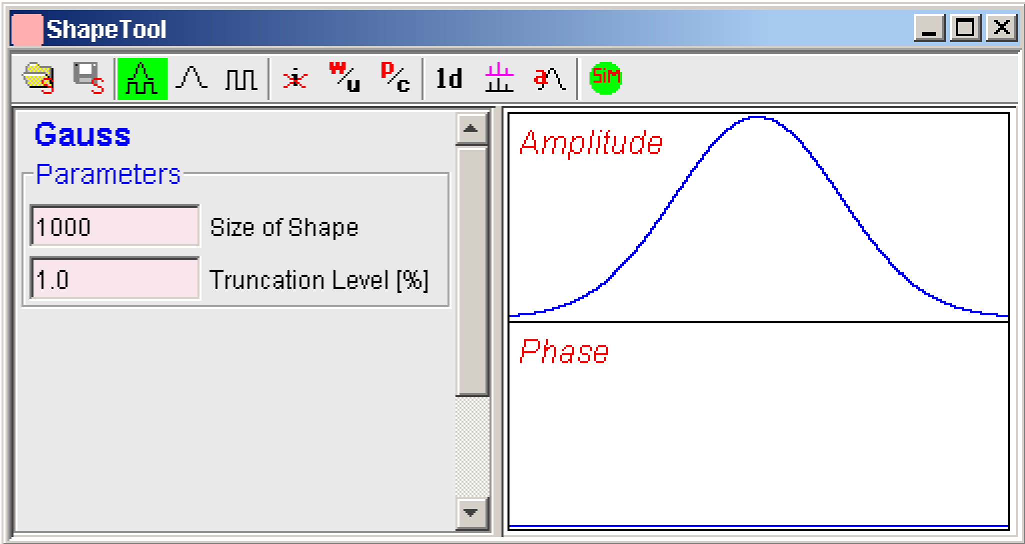
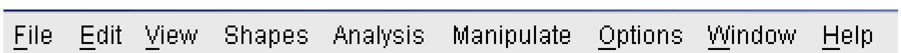


Figure 2.1

By default, a 1000 point Gauss shape is displayed with Truncation level 1.0.

The TOPSPIN menu is changed showing the additional ***Shapes*** and ***Manipulate*** menus and the adjusted ***File***, ***Analysis*** and ***Options*** menus.

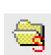


Note that all functions of the interactive Shape Tool can also be performed non-interactively with the TOPSPIN command st. This command must entered with the appropriate arguments on the command line while the associated dataset is displayed and selected. For a description of the st command see:

+ ***Help*** ' ***Application manuals*** ' ***Shape Tool***

2.1 Opening a Shape/Gradient

To open an existing shape/gradient, click the button:

 Open a shape or gradient.

select ***Shape*** or ***Gradient***, select a file from the appearing file list and click ***OK***. The selected shape/gradient will appear in the data section.

2.2 Using Shape Tool Display Options

The Shape Tool toolbar offers the following display options:

 Display amplitude and phase.

 Display amplitude only.

 Display phase only.

 Toggle cursor information on/off. Cursor information consists of the point number and amplitude/phase value.

 Wrap/unwrap phase (actual phase/phase modulo 360°).

 Toggle between polar and cartesian coordinates.

2.3 Saving a Shape/Gradient as a 1D dataset

To save the current shape/gradient stored under a procno of the associated dataset, click:

 Save shape/gradient as a 1D dataset.

2.4 Superimposing Multiple Shapes/Gradients

Several shapes/gradient can be displayed superimposed using the following buttons:

 Add the currently displayed shape to multiple display.

 Switch to multiple display mode. This shows all ’added’ shapes/gradients superimposed.

2.5 Saving a Shape/Gradient

To save a shape/gradient, click the button:

 Save a Shape or Gradient or a fraction of it.

and select ***Save Shape***, ***Save Gradient*** or ***Save Fraction***. A dialog window appears where you can enter a (File)*Name*, *Title*, *Flip Angle* and the *Type of Rotation*.

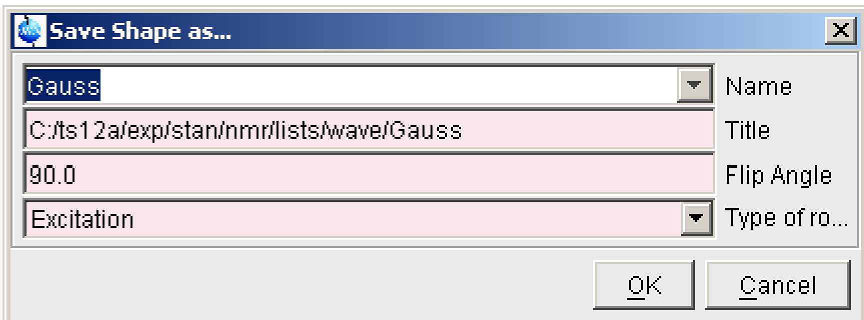
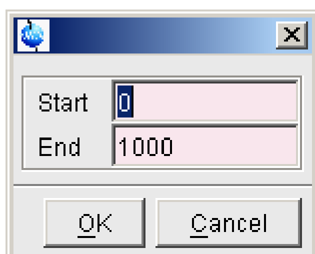


Figure 2.2

If you save a fraction of a shape or gradient, the above dialog is preceded by the following dialog:



Enter the *Start* and *End* point and click ***OK***.

2.6 Generating Shapes/Gradients

The Shape Tool allows you to generate RF and gradients shapes. Various

Basic, *Classical* or *Adiabatic* shapes can be created from the ***Shapes*** menu. Additionally *Solids*, *Imaging* and *Decoupling* shapes are available.

How to Generate a Gauss shape

To generate a Gauss shape:

+ Click ***Shapes*** ’ ***Classical Shapes*** ’ ***Gauss***

A Gaussian shaped curve will appear in the data section. The parameter section shows the two parameters that can be set for a Gauss:

Size of Shape: the number of shape data points

Truncation level: the minimum amplitude at the edge of the shape

If you change these parameters, the displayed shape will automatically be updated. To save the shape, click , enter a *Name*, e.g. *mygauss*, *Title*, *Flip Angle* and the *Type of Rotation* (see chapter 2.5) and click ***OK***.

How to Generate a ShapFour shape

To generate an RF shape that is defined by Fourier coefficients:

+ Click ***Shapes*** ’ ***Classical Shapes*** ’ ***ShapFour***

The following dialog box will appear:

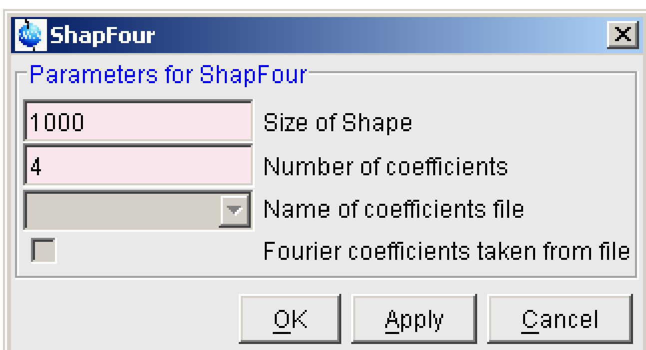


Figure 2.3

Here you can enter the *Size of Shape* and the *Number of coefficients*. Clicking ***OK*** or ***Apply*** will open a further dialog box (see Fig. 2.4), where you can enter the required coefficients. A ShapFour shape is defined by two coefficients arrays a[0,1,...] and b[1,...]. Note that the element a[0] is listed separately.

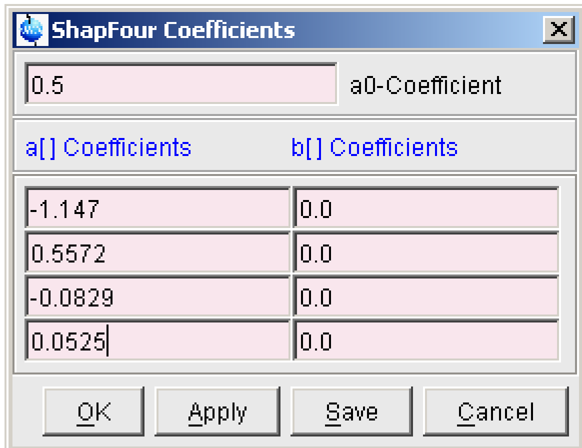


Figure 2.4

Here, you can enter the desired coefficients and then click:

Save to store the coefficients for later usage. You will be prompted for a filename which will be stored as:

<*user-home*>/.topspin-<hostname>/shapetool

Apply to display the shape while keeping the dialog box open for possible further changes.

OK to display the shape and close the dialog box.

With the coefficients above you have created a *Rsnob* shape.

To save it:

Click  , enter a *Name*, e.g. *myrsnob*, *Title*, *Flip Angle* and the *Type of Rotation* (see chapter 2.5) and click ***OK***.

2.7 Analysing Shapes

The Shape Tool interface offers several functions to analyse shapes. Most of these functions are only meaningful for RF shapes.

To access these functions:

+ Click ***Analysis***

in the TOPSPIN menu bar. This will open the pull-down menu shown in Fig. 2.5.

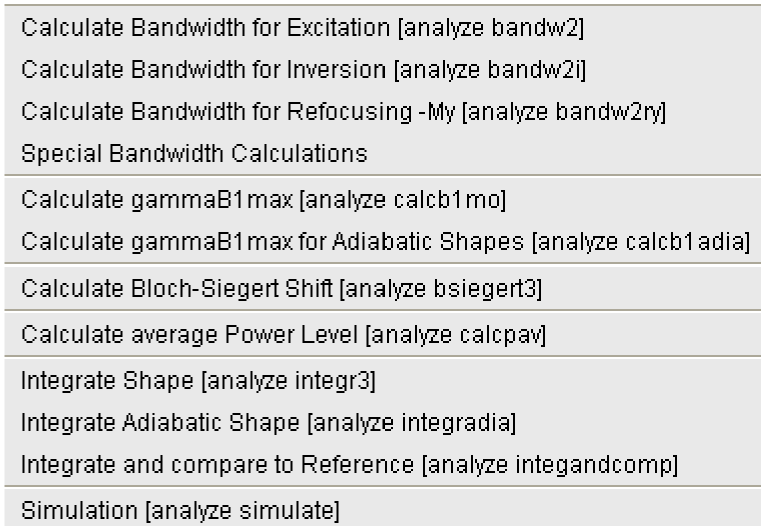


Figure 2.5

From here, you can start the analysis functions discussed below.

How to Calculate the Bandwidth for Excitation

To calculate the excitation band width factor $\Delta\omega * \Delta T$:

+ click ***Analysis*** → ***Calculate Bandwidth for Excitation*** [analyze bandw2]

For the excitation band width, the $\sqrt{(Mx^2 + My^2)}$ magnetization is used.

Fig. 2.6 shows the resulting parameter section for a Gauss shape.

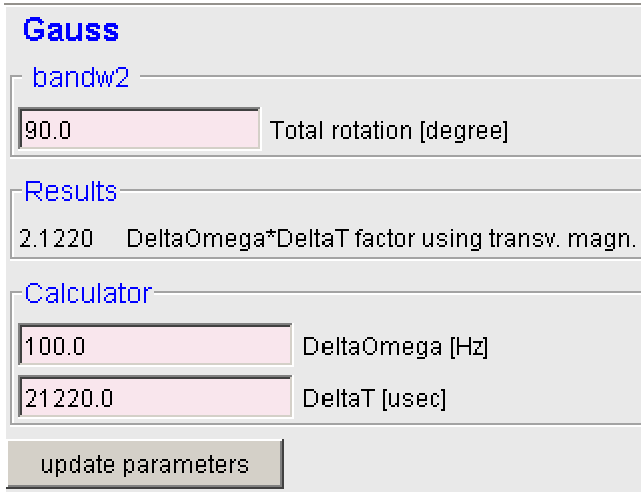


Figure 2.6

As you can see, for a 90° Gaussian shape the bandwidth factor is 2.122.

The bandwidth factor is the product of the width of excitation (DeltaOmega) and the pulse length (DeltaT).

This means a pulse length of 21220 μsec gives a band width ($\Delta\omega$) of 100.0 Hz. The bandwidth is the excitation width at the 3 dB point, i.e. the point where the magnetization has dropped to 70.8 %.

When you change one of the parameters in the parameter section, the others are automatically adjusted. Clicking the ***Update Parameters*** button will store the length of the shaped pulse (DeltaT) to the associated dataset parameter (default P11).

How to Calculate the Bandwidth for Inversion

To calculate the inversion band width factor $\Delta\omega * \Delta T$:

+ Click ***Analysis*** ’ ***Calculate Bandwidth for Inversion*** [analyze bandw2i]

For the inversion band width, the Mz magnetization is used.

How to Calculate Bandwidth for Refocusing

To calculate the refocusing band width factor $\Delta\omega * \Delta T$:

+ Click ***Analysis* ’ *Calculate Bandwidth for Refocusing*** [analyze bandw2ry]

For the refocusing band width, the -My magnetization is used.

How to Calculate Special Bandwidths

Further routines for the evaluation of various magnetization components are available under the menu item ***Special Bandwidth Calculations***.

How to Calculate the Maximum RF Field Strength for Classical Pulses

To calculate the RF field strength for classical pulses:

+ Click ***Analysis* ’ *Calculate gammaB1max*** [analyze calcb1mo]

Fig. 2.7 shows the resulting parameter section for a Gauss shape.

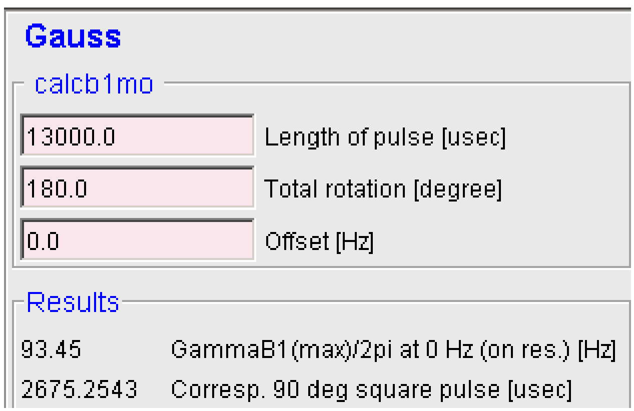


Figure 2.7

The result consists the field strength (γB1max/2π) and the corresponding 90° square pulse length. To obtain this result, the integral of the shaped pulse is compared to that of a square pulse of same length, with the latter being normalized to 1.

The maximum power is:

$$\gamma B1(max)/2\pi = \gamma B1/2\pi \text{ (square pulse of same length) / integral ratio}$$

where

$\gamma B1/2\pi$ (square pulse of same length) = (1 / pulse length * (360°/ flip angle))

How to Calculate the Maximum RF Field Strength for Adiabatic Pulses

To calculate the RF field strength for adiabatic pulses:

+ Click ***Analysis*** ' ***Calculate gammaB1max for Ad. shapes*** [analyze calcb1adia]

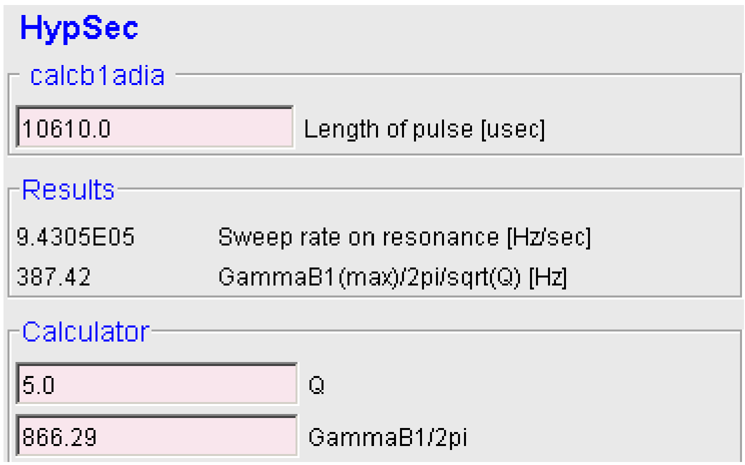


Figure 2.8

Fig. 2.8 shows the resulting parameter section for a *HypSec* shape.

The result $\gamma B1(max)/2\pi / \sqrt{(Q)}$ is calculated from the on-resonance sweep rate.

Q(t) is the quality or adiabaticity factor during the shape. After entering the appropriate value for Q with respect to the middle of the shape, the value for $\gamma B1(max)/2\pi$ is obtained. As a rule of thumb Q is set to 5 for inversion pulses. However, for decoupling pulses, Q should be set between 2 and 3 to allow a lower decoupling power.

How to Calculate the Bloch-Siegert Shift

To calculate the phase difference due to the Bloch-Siegert shift:

+ Click ***Analysis*** ' ***Calculate Block-Siegert Shift*** [analyze bsiegert3]

Input parameters are the length of the shaped pulse in μs, γB1(max) in Hz and the offset of a theoretical signal relative to the frequency of the RF-pulse in Hz. The result consists of the phase difference due to Bloch-Siegert shift in Degree and the corresponding frequency shift in Hz.

How to Calculate the Average Power Level

To calculate the average power:

+ Click ***Analysis*** ’ ***Calculate average Power Level*** [analyze calcpav]

The result is the percentage of the average power of a square pulse of the same length.

How to Integrate Classical Shapes

To calculate the power level required for a classical shaped pulse:

+ Click ***Analysis*** ’ ***Integrate Shape*** [analyze integr3]

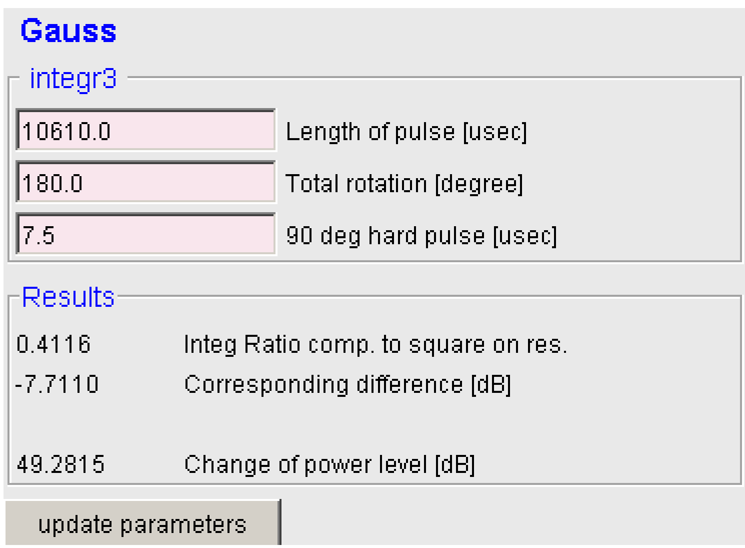


Figure 2.9

Fig. 2.9 shows the parameter section where you can enter the length of the soft pulse, the flip angle and the length of the 90° hard pulse. Soft pulse and hard pulse length are initialized with the values of the corresponding parameters of the associated dataset. If these values are zero or if no dataset is associated, default values are taken, a 10000 μs soft pulse and 50 μs hard pulse.

The result for a Gaussian shape with 1000 points and 1% truncation is shown. The *Integral ratio* and the *Corresponding difference* in dB are calculated from shape amplitude and phase, assuming equal pulse length and flip angle for soft and hard pulse. The *Change in power level,* however, is calculated from the specified pulse lengths and rotation.

Clicking the ***Update Parameters*** button saves the length of the shaped pulse and the change in required power level to the corresponding parameters of the associated dataset. Note that the latter is the sum of the shown *Change of power level* and the current hard pulse power level (e.g. PL1).

How to Integrate Adiabatic Shapes

To calculate the power level required for an adiabatic shaped pulse:

+ Click ***Analysis*** ’ ***Integrate Adiabatic Shape*** [analyze integradia]

The change of power level is calculated from the length of the corresponding 90° pulse and the length of the hard pulse.

Clicking the ***Update Parameters*** button saves the length of the shaped pulse and the required power level to the corresponding parameters of the associated dataset.

How to Start Simulation

To evaluate the shape behaviour, you can start the TOPSPIN NMRSIM routine:

+ Click ***Analysis*** ’ ***Simulation*** [analyze simulate]

This allows you for example, to view the excitation profile, or, for adiabatic pulses, check the adiabaticity.

2.8 Manipulating Shapes

Shapes can be manipulated in various ways. Most of these functions are only meaningful for RF shapes.

Frequency Encoding

To perform a phase (and amplitude) modulation encoding one or more offset frequencies:

+ Click ***Manipulate* ’ *Phase modulation acc. to Offset Freq.*** [manipul offs]

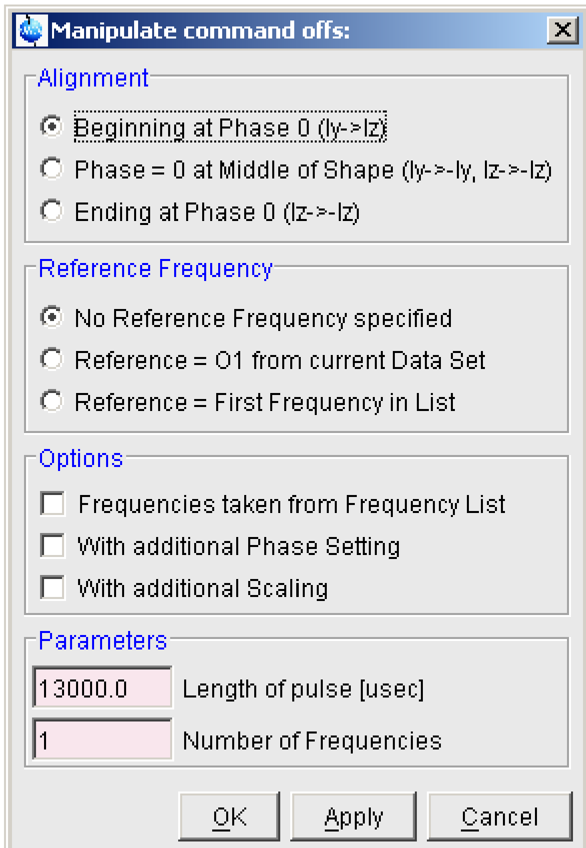


Figure 2.10

A dialog box will appear (see Fig. 2.10) where you can set the required parameters.

The **Alignment** radio buttons allow you to define the position of phase 0; the beginning, middle or end of the shape.

The **Reference Frequency** radio buttons allow you to choose whether the reference frequency:

- is not used
- is set to O1 of the associated dataset
- is set to the first entry of the frequency list. The ***Option*** *’Frequencies taken from Frequency’ List* will automatically be checked.

The **Options** check boxes allow you to set:

- *Frequencies taken from a Frequency list*. The **Parameter** *Name of Frequency List* will automatically appear. Frequency lists can be set up from the TOPSPIN interface with the command ***edlist*** or, interactively, by clicking the  button.
- *With additional Phase Setting*
- *With additional Scaling (0-100%)*: the relative amplitude for each excitation region. The overall amplitude will be divided by the number of frequencies. For example, for 3 frequencies with equal scaling factors, each frequency will contribute 33%.

The **Parameters** fields:

- The *Length of Pulse*
- The *Number of Frequencies* or, when the **Option** *Frequencies taken from a Frequency list* is checked, *Name of the Frequency List*.

Clicking ***Apply*** or ***OK*** will open a new dialog box where the selected parameters are shown.

If no reference frequency is used, the values entered as frequencies have to be difference frequencies.

How to Calculate a Shape from an Excitation Region

A shape can be modulated according to specific regions in a spectrum. To do that, take the following steps:

1. Switch to the associated dataset.
2. Determine the integral regions interactively.
3. Switch back to the Shape Tool interface.
4. Click ***Manipulate*** ’ ***Calc. Shape from excitation Region*** [manipul

region].

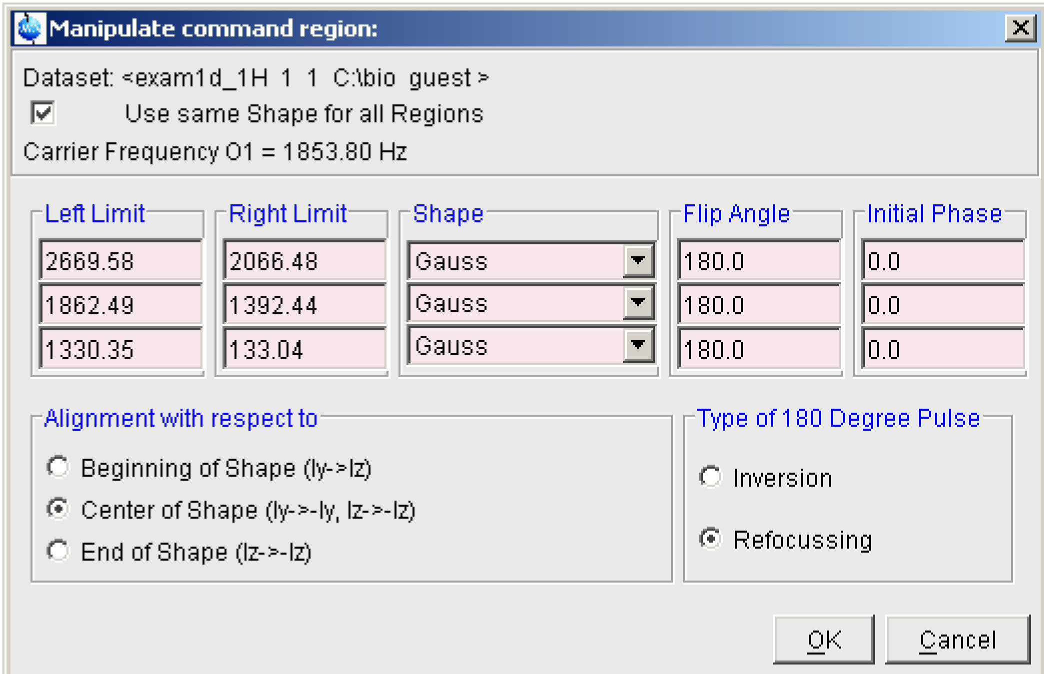


Figure 2.11

If the `intrng` file does not exist, you will be prompted for the number of regions and the carrier frequency O1. In that case, the fields **Left Limit** and **Right Limit** are empty. Note that overlapping regions are not allowed.

In Fig. 2.11 the default values for Flip Angle, Initial Phase, Alignment and Type of 180 Degree Pulse are shown. Depending on the application these settings have to be modified accordingly.

You can use the same shape for each region of all different shapes. In the latter case, the check box *Use same Shape for all Regions* must be unchecked.

How to Add Shapes

To add multiple shapes:

+ Click ***Manipulate*** ' ***Add Shapes*** [manipul addshapes]

A dialog box will appear where you can select up to 10 shapes from the available shape files.

A minimum of two shapes must be selected. Note that the selected shapes replace the current shape.

The file size of each shape is shown in the *Size* column. Note that if the sizes differ, the desired alignment must be selected.

For each added shape, you can specify a scaling factor between 0 and 100% in the *Scaling* column.

The *Scale resulting shape* radio button allows you to rescale the resulting shape:

- to 100%
- to the average of the individual scaling factors

The alignment of the added shapes may be with respect to the ***Beginning of Shape***, the ***Center of Shape*** or the ***End of Shape***. If ***Arbitrary Alignment*** is selected, the start point must be entered for each shape in the *Start* column. In other cases the *Start* entry is deactivated.

How to Perform Single Sine Modulation

To perform an amplitude modulation such that the pulse excites at two symmetric sidebands (+/- offset) with opposite phase:

+ Click ***Manipulate*** ' ***Single Sine Modulation*** [manipul sinm2]

and set *Offset frequency* to be relative to the carrier frequency.

How to Perform Single Cosine Modulation

To perform an amplitude modulation such that the pulse excites at two symmetric sidebands (+/- offset) with the same phase:

+ Click ***Manipulate*** ' ***Single Cosine Modulation*** [manipul cosm2]

and set *Offset frequency* to be relative to the carrier frequency.

How to Create a Shape with a Linear Sweep

To create a shape with a phase modulation according to a linear frequency sweep:

+ Click ***Manipulate*** ' ***Linear Sweep*** [manipul sweep]

and set the pulse length and sweep width.Then specify the Q factor to obtain the value for γB1(max)/2π. Q is the quality or adiabaticity factor which, as a rule of thumb Q is set to 5 for inversion pulses and between 2 and 3 for decoupling pulses.

How to Create a Shape with Const. Adiabaticity Sweep

To create a shape with a phase modulation according to a constant adiabaticity sweep:

+ ***Manipulate*** ' ***Const. Adiabaticity Sweep*** ' [manipul caSweep]

and set the pulse length and sweep width.Then specify the Q factor to obtain the value for γB1(max)/2π. Q is the quality or adiabaticity factor which, as a rule of thumb Q is set to 5 for inversion pulses and between 2 and 3 for decoupling pulses.

How to Calculate a Shape with Amplitude to the Power x

To create a shape with an amplitude to the power of a specified exponent:

+ Click ***Manipulate*** ' ***Power of Amplitude*** [manipul power]

and enter the desired exponent.

How to Scale the Amplitude

To scale the amplitude of a shape to a specified percentage:

+ Click ***Manipulate*** ' ***Scale Amplitude*** [manipul scale]

and enter the desired scaling factor (percentage).

How to Add Constant Phase

To add a constant phase to the shape:

+ Click ***Manipulate*** ' ***Add constant Phase*** [manipul addphase]

and enter the phase to be added.

How to Perform Time Reversal

To time reverse a shape:

+ Click ***Manipulate*** ' ***Time Reversal*** [manipul trev]

How to Expand Shape

To expand a shape according to a specified phase list (supercycle):

+ Click ***Manipulate*** ’ ***Expand Shape*** [manipul expand]

and selected a phase cycle. The following standard phase cycles are offered:

mlev4, mlev16, p5(150 deg), p5(330 deg), p5m4, p5m16, p9, **p9m16, p5p9**

For example, **mlev4** has the following supercycle: 0 0 180 180

In addition, the entry **YourOwn** appears, which allows you to define your own phase cycles. These can be saved for later usage. The specified file must have the extension `.expand`. It is stored in the directory:

`<user-home>/.topspin-<hostname>/shapetool`

2.9 Setting Shape Tool Options

When the Shape Tool window is selected, the upper three entries in the TOPSPIN ***Options*** menu concern the Shape Tool.

How to Change the Relation between Shape Tool and TOPSPIN parameters

To define the relation between Shape Tool parameters and TOPSPIN acquisition parameters:

+ Click ***Options*** ’ ***Define Parameter Table***

A dialog box will appear with a list box for each parameter (see Fig. 2.12).

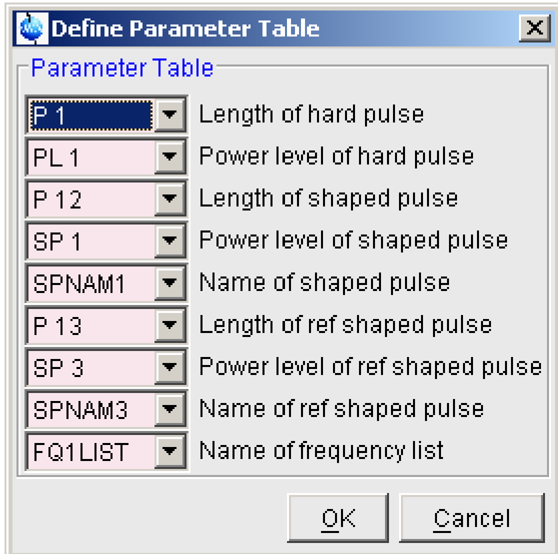


Figure 2.12

Make any changes you want and click ***OK***. The acquisition parameters of the associated dataset can be set/viewed from the TOPSPIN interface by clicking ***AcquPars*** or entering eda.

How to Change the Shape Storage Directory

To change the shape storage directory:

+ Click ***Options*** ' ***Set path to Shape Directory***

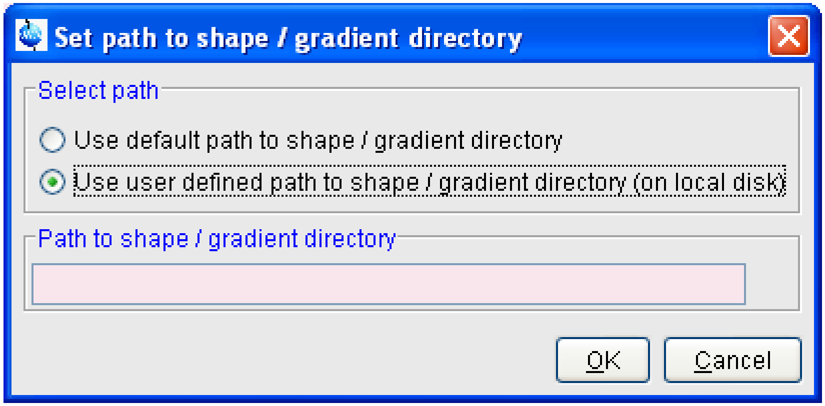


Figure 2.13

In the appearing dialog box, you can select the default path or select and specify a different path. Note that a shape base directory must be `shape` and a gradient base directory must be `gp`. Opening and saving shapes/gradients will access the specified directory.

How to select the Associated Dataset

To set the dataset associated to the Shape Tool interface:

+ Click ***Options*** ’ ***Select associated dataset***

A list of open datasets will appear. Select the desired dataset and click ***OK***.

2.10 Examples of using the Shape Tool

Example 1: Create a Shaped Pulse for Multiple Solvent Suppr. using WET

To create a shaped pulse:

1. Acquire a reference 1D spectrum.
2. Click  to switch to frequency list mode.
   - Select the frequency list type and enter the list name *freqlist*. If you get a message that this list already exists, click ***Overwrite*** to over-write the existing list or click ***Cancel*** and specify a new name.

- Move the vertical cursor line to the desired frequencies.
- Left-click the desired frequencies.
- Click  to save the frequency list and return.

3. To view the frequency list:

\+ Enter edlist f1 freqlist and click ***OK***.

It should look, for example, like this:

```
O 300.19
3759.74
8775.99
8712.96
```

Click ***Cancel*** to close the list.

4. Enter stdisp to start the Shape Tool interface.

5. Proceed as follows:

\+ Click  , choose ***Open Shape***, select *Sinc1.1000* and click ***OK***

or

\+ Click ***Shapes*** ' ***Classical Shapes*** ' ***Sinc*** and enter:

Size of shape: 1000

Number of cycles: 1

in the parameter section.

6. Click ***Manipulate*** ' ***Phase modulation acc. to Offset Freq.*** [manipul offs]

In the appearing dialog box (see Fig. 2.14):

- Select **Ending at Phase 0**.
- Select **Reference = O1 from current Data Set**.
- Check the box **Frequencies taken from Frequency List**.
- Set **Length of Pulse** to **10000**.
- Set **Name of Frequency List** to **freqlist** or the name you specified in step 2.
- Click **OK**.

7. Check the frequency values in the appearing dialog box (see Fig.

2.15) and click ***OK***.

8. Click  and click ***Save Shape***, enter a *Name* and *Title*, set the *Flip Angle* to *90°* and the *Type of Rotation* to *excitation*

Now you have created a shape that can be used in a WET experiment.

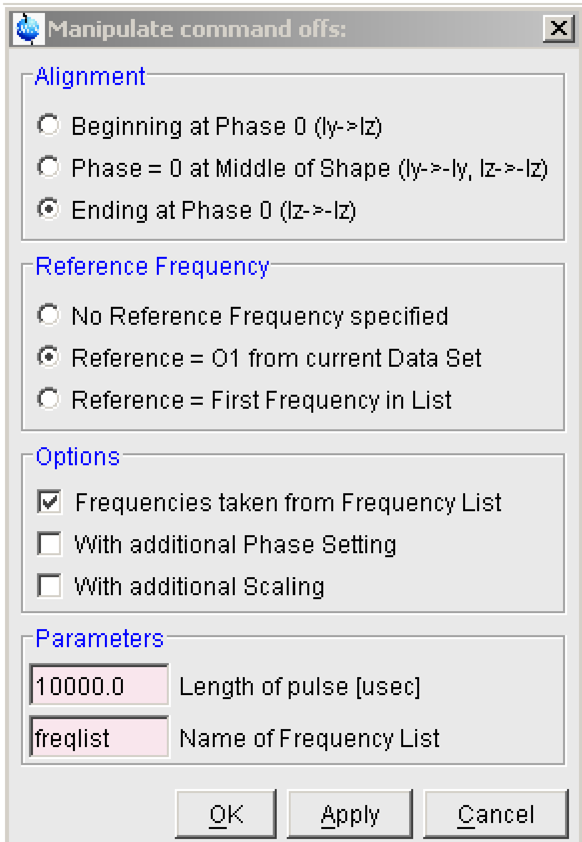


Figure 2.14

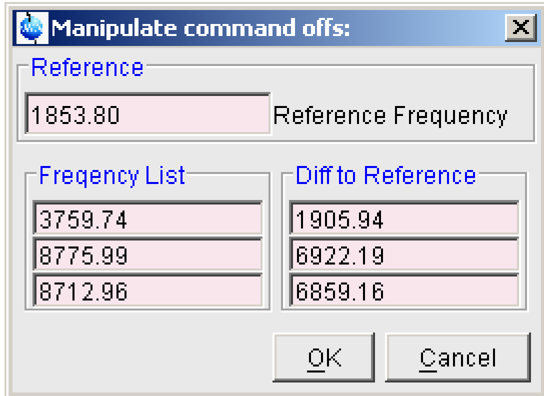


Figure 2.15

Example 2: Two-step Procedure to a Selective Experiment

1. Read/acquire a 1D reference spectrum.
2. Determine the width of the region to be excited. Let's assume this is 40 Hz.
3. Create a new dataset.
4. Read the pulse program *selgpse.*
5. Enter ased and set all acquisition parameters for *selgpse*, except for the shaped pulse parameters.
6. Enter stdisp to start the Shape Tool interface.
7. Click ***Shapes*** ’ ***Classical Shapes*** ’ ***Gauss***
8. In the parameter section, enter:

   Size of shape: 1000

   Truncation level : 1
9. Click ***Options*** ’ ***Define Parameter Table***
   - Set *Length of shaped pulse* to P12
   - Set *Power level of shaped pulse* to SP2
   - Set *Name of shaped pulse* to SPNAM2

   and click ***OK***.
10. Click ***Analysis*** ’ ***Calculate Bandwidth for Refocusing -My***

- Enter **Total Rotation**: 180

  this calculates the bandwidth factor, which is the product of the width of excitation (DeltaOmega) and the pulse length (DeltaT).
- Enter **Delta Omega**: 40 (the bandwidth determined in step 2)

  this calculates the shaped pulse length DeltaT !!!
- Click ***update parameters*** to store this pulse length as P12.

11. Click ***Analyses* ’ *Integrate Shape***

- Click ***update parameters*** to store the name of the shaped pulse to SPNAM2

12. On the associated dataset: enter the command ased and check the values of P12 and SP2. If the steps above were performed correctly, they should have the values of *DeltaT* and *Change of power level* (+ hard power level), respectively.

Note that if the peak is off-resonance, you need to determine the chemical shift difference between the peak and O1 and set the parameter SPOFFS2 accordingly. To determine the proper value, click , put the cursor on the desired peak and subtract the value of SFO1 from the MHz value displayed in the upper left of the data field.

Example 3: Create a Shaped Pulse for Sel. Excitation from Integral Regions

1. Read/acquire a 1D reference spectrum.

2. Click to switch to integration mode.

3. Click to define regions around the peaks to be excited.

4. Click to save these regions and return.

5. Create a new dataset.

6. Read the pulse program *selgpse.*

7. Enter ased and set all acquisition parameters for *selgpse*, except for the shaped pulse parameters.

8. Switch back the reference spectrum.

9. Enter stdisp to start the Shape Tool interface.

10. Click ***Shapes* ’ *Classical Shapes* ’ *Gauss***

11. In the parameter section, enter:

    Size of shape: 1000

    Truncation level : 1

12. Click ***Options* ’ *Define Parameter Table***
    - Set *Length of shaped pulse* to P12
    - Set *Power level of shaped pulse* to SP2
    - Set *Name of shaped pulse* to SPNAM2

13. Click ***Manipulate* ’ *Calc. Shape from excitation Region*** [manipul region]

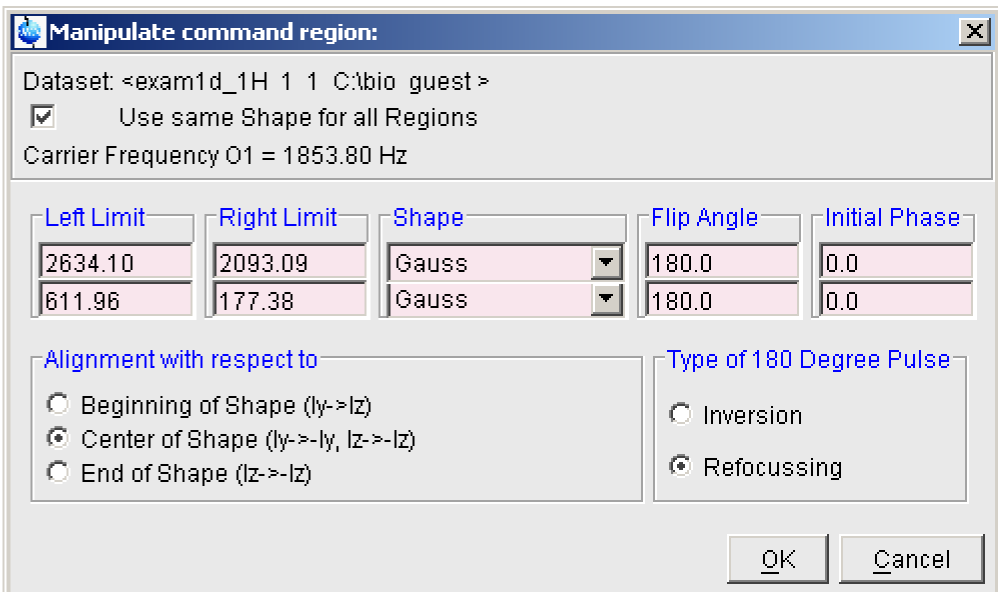


Figure 2.16

14. Click ***OK***

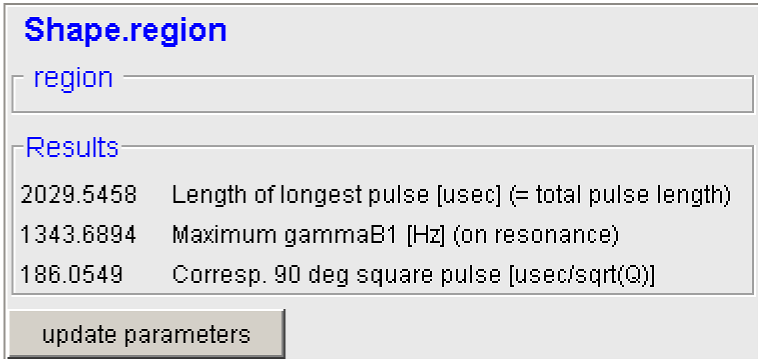


Figure 2.17

15. Click ***Options*** ’ ***Select associated dataset*** and select the *selgpse* dataset.

16. Click ***update parameters***, specify a name for the shaped pulse and click ***OK***.

17. Now switch to the *selgpse* dataset and start the experiment.

Chapter 3

Generating Shapes with st

3.1 Introduction

Syntax

st generate <shape type> <further parameters>

Example

st generate Gauss 1000 1 filename=Gauss.new -nobwcalc

By default, output files are stored under the name <shape type>. If you prefer a different filename, this must be specified with the option:

<filename=*newname*>

The option <-*nobwcalc*> will prevent automatic calculation of the bandwidth factor: ##$SHAPE_BWFAC= 0.0

This example will generate a Gaussian Shape with 1000 points and a truncation level of 1%. The shape is stored as `Gauss.new`. No automatic calculation of the bandwidth factor is done.

3.2 Basic Shapes

3.2.1 Rectangle Shape

Syntax

st generate Rectangle <size> <amplitude>

int <size> = shape size in number of points
double <amplitude> = amplitude in %

Example

RF shape: st generate Rectangle 256 100

Gradient: st generate Rectangle 256 false 100

3.2.2 Exponential Function (Efunc)

Syntax

st generate Efunc <size> <trunclevel>

or

st generate Efunc <size> <linebroadening> <sweepwidth>

int <size> = shape size in number of points
double <trunclevel> = truncation level in %

Conversion: trunclev <-> linebroadening / sweepwidth

trunclev = exp (-beta * (size-1)) * 100
beta = (linebroadening * π) / (2 * sweepwidth)

Example

RF shape: st generate Efunc 256 0.1
st generate Efunc 256 44 10000

Gradient: st generate Efunc 256 false 0.1
st generate Efunc 256 false 44 1000

3.2.3 Ramp Shape

Syntax

st generate Ramp <size> <start> <end>

int <size> = shape size in number of points
double <start> = start amplitude in %
double <end> = end amplitude in %

Example

RF shape: st generate Ramp 256 10 80

Gradient: st generate Ramp 256 false 10 80

3.2.4 Quadratic Ramp (QRamp)

Syntax

st generate QRamp <size> <start> <end>

int <size> = shape size in number of points
double <start> = start amplitude in %
double <end> = end amplitude in %

Example

RF shape: st generate QRamp 256 10 80

Gradient: st generate QRamp 256 false 10 80

3.2.5 Sine Shape (Sinus)

Syntax

st generate Sinus <size> <cycnum> <phase>

int <size> = shape size in number of points
int <cycnum> = number of cycles to be calculated
double <phase> = phase angle in degree (0.0 <= p <= 360.0)

Example

RF shape: st generate Sinus 256 8 180.0

Gradient: st generate Sinus 256 false 8 180.0

3.2.6 Trapezoid Shape

Syntax

st generate Trapezoid
<size> <startAmpl> <leftLimit> <centerAmpl> <rightLimit> <endAmpl>

int <size> = shape size in number of points.
double <startAmpl> = Amplitude at Start of Shape (in %).
double <leftLimit> = Left Limit of center region in Points.
double <centerAmpl> = Amplitude at Center of Shape (in %).
double <rightLimit> = Right Limit of center region in Points.
double <endAmpl> = Amplitude at the End of Shape (in %).

Example

RF shape: st generate Trapezoid 1000 0 300 100 700 0

Gradient: st generate Trapezoid 1000 false 0 300 0 100 700 0

3.2.7 Triangle Shape

Syntax

st generate Triangle <size>

int <size> = shape size in number of points

Example

RF shape: st generate Triangle 256

Gradient: st generate Triangle 256 false

3.3 Classical Shapes

3.3.1 Burp Shapes

Syntax

RF shape: st generate <shape type> <size>

int <size> = shape size in number of points
string <shape type> = {EBurp1 | EBurp2 | IBurp1 | IBurp2 | ReBurp | UBurp1}

Gradient: st generate <shape type> <size> false

Example

st generate IBurp1 256

Literature

H. Geen & R. Freeman,
J. Magn. Reson. 93, 93-141 (1991)

3.3.2 Gauss Shape

Syntax

RF shape: st generate Gauss <size> <trunclevel>

Gradient: st generate Gauss <size> false <trunclevel>

int <size> = shape size in number of points
double <trunclevel> = truncation level in %

Example

st generate Gauss 256 10

Literature

C. Bauer, R. Freeman, T. Frenkiel, J. Keeler & A.J. Shaka,
J. Magn. Reson. 58, 442-457 (1984)
L. Emsley & G. Bodenhausen,

J. Magn. Reson. 82, 211-221 (1989)

3.3.3 GaussCascade Shapes

Syntax

RF shape: st generate <shape type> <size>

Gradient: st generate <shape type> <size> false

string <shape type> = {GaussCascadeG3 | GaussCascadeG4 | GaussCascadeQ3| GaussCascadeQ5}
int <size> = shape size in number of points

Example

st generate GaussCascadeG4 256

Literature

GaussCascadeG3, GaussCascadeG4:
L. Emsley & G. Bodenhausen,
Chem. Phys. Lett. 165, 469 (1990)

GaussCascadeQ3, GaussCascadeQ5:
L. Emsley & G. Bodenhausen,
J. Magn. Reson. 97, 135-148 (1992)

3.3.4 HalfGauss Shape

Syntax

RF shape: st generate HalfGauss <size> <trunclevel>

Gradient: st generate HalfGauss <size> false <trunclevel>

int <size> = shape size in number of points
double <trunclevel> = truncation level in %

Example

st generate HalfGauss 256 10

Literature

J. Friedrich, S. Davies & R. Freeman,

J. Magn. Reson. 75, 390-395 (1987)

3.3.5 Hermite Shape

Syntax

RF shape: st generate Hermite <size> <trunclevel> <quadcoeff>

Gradient: st generate Hermite <size> false <trunclevel> <quadcoeff>

int <size> = shape size in number of points
double <trunclevel> = truncation level in %
double <quadcoeff> = coefficient of quadratic term (-4.0 .... +6.0)

Example

st generate Hermite 256 10 1.0

Literature

W.S. Warren,
J. Chem. Phys. 81, 5437-5448 (1984)

3.3.6 Seduce Shapes

Syntax

st generate <shape type> <size>

int <size> = shape size in number of points
string <shape type> = {Seduce1 | Seduce3}

Example

RF shape: st generate Seduce1 1000

Gradient: st generate Seduce1 1000 false

Literature

M.A. McCoy & L. Mueller,
J. Magn. Reson. A 101, 122-130 (1993)

3.3.7 Sinc Shape

Syntax

st generate Sinc <size> <cycnum>

int <size> = shape size in number of points
int <cycnum> = cycnum number of cycles to be calculated

Example

RF shape: st generate Sinc 256 8

Gradient: st generate Sinc 256 false 8

Literature

A.J. Temps Jr. & C.F. Brewer,
J. Magn. Reson. 56, 355-372 (1984)

3.3.8 Sneeze Shape

Syntax

st generate Sneeze <size>

int <size> = shape size in number of points

Example

RF shape: st generate Sneeze 256

Gradient: st generate Sneeze 256 false

Literature

J. M. Nuzillard & R. Freeman,
J. Magn. Reson. A 110, 252-256 (1994)

3.3.9 Snob Shapes

Syntax

st generate <shape type> <size>

int <size> = shape size in number of points string <shape type> = {ESnob | ISnob2 | ISnob3 | RSnob | DSnob}

Example

RF shape: st generate DSnob 256

Gradient: st generate ISnob2 256 false

Literature

E. Kupce, J. Boyd & I.D. Campbell,
J. Magn. Reson. B 106, 300-303 (1995)

3.3.10 Vega Shapes

Syntax

st generate <shape type> <size>

int <size> = shape size in number of points
string <shape type> = {EVega1 | EVega2 | IVega}

Example

RF shape: st generate EVega1 256

Gradient: st generate IVega 256 false

Literature

D. Abramovich & S. Vega,
J. Magn. Reson. A 105, 30-48 (1993)

3.3.11 Shapes defined by Fourier Coefficients (ShapFour)

Syntax

st generate ShapFour <size> <n> <a0> <a1>....<an> <b1>....<bn>

int <size> = shape size in number of points
int <n> = number of coefficients
double <a0> = 0. a-coefficient
double <a1> = 1. a-coefficient
..
..

double <an> = n. a-coefficient
double <b1> = 1. b-coefficient
..
..
double <bn> = n. b-coefficient

Example

st generate ShapFour 256 4 0.5 -1.147 0.5572 -0.0829 0.0525 0 0 0 0 0

generates a RSnob shape

3.4 Adiabatic Shapes

3.4.1 Hyperbolic Secant Shape (HypSec)

Syntax

st generate HypSec <size> <SW> <trunclevel> <full/half> <sweepDir>

int <size> = shape size in number of points
double <SW> = sweep width based on 1sec pulse
double <trunclevel> = truncation level in %
boolean <full / half > = full or half passage (true / false)
int <sweepDir> = Direction of sweep: 1= high to low, -1 = low to high field.

Example

RF shape: st generate HypSec 256 6.75 1.0 true -1

Gradient: st generate HypSec 256 false 6.75 1.0 true -1

Literature

M.S. Silver, R.I. Joseph & D.I. Hoult,
J. Magn. Reson. 59, 347 (1984)

3.4.2 SinCos Shape

Syntax

RF shape: st generate SinCos <size> <trunclevel> <full/half> <sweep-

Dir>

Gradient: st generate SinCos <size> false <trunclevel> <full/half> <sweepDir>

int <size> = shape size in number of points
double <factor> = phase amplitude factor (0.0 <= p <= 16.0)
boolean <full / half > = full or half passage (true / false)
int <sweepDir> = Direction of sweep: 1= high to low, -1 = low to high field.

Example

RF shape: st generate SinCos 256 8 true -1

Gradient: st generate SinCos 256 false 8 true -1

Literature

M.R. Bendall & D.T. Pegg,
J. Magn. Reson. 67, 376-381 (1986)

3.4.3 SmoothedChirp Shape

Syntax

st generate SmoothedChirp <size> <SW> <length> <smoothed> <sweepDir>

int <size> = shape size in number of points
double <SW> = Total Sweep Width (in Hz)
double <length> = length of pulse (in usec)
double <smoothed> = % to be smoothed
int <sweepDir> = Direction of sweep: 1= high to low, -1 = low to high field.

Example

RF shape: st generate SmoothedChirp 256 40000.0 1500.0 10.0 -1

Gradients: st generate SmoothedChirp 256 false 40000.0 1500.0 10.0 -1

Literature

J. M. Boehlen & G. Bodenhausen,
J. Magn. Reson. A 102, 293 (1993)

3.4.4 CompositeSmoothedChirp Shape

Syntax

st generate CompositeSmoothedChirp <size> <SW> <length> <smoothed> <sweepDir>

int <size> = shape size in number of points
double <SW> = Total Sweep Width (in Hz)
double <length> = length of pulse for basic element (in usec)
double <smoothed> = % to be smoothed
int <sweepDir> = Direction of sweep: 1= high to low, -1 = low to high field.

Example

RF shape: st generate CompositeSmoothedChirp 256 40000.0 375.0 10.0 -1

Gradient: st generate CompositeSmoothedChirp 256 false 40000.0 375.0 10.0 -1

Literature

T.L. Hwang, P.C.M van Zijl & M. Garwood
J. Magn. Reson. 124, 250 (1997)

3.4.5 TanhTan Shape

Syntax

st generate TanhTan <size> <total SW> <length> <zeta> <tan(kappa)>

int <size> = shape size in number of points
double <total SW> = Total Sweep Width
double <length> = Length of Pulse (in usec)
double <zeta> = Value for zeta.
double <tan(kappa)> = Value for tan(kappa).

Example

RF shape: st generate TanhTan 2000 1000000.0 500.0 10.0 20.0

Gradient: st generate TanhTan false 2000 1000000.0 500.0 10.0 20.0

Literature

R.S. Staewen, A.J. Johnson, B.D. Ross, T. Parrish, H. Merkle & M. Garwood,
Invest. Radiol. 25, 559-567(1990)
M. Garwood & Y. Ke,
J. Magn. Reson. 94 511-525(1991)

3.4.6 Wurst Shape

Syntax

st generate Wurst <size> <total SW> <length> <power index> <sweep-Dir>

int <size> = shape size in number of points
double <total SW> = Total Sweep Width
double <length> = Length of Pulse (in usec)
double <power index> = Amplitude Power Index
int <sweepDir> = Direction of sweep: 1= high to low, -1 = low to high field.

Example

RF shape: st generate Wurst 256 40000.0 1500.0 20.0 -1

Gradient: st generate Wurst 256 false 40000.0 1500.0 20.0 -1

Literature

E. Kupce & R. Freeman,
J. Magn. Reson. A 115, 273-276 (1995)

3.4.7 Constant-Adiabaticity Shapes

The following constant adiabaticity shapes are implemented:

- CaPowHsec (constant adiabaticity hyperbolic secant shape)
- CaWurst (constant adiabaticity wurst shape)
- CaSmoothedChirp(constant adiabaticity smoothed chirp shape)
- CaGauss (constant adiabaticity gauss shape)
- CaLorentz (constant adiabaticity lorentz shape)

Syntax

st generate <shape type> <size> <additional parameters>

For the additional parameters see the corresponding adiabatic shapes in chapter 3.4. However, for CaGauss and CaLorentz, the additional parameters are:

<SW> <length> <trunclev> <sweepDir>

Example

st generate CaWurst 1000 40000.0 1500.0 2.0

Literature

A. Tannus & M. Garwood,
J. Magn. Reson. A 120, 133-137 (1996)

3.5 Special Shapes for Solids Applications

3.5.1 Sines Shape

Syntax

st generate Sines <size> <cycnum> <phase> <average> < mod.>

int <size> = shape size in number of points
double <cycnum> = number of cycles to calculate
double <phase> = initial phase angle (0.0 <= p <= 360.0)
double <average> = average amplitude
double <mod> = amplitude of modulation

Example

RF shape: st generate Sines 256 2.0 0.0 80.0 10.0

Gradient: st generate Sines 256 false 2.0 0.0 80.0 10.0

Literature

S.Hediger, B.H.Meier, R.H. Ernst,
J. Chem. Phys. 102, 4000-4011 (1995)

3.5.2 TangAmplitudeMod Shape

Syntax

st generate TangAmplitudeMod <size> <modulation> <phase> <ampl.>

int <size> = shape size in number of points
double <modulation> = Amplitude of Modulation
double <phase> = Phase Value (max. 95 degree)
double <ampl.> = Average Amplitude

Example

RF shape: st generate TangAmplitudeMod 256 5000.0 26.56 50000.0

Gradient: st generate TangAmplitudeMod 256 false 5000.0 26.56 50000.0

Literature

M. Baldus, D.C. Geurts, S.Hediger, B.H.Meier,
J. Magn. Reson. A 118, 140-144 (1996)

3.6 Special Shapes for Imaging Applications

3.6.1 CosSinc Shapes

Syntax

RF shape: st generate CosSinc <size> <cycles> <window size>

Gradient: st generate CosSinc <size> false <cycles> <window size>

int <size> = shape size in number of points
double <cycles> = number of cycles to calculate
double <window size> = window size in %

Example

st generate CosSinc 1000 4 50

Literature

G.J. Galloway, W.M. Brooks, J.M. Bulsing, I.M. Brereton,

J. Field, M. Irving, H. Baddeley & D.M. Doddrell,
J. Magn. Reson. 73, 360-368 (1987)

3.6.2 Sine * Sinc Shape (SineSinc)

Syntax

st generate SineSinc <size> <cycnum>

int <size> = shape size in number of points
int <cycnum> = number of cycles to calculate

Example

RF shape: st generate SineSinc 256 8

Gradient: st generate SineSinc 256 false 8

Literature

D.M. Doddrell, J.M. Bulsing, G.J. Galloway, W.M. Brooks, J. Field, M. Irving, & H. Baddeley,
J. Magn. Reson. 70, 319-326 (1986)

3.7 Special Shapes for Decoupling

3.7.1 Swirl Shapes

Syntax

st generate <shape type> <size>

int <size> = shape size in number of points
string <shape type> = {Swirl11 | Swirl12 | Swirl17}

Example

RF shape: st generate Swirl11 256

Gradient: st generate Swirl17 256 false

Literature

H. Geen & J.-M. Boehlen,

J. Magn. Reson. 125, 376-382 (1997)

Chapter 4

Manipulating Shapes with st

4.1 Introduction

Syntax

st manipulate <shape type> <command> <further parameter>

The following manipulating commands are implemented:

- offs - phase modulation according to offset frequencies
- sinm2 - single sine modulation (+/- offset)
- cosm2 - single cosine modulation (+/- offset)
- sweep - modulation according to linear frequency sweep
- caSweep - modulation according to constant adiabticity frequency sweep
- power - calculate power of amplitude
- scale - scale the amplitude of a shape
- addphase - add constant phase
- trev - time reverse a shape
- expand - expand shape according to supercycle

4.2 Command offs

Calculates a phase modulation according to offset frequencies.

The manipulate command offs has following subcommands:

b - phase modulation beginning at phase 0
m - phase modulation with phase of 0 at middle of shape
e - phase modulation ending at phase 0

Syntax

st manipulate <shape type> offs b <pulDur> <n> <f1>...<fn>

double <pulDur> = pulDur = length of shaped pulse (in us)
int <n> = number of offset frequencies
double <f1> = offset frequency 1 (in Hz)
double <f2> = offset frequency 2 (in Hz)
....
....
double <fn> = offset frequency n (in Hz)

Example

st manipulate Gauss offs b 100 2 2000 3000

calculates phase modulation beginning at phase 0.

Optional commands are:

f - frequencies taken from frequency list
p - additional phase setting
s - additional scaling

Syntax

st manipulate <shape type> offs b f <pulDur> <freqlist>
string <freqlist> = file with frequency-list

Example

st manipulate Gauss offs b f 100 freqlist

Syntax

st manipulate <shape type> offs m p <pulDur> <n> <f1> <p1>...<fn> <pn>

double <pulDur> = pulDur = length of shaped pulse (in us)
int <n> = number of offset frequencies
double <f1> = offset frequency 1 (in Hz)
double <p1> = initial phase 1 (in degree)
double <f2> = offset frequency 2 (in Hz)
double <p2> = initial phase 2 (in degree)
....
....
double <fn> = offset frequency n (in Hz)
double <pn> = initial phase n (in degree)

Example

st manipulate Gauss offs m p 100 2 2000 90 3000 300

Syntax

st manipulate <shape type> offs e s <pulDur> <n> <f1> <s1> <f2> <s2>

double <pulDur> = pulDur = length of shaped pulse (in us)
int <n> = number of offset frequencies
double <f1> = offset frequency 1 (in Hz)
double <s1> = scaling factor 1 (in %)
double <f2> = offset frequency 2 (in Hz)
double <s2> = scaling factor 2 (in %)
....
....
double <fn> = offset frequency n (in Hz)
double <sn> = scaling factor n (in %)

Example

st manipulate Gauss offs e s 100 2 2000 50 3000 75

Note that multiple optional commands can be used, for example:

st manipulate Gauss offs m f s 100 50 75 freqlist

st manipulate Gauss offs e f p 100 90 180 freqlist

4.3 Command sinm2

Calculates an amplitude modulation such that the pulse excites at two symmetric sidebands (+/- offset) with opposite phase.

Syntax

st manipulate <shape type> sinm2 <pulDur> <offset>

double <pulDur> = length of shaped pulse (in us)
double <offset> = offset frequency (in Hz)

Example

st manipulate Gauss sinm2 1000 3000

4.4 Command cosm2

Calculates an amplitude modulation such that the pulse excites at two symmetric sidebands (+/- offset) with the same phase.

Syntax

st manipulate <shape type> cosm2 <pulDur> <offset>

double <pulDur> = pulDur = length of shaped pulse (in us)
double <offset> = offset frequency (in Hz)

Example

st manipulate Gauss cosm2 1000 3000

4.5 Modulation according to Frequency Sweep

4.5.1 Command sweep

Calculates a phase modulation according to a linear frequency sweep.

Syntax

st manipulate <shape type> sweep <pulDur> <sw>

double <pulDur> = length of shaped pulse (in us)
double <sw> = total sweep-width (in Hz)

Example

st manipulate Gauss sweep 1000 5000

4.5.2 Command caSweep

Calculates a phase modulation according to a constant adiabaticity frequency sweep: phase(t) = ∫ frequency(t) = ∬ amplitude(t)

Syntax

st manipulate <shape type> caSweep <pulDur> <sw>

double <pulDur> = length of shaped pulse (in us)
double <sw> = total sweep-width (in Hz)

Example

st manipulate Gauss caSweep 1000 5000

4.6 Command power

Calculate the power of an amplitude. This allows you to compare a theoretical shape with an observed shape on the scope.

Syntax

st manipulate <shape type> power <exponent>

double <exponent> = exponential factor

Example

st manipulate Gauss power 2

4.7 Command scale

Scale the amplitude of a shape to a given percentage.

Syntax

st manipulate <shape type> scale <scale>

double <scale> = new scaling in %

Example

st manipulate Gauss scale 50.0

If the maximum amplitude after scaling exceeds 100%, it will be rescaled to 100% during execution.

4.8 Command addphase

Adds a constant phase to a shape.

Syntax

st manipulate <shape type> addphase <phase>

double <phase> = phase constant to be added in degree

Example

st manipulate Gauss 90.0

4.9 Command trev

Time reverse a shape. Since shapes are often optimized for a particular rotation (e.g. Iz ’ - Iy , excitation) , reversing the rotation (Iy ’ Iz , flipback) will only work reliably if the shape is time reversed as well.

Syntax

trev needs no additional parameters.

Example

st manipulate HalfGauss trev

4.10 Command expand

Expand shape according to a phase list (supercycle).

Syntax

st manipulate <shape type> expand <n> <phase1> ... <phasen>

int <n> = number of phases to expand
double <phase1> = first phase value
.
.
double <phasen> = nth phase value

Example

st manipulate Gauss expand 4 0 0 180 180

Chapter 5

Analyzing Shapes with st

5.1 Introduction

Syntax

st analyze <shape type> <analyze command> <further parameter>

The following analyzing commands are available:

- bandw2 calculate bandwidth for excitation (√(Mx2+My2)
- bandw2i calculate bandwidth for inversion (-Mz)
- bandw2ry calculate bandwidth for refocusing (-My)
- Special Bandwidth Calculations:

  bandw2e calculate bandwidth for excitation (-My)
  bandw2r calculate bandwidth for refocusing (My'√(Mx2+My2))
  bandw2rx calculate bandwidth for refocusing (+Mx)
- calcb1mo calculate γB1(max)/2π at offset
- calcb1adia calculate γB1(max)/2π for adiabatic shapes
- bsiegert3 - calculate Bloch-Siegert shift
- calcpav calculate average power level

- integr3 - integrate shape and calculate power level compared to hard pulse
- integradia - integrate adiabatic shapes and calculate power level compared to hard pulse.

The following commands are only available for the st analyze command. In the stdisp graphical interface, they have been replaced (see chapter 5.12).

- integr integrate shape and compare to square.
- integr2 calculate power level compare to hard pulse.
- calcb1m calculate $\gamma B1(max)/\pi$ on resonance.

5.2 Command bandw2

Calculate the bandwidth for excitation ($\sqrt{}$(Mx2+My2).

Syntax

st analyze Gauss bandw2 <rotation>

double <rotation> = total rotation (in degree)

Example

st analyze Gauss bandw2 90

Result: bandwidth factor $\Delta\omega$ * ΔT.

5.3 Command bandw2i

Calculates the bandwidth for inversion (-Mz).

Syntax

st analyze Gauss bandw2i <rotation>

double <rotation> = total rotation (in degree)

Example

st analyze Gauss bandw2i 180

Result: bandwidth factor $\Delta\omega * \Delta T$.

5.4 Command bandw2ry

Calculates bandwidth for refocusing (-My).

Syntax

st analyze Gauss bandw2ry <rotation>

double <rotation> = total rotation (in degree)

Example

st analyze Gauss bandw2ry 180

Result: bandwidth factor $\Delta\omega * \Delta T$.

5.5 Special Bandwidth Calculations

bandw2e: calculate bandwidth for excitation (-My)

bandw2r: calculate bandwidth for refocusing (My ’ √(Mx2+My2)

bandw2rx calculate bandwidth for refocusing (+Mx)

Syntax and Result of these commands are identical to the bandwidth calculation commands described above.

5.6 Command calcb1mo

Calculates γB1(max)/π at offset.

Syntax

st analyze Gauss calcb1mo <pulDurShape> <rotation> <offset>

double <pulDurShape> = length of shaped pulse (in us)
double <rotation> = total rotation (in degree)
double <offset> = offset (in Hz)

Example

st analyze Gauss calcb1mo 100 90 3000

Result:

- maximum gB1/2π (on resonance)
- corresponding 90 degree square pulse

5.7 Command calcb1adia

Calculates γB1(max)/2π/√(Q) for adiabatic shapes.

Syntax

st analyze SmoothedChirp calcb1adia <pulDurShape>

double <pulDurShape> = length of shaped pulse (in us)

Example

st analyze SmoothedChirp calcb1adia 10000

Result:

- sweep rate on resonance (in Hz/sec)
- maximum γB1/2π/√(Q) (on resonance)

5.8 Command bsiegert3

Calculates the Bloch-Siegert shift.

Syntax

st analyze <shape type> bsiegert3 <pulDur> <γB1> <offset>

double <pulDur> = length of shaped pulse (in us)
double <γB1> = γB1(max) (in Hz)
double <offset> = offset relative to frequency of RF-pulse (in Hz)

Result:

- phase difference due to Bloch-Siegert shift (in degree)

- corresponding frequency shift (in Hz)

5.9 Command calcpav

Calculates the average power.

calcpav needs no additional parameters.

Example

st analyze Gauss calcpav

Result:

- amplitude relative to a square pulse of 100%
- corresponding difference in dB.
- power relative to a square pulse of 100%

5.10 Command integr3

Integrates shape and calculates power level compared to hard pulse.

Syntax

st analyze Gauss integr3 <pulDurShape> <pulDurHard> <totRot>

double <pulDurShape> = length of shaped pulse (in us)
double <pulDurHard> = length of reference hard pulse (in us)
double <totRot> = total rotation (in degree).

Example

st analyze Gauss integr3 10000 6.6 180

Result:

- integral ratio compared to a square pulse of 100% (Flip angle not evaluated)
- corresponding difference in dB. (Flip angle not evaluated)
- change of power level compared to level of hard pulse in dB

5.11 Command integradia

Integrates adiabatic shapes and calculates power level compared to hard pulse.

Syntax

st analyze <adiabatic shape> integradia <pulDurShape> <pulDurHard>

double <pulDurShape> = length of shaped pulse (in us)
double <pulDurHard> = length of reference hard pulse (in us)

Example

st analyze SmoothedChirp integradia 10000 8

Result:

- sweep rate on resonance (in Hz/sec)
- γB1(max)/2π / $\sqrt{}$(Q)

5.12 Routines which have been replaced in stdisp

The commands integr and integr2 are available for st, but have been replaced by analyze integr3 in stdisp. The command calcb1m for st has been replaced by analyze calcb1mo with offset = 0 in stdisp

5.12.1 Command integr

Integrates shape and compare to square.

integr needs no additional parameters

Example

st analyze Gauss integr

Result:

- integral ratio compared to a square pulse of 100%
- corresponding difference in dB

5.12.2 Command integr2

Calculates the power level compared to a hard pulse.

Syntax

st analyze <shape type> integr2 <pulDurShape> <pulDurHard>

double <pulDurShape> = length of shaped pulse (in us)
double <pulDurHard> = length of reference hard pulse (in us) of same flip angle

Example

st analyze Gauss integr3 10000 6.6 180

Result:

- integral ratio compared to a square pulse of 100%
- corresponding difference in dB.
- change of power level compared to level of hard pulse in dB.

5.12.3 Command calcb1m

Calculates γB1(max)/2π on resonance.

Syntax

st analyze Gauss bandw2i <rotation>

double <pulDurShape> = length of shaped pulse (in us)
double <rotation> = total rotation (in degree)

Example

st analyze Gauss calcb1m 100 180

Result:

- maximum γB1 (on resonance).
- corresponding 90 degree square pulse

Chapter 6

Miscellaneous st functions

6.1 Introduction

- add - add shapes (up to 10).
- convert, convertgr - convert shapes/gradients from conventional ASCII format to JCAMP-DX format.

6.2 Commands convert, convertgr

This commands convert shapes/gradients from conventional ASCII format to JCAMP-DX format.

Syntax

st convert <input> <output> <type> <#freq> [<deltaOmega*deltaT>]

string <type> = types are: Universal, Excitation, Inversion, etc.
string <input> = input filename
string <output> = output filename
int <#freq> = number of off resonance frequencies in shape
double <deltaOmega*deltaT> = value for deltaOmega*deltaT (this parameter is optional)

Examples

st convert Gauss.ascii Gauss.jcamp Excitation 0
st convertgr Gauss.ascii Gauss.jcamp

Required format of the ascii input files:

RF-shapes	Gradients
RFVERSION_F	GRADIENT
-5.14574 0.0000	1.000000e-02
...	...
-5.16086 0.0000	1.000000e-02

6.3 Command add

Add existing shapes to form a new shape.

Syntax

st add <alignment> <n> <input1> <scale1> ... <inputn> <scalen> <result>

int <alignment> = with respect to beginning = 0, center = 1, end = 2 of shape
int <n> = number of shapes to be added (max. 10 shapes are allowed)
string <input1> = filename of first shape to be added
double <scale1> = scaling of first shape
...
...
string <inputn> = filename of nth shape to be added
double <scalen> = scaling of nth shape
string <result> = result of the addition

Example

st add 0 2 Gauss.1 100 Gauss.2 50 Gauss.result

Chapter 7

Shapes in AU programs

7.1 Using Shape Tool commands in AU Programs

Here you find an example of an AU program using Shape Tool commands.

```
#include <stdio.h>
#include <stdlib.h>
#include <strings.h>
#include <limits.h>
#include <ShapeIO/ShapeIOC.h>

#define MAX_ANZ                  20

char result[PATH_MAX];
char filename[PATH_MAX];
char *singleResult;
int i, numbOfParams;
double retValue[MAX_ANZ];
double bandWidthFactor;

/* read gaussian shape and call analyze command bandw2 */

(void)sprintf(filename,"%slists/wave/Gauss",getstan(0, 0));
```

```
numbOfParams = analyzeShapeC(filename, "bandw2", "90",
&result[0]);

if (numbOfParams <= MAX_ANZ)
{
      i = 0;
       singleResult = strtok(result, ",");            /* scan result string for
results */
       retValue[i] = atof(singleResult);

      while ((singleResult = strtok(0, ", ")))
      {
          retValue[++i] = atof(singleResult);
                if (i >= numbOfParams)       break;
      }
      bandWidthFactor = retValue[0];
}
/* do further calculations with bandWidthFactor */
........
........
QUIT
```

In this example the command analyzeShapeC(...) reads a gaussian shape and applies the command bandw2 with the parameter total rotation = 90° and stores the result of the calculation into the char [ ] result. The return value of analyzeShapeC is the number of results calculated. In the case of bandw2 only one result, the bandWidthFactor $\Delta\omega$ * ΔT is returned. Now the Bandwidth factor can be used for further calculations in the AU program.

Most of the analyze commands return more than one result. These are then separated by semicolons in the returned char [ ] result. The while loop in the example scans this array and copies the single results to the double array retValue. Now all results of the analyze command are available for further calculations.

Chapter 8

Shape File Format

8.1 Format of a Gaussian Shape File

```
##TITLE= /tshome/exp/stan/nmr/lists/wave/Gauss
##JCAMP-DX= 5.00 Bruker JCAMP library
##DATA TYPE= Shape Data
##ORIGIN= Bruker Analytik GmbH
##OWNER= <wk>
##DATE= 00/03/23
##TIME= 08:19:08
##$SHAPE_PARAMETERS= Type: Gauss ; Truncation Level: 1
##MINX= 1.000000e+00
##MAXX= 9.999954e+01
##MINY= 0.000000e+00
##MAXY= 0.000000e+00
##$SHAPE_EXMODE= Universal
##$SHAPE_TYPE=
##$SHAPE_USER_DEF=
##$SHAPE_REPHFAC=
##$SHAPE_TOTROT= 9.000000e+01
##$SHAPE_BWFAC= 2.122000e+00
##$BWFAC50 =
```

```
##$SHAPE_INTEGFAC= 4.115776e-01
##$SHAPE_MODE= 0
##NPOINTS= 1000
##XYPOINTS= (XY..XY)
1.000000e+00, 0.000000e+00
1.018591e+00, 0.000000e+00
1.037490e+00, 0.000000e+00
1.056700e+00, 0.000000e+00
1.076227e+00, 0.000000e+00
1.096073e+00, 0.000000e+00
1.116245e+00, 0.000000e+00
1.136746e+00, 0.000000e+00
1.157580e+00, 0.000000e+00
1.178753e+00, 0.000000e+00
1.200269e+00, 0.000000e+00
...
...
...
1.200269e+00, 0.000000e+00
1.178753e+00, 0.000000e+00
1.157580e+00, 0.000000e+00
1.136746e+00, 0.000000e+00
1.116245e+00, 0.000000e+00
1.096073e+00, 0.000000e+00
1.076227e+00, 0.000000e+00
1.056700e+00, 0.000000e+00
1.037490e+00, 0.000000e+00
1.018591e+00, 0.000000e+00
1.000000e+00, 0.000000e+00
##END=
```