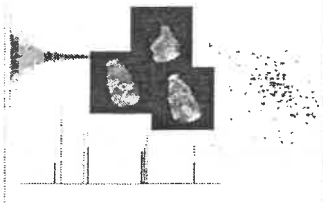

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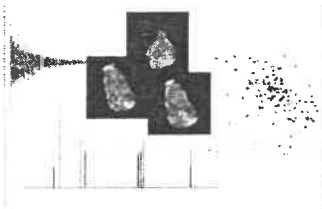

1 - Main NTNMR Window

1.1 Introduction

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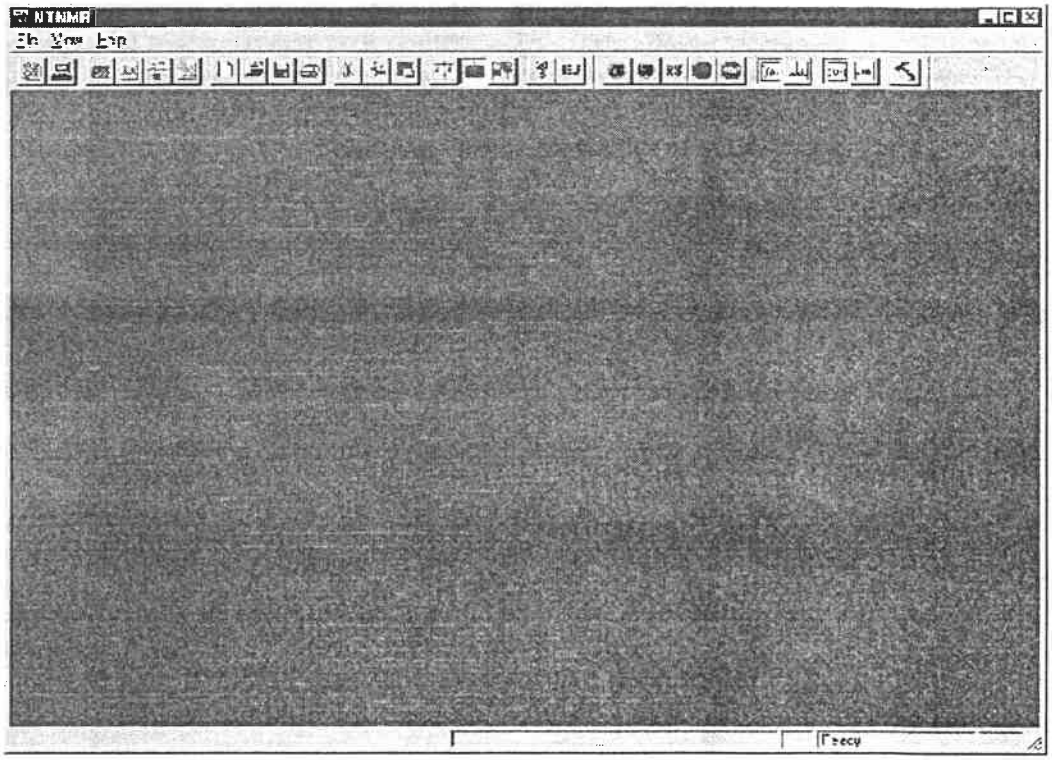
The NTNMR window, shown below, contains the menus and toolbars for the application. The menus and toolbars conform to the Windows standards. Data files are opened as document windows as with other Windows applications.



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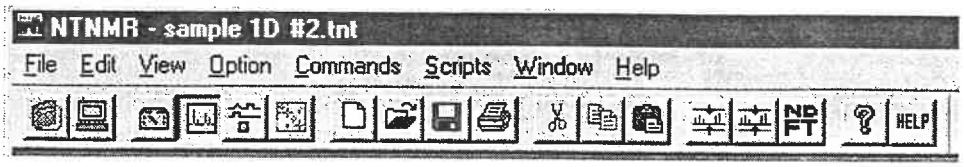
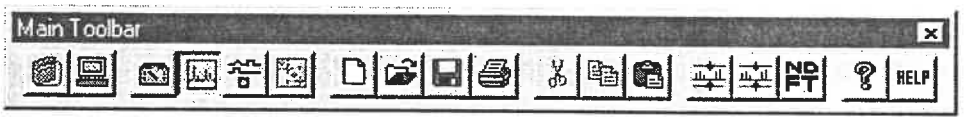
Main Toolbar

The Main NTNMR Toolbar (shown below) is a "dockable" toolbar that controls several of the most commonly accessed features of NTNMR. Each button on the Main Toolbar is discussed below.



The Main NTNMR Toolbar can be "undocked" by left-clicking and dragging to anywhere on the Toolbar. The "undocked" toolbar can be positioned anywhere on the desktop. Additionally, the Main Toolbar (as well as other Toolbars) can be docked on the bottom of the NTNMR window or on either side. Double-clicking on the Toolbar title bar while it is "undocked" will pop the Toolbar back to its last "docked" position.

The Main Toolbar "undocked."



The Comment Button

Click once on the Comment button to make the Comment window appear. The Comment window is a floating, editable, text window containing descriptive information that is stored with each NTNMR data file.

> *Choosing Comment under the Window menu will also make the Comment window appear.*

The Console Button

The Console button activates the NTNMR hardware Console for the current hardware type. Consult the Users guide for your hardware type for details about the Console window.

The Dashboard Button 

Click once on the Dashboard button to make the Dashboard window appear. The Dashboard is a "dockable" window that appears at the bottom of the Main Window by default and is always associated with the active data file. When another data file is opened, the contents of the Dashboard window will automatically update to reflect the new data file. See the section below entitled Dashboard Window for details about the NTNMR Dashboard.

> *Choosing **Dashboard** under the **Windows** menu will also activate the Dashboard window.*

The Data and Pulse Sequence Buttons

These two buttons allow the Pulse Sequence and Data windows to be toggled to the front. Clicking once on the Pulse Sequence button causes the associated Pulse Sequence window to appear. For detailed information about Pulse Sequences, see the associated chapter.

2D Display Button 

If a 2D data set is loaded and front most, the 2D Display button will be active. Clicking on the 2D Display button will activate the 2D Display mode. The default drawing mode (contours or continuous colors) is set in the **2D** tab of the preferences dialog (**Edit | Preferences...**). The 2D drawing mode can also be set by [SHIFT]-clicking on the 2D Display button, which calls a 2D setup dialog. See the chapter on 2D Display for more information.

Common Windows Buttons 

The next several buttons are common Microsoft Windows buttons:

- "New" button: this button opens a new blank NTNMR document. Same as **File|New**.
- "Open" button: present the Open File dialog. Same as **File|Open**.
- "Save" button: when previously unsaved data file is on the front, this button will present the standard

"Save As" dialog: in this case, the Save button is identical to **File|Save** and **File|Save As...**. If the data file has already been saved, the Save button simply saves the file, *overwriting the last saved version*. In this case, the Save button is the same as **File|Save**.

- "Print" button: sends the current data file to the currently selected printer. Same as **File|Print...**.
- "Cut" button: same as **Edit|Cut**.
- "Copy" button: same as **Edit|Copy**.
- "Paste" button: same as **Edit|Paste**.

Fit to Window Button 

Clicking on the Fit To Window button will auto scale the data currently displayed one time without activating Auto Scale mode (see below). If a zoom region is selected, the data in the zoom will be scaled to fit the window. Same as View | Fit to Window.

Auto Scale Button 

Activates the auto scale mode. The data in the window will always be scaled to fit the window. The auto scale is based on the entire data set and not the current zoom. Thus, if auto scale is active and a zoom is active, it may appear that the data is not scaled properly. The Fit to Window function will always override the auto scale.
The data is scaled based on the data type that is displayed (i.e. real, imaginary, or magnitude). If more than one type of data is displayed, the following hierarchy is used to determine the data scaling: real, imaginary and magnitude. Therefore, if the real and magnitude data is displayed simultaneously, and the auto scale mode is active, the data will be scaled based on the real data only.

nDFT Button

Executes a processing template. [SHIFT]-click to configure the NDFT processing template. See the Chapter on Commands for detailed information.

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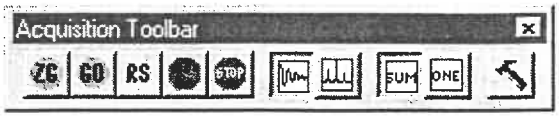
Acquisition Toolbar

The Acquisition Toolbar is dockable and has behaves the same way as the Main Toolbar; it can be "undocked" and "re-docked" in different locations or "undocked" and allowed to float anywhere on the desktop. The Acquisition Toolbar is shown below. Each button is discussed in turn below.



ZG Button 

Zeroes the signal averager memory and Starts an acquisition. Same as Commands|Acquisition Commands…|Zero and Go and (Ctrl + Z).

GO Button 

Starts an acquisition without zeroing the memory (i.e. "continue"). Same as Commands|Acquisition Commands…|Go and (Ctrl + G).

RS Button 

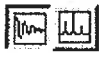
Starts the "Repetitive Scan" mode. This command begins zeroes the memory, begins acquisition and repeats until stopped by the user. Same as Commands|Acquisition Commands…|Repeat Scan and (Ctrl + R).

Soft Stop Button 

Stops the acquisition *after completion* of the current receiver phase cycle. Same as Commands|Acquisition Commands…|Stop and (Ctrl + ESC). This button will be grayed (as in the Acquisition Toolbar figure above) unless an acquisition is in progress.

Stop Button 

Aborts the acquisition *immediately*. Same as Commands | Acquisition Commands ... | Abort and (ESC). This button will be gray (as in the Acquisition Toolbar figure above) unless it stops an acquisition in progress.

Show FID/Show Spectrum Toggle Buttons 

These buttons act as a pair in toggle mode. When the "FID" button (left) is active, NTNMR displays time domain data. When the "Spectrum" button (right) is active, NTNMR will display the transformed spectrum (performs BC - FT). In both cases, the display will be updated after every scan. These buttons are used in conjunction with the SHOW SUM/SHOW ONE buttons discussed below.

Show Sum/Show One Toggle Buttons 

These buttons act as a pair in toggle mode. When the "SUM" button is active, as in the picture above, NTNMR will display the accumulated data after each scan. When the "ONE" button is active, NTNMR will show the last single shot acquired and *not* the accumulated data. These buttons are used in conjunction with the SHOW FID/SHOW SPECTRUM buttons above.

Reset Button 

This button resets the hardware and reloads all default configuration files.

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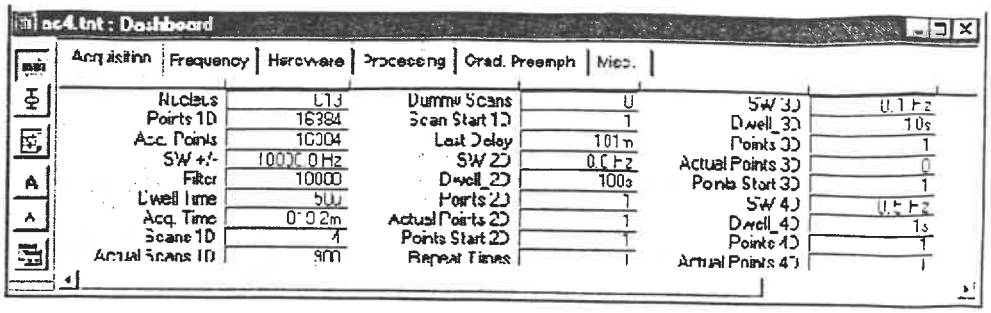
NTNMR Dashboard Window



When the Dashboard button is activated and the Dashboard window is opened, parameters from the data file will appear. This window displays a categorized list of parameters for acquisition and processing.

> *The Dashboard window displays the parameters that are read from the data file. Changing the values for parameters displayed in the Dashboard window does not affect the parameters stored with the data file, unless the data is written to a file by using the* ***Save*** *command.*

Working With the Dashboard

The dashboard contains several tools that facilitate quick access to information available as well as manipulation of the appearance of the Dashboard.

Re-sizing the Dashboard

Use the size control in the lower right corner of the Dashboard window to alter the size of the window. If there are too many parameters to display, a scroll bar will be activated at the bottom of the window to allow scrolling to the parameters out of the current view.

Tabs

The parameters in the dashboard are organized under several categories that appear as a row of tabs along the top of the dashboard. Left-clicking on any tab will update the display to show all of the parameters in that category. Note that not all parameters are editable. Some parameters such as "Actual Scans 1D" are provided for informational purposes and are not editable.

The Tab Button: 

Clicking on the Tab button will hide the category tabs along the top of the Dashboard.

The Scroll Button: 

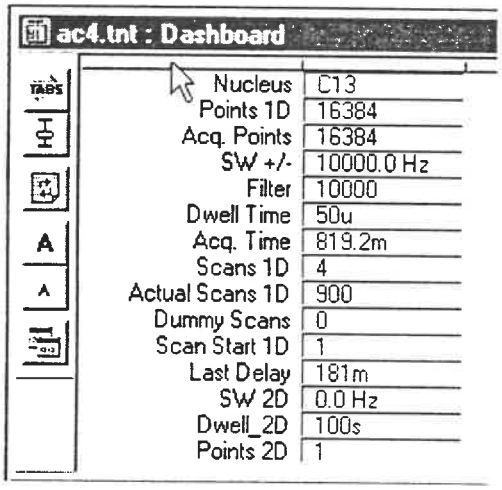
The Scroll button can be used to page through the various Dashboard parameter display categories. Each left-click will cause the display to jump to the next tab and update the display. This button is functional regardless of whether the tabs are currently visible.

The Text Size Buttons: 

The up and down size buttons allow the size of the Dashboard text to be increased and decreased. Left-clicking either size button will cause the display to be refreshed with an increase or decrease of 1 point in the font size.

The Justification Bars: (See graphic below)

Left-clicking on the Justification bars above the parameter descriptions and values will alternately change the justification from left to right.



When the Dashboard window is active, use the [TAB] key to scroll through the list or select a field by left-clicking. Key [RETURN] or [ENTER] to complete any entry.

Real Time Adjustment Mode Button 

This button activates the Real Time Adjustment Mode for interactively adjusting experimental parameters. See the Chapter on Pulse Sequences for more information.

Customizing the Dashboard

Clicking on the  button (Dashboard Customize) in the Dashboard toolbar will launch the Dashboard Customize applet which allows the user to choose from a pre-saved list of dashboard configurations, load a pre-saved dashboard configuration from disk, or to customize and save a new dashboard configuration.

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Dashboard Parameters

Master Parameters

The table below lists all of the available dashboard parameters in NTNMR. Keep in mind that the dashboard that appears in NTNMR will most likely not display all of the parameters listed and that parameters may be stored (and even duplicated) under any tab. Custom tabs with unique names can also be created.

Sequence Parameters

An additional tab labeled "Sequence" will often be visible. This tab contains user definable Sequence Parameters. If a sequence file is loaded that contains variables, the sequence tab will appear in the dashboard. Consult the chapter on Pulse Sequences for more information.

Dashboard parameters that represent time or frequency must be followed by a unit (such as n for nanoseconds, u for microseconds, m for milliseconds and s for seconds). Scientific notation, like 1e-5, is also allowed.

> *Sweep width (SW +\-) will be updated after each Dwell Time Character is entered. Acquisition Time will be updated for any change in Acquisition Points, Dwell Time or SW +\-.*

*The following codes are used to indicate the functionality of dashboard parameters:

- 1 = editable by the user
- 2 = not editable by the user
- 3 = information field only, no hardware significance
- 4 = may not be functional on all hardware types

Dashboard Parameters

Parameter	Function	Default Tab	Info*
Date	Display the NTNMR file creation date	Misc.	1,3
Magnet Field	Magnetic field in Tesla	Misc.	1,3
F1 Ref. Freq.		Misc.	1
Absolute Freq.		Misc.	2
Exp. Start Time	Time the current experiment was started	Misc.	2
Exp. Finish Time	Estimated time the current experiment will finish	Misc.	2
Exp. Elapsed Time	Estimated time the current experiment has been running	Misc.	2
Trans. Gain	Transmitter power	Hardware	1
Receiver Gain	Receiver gain	Hardware	1
DEC Attn	Parameter for the decoupler power	Hardware	1, 4
DEC BW	Modulation for the decoupler power	Hardware	1, 4
Set Temp	VT temperature parameter (K)	Hardware	1, 4
Actual Temp		Hardware	2, 4
Set Spin Rate	Sample spinning speed	Hardware	1, 4
Actual Spin Rate		Hardware	2, 4

Dashboard Parameters cont.			
Parameter	**Function**	**Default Tab**	**Info***
Lock Solvent	Lock Solvent	Hardware	1, 4
Lock Field		Hardware	1, 4
Lock Power	Lock transmitter value, as shown in the Lock Console (see Chapter 2)	Hardware	1, 4
Lock Gain	Lock receiver value, as shown in the Lock Console (see Chapter 2)	Hardware	1, 4
Lock Phase	Lock phase value, as shown in the Lock Console (see Chapter 2)	Hardware	1, 4
Lock PPM		Hardware	1, 4
Shim Units	The sum of the magnitude calculations for all points, used as a shimming rating	Hardware	2
Observe Freq.	Observe frequency in MHz determined by the Observe Ch.	Frequency	1
Observe Ch.	Assigns which transmitter channel is assigned for 'observe' (1-4)	Frequency	1
F1 Freq.	F1 frequency in MHz (F1 base + F1 offset)	Frequency	1
F1 Base	Base observe frequency in MHz	Frequency	1
F1 Offset	Added observe frequency in kHz	Frequency	1
Fn Freq.	Fn frequency in MHz (Fn base + Fn offset)	Frequency	1, 4
Fn Base	Base Fn frequency in MHz	Frequency	1, 4
Fn Offset	Added Fn frequency in kHz	Frequency	1, 4
Nucleus	Display the observation nucleus	Acquisition	3
Points 1D	Number of complex data points (input is adjusted to 2n), any change to this will change Acquisition Points if the Hardware Preference is on for tracking	Acquisition	
Acq. Points	number of complex data points actually sampled (not necessarily 2n, but must be less than or equal to Points 1D), any change will not change Points 1D	Acquisition	
SW +/-	spectral width in Hz, +/- (editing SW+/- will also change the Dwell Time)	Acquisition	1
Filter	audio filter setting	Acquisition	
Dwell Time	time per complex point in seconds given by (2*SW+/-)-1 (editing Dwell Time will also change the SW+/-)	Acquisition	1

Dashboard Parameters cont.

Parameter	Function	Default Tab	Info*
Acq. Time	Displays the Points 1D * Dwell Time	Acquisition	2
Scans 1D	Number of averages/accumulations requested	Acquisition	1
Actual Scans 1D	Number of averages/accumulations actually completed	Acquisition	2
Dummy Scans	Number of scans without data averaging before acquisition starts	Acquisition	1
Scan Start 1D	Sets the starting scan number (1D)	Acquisition	1
Last Delay	The delay of the last event in a pulse sequence (entered in as a number followed by a unit), used to set the delay between scans	Acquisition	1
SW nD	Spectral width for the n dimension (where n can equal 2, 3, or 4).	Acquisition	1
Dwell_nD	Dwell time for the n dimension	Acquisition	1
Points nD	Number of data points in the n dimension	Acquisition	1
Actual Points nD	Number of points actually collected in the n dimension	Acquisition	2
Points Start nD	Starting point for the n dimension	Acquisition	1
Repeat Times	Number of times to repeat the entire experiment. Used for nD experiments only. Data from each dimension will be added Repeat Times value number of times	Acquisition	1
S.A. Dimension	Sets the dimension (1-4) in which the signal averager will accumulate data- see the pulse sequence chapter for more information.	Acquisition	1
S.A. Mode	Sets behavior of the Signal averager for the dimension specified in S.A.Dimension- see the pulse sequence chapter for more information.	Acquisition	1
DC.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
A0.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
A1.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
A2.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
A3.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
T1.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4

Dashboard Parameters cont.			
Parameter	**Function**	**Default Tab**	**Info***
T2.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
T3.(x, y, z, 0)	Gradient pre-emphasis parameters	Grad. Preemph.	1, 4
Shift # Pts.	Goints value used by left/right shift command	Processing	1
LB nD	Line broadening constant in Hz used during exponential multiplication	Processing	1
GB nD	Line broadening constant in Hz used during Gaussian multiplication	Processing	1
DM nD	Line broadening constant in Hz used for double exponential multiplication	Processing	1
SB Shift nD	Phase shift for sin bell multiplication	Processing	1
SB Width nD	Window points for sin bell multiplication	Processing	1
SB Skew nD	Skew factor for sin bell multiplication	Processing	1
TZ 1-4 nD	Points used for a trapezoidal apodization	Processing	1
Traf nD	Estimated T2 used during Traficante-Ziessow apodization	Processing	1
Sys. Phase 0 nD	Zeroth order phase value stored in the system	Processing	2
Sys. Phase 1 nD	First order phase value stored in the system	Processing	2
Phase 0 nD	Zeroth order phase value	Processing	1
Phase 1 nD	First order phase value	Processing	1
Echo Center nD	Center of echo used in Echo Zero Fill, Echo FFT, and other Echo commands	Processing	1

Not all parameters are active for all systems.

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Status Bar and Tool Tips

Status Bar

The Status bar appears at the bottom of the Main NTNMR window (*not the data window*) and displays various information about the program.

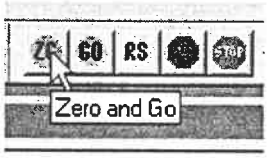
- On the left side of the example above, a description is displayed of the NTNMR object that the mouse is currently over. In this case, the information displayed is a description of the **ZG** button. Look for information about the various components of NTNMR at this location while using NTNMR.

- In the center of the Status Bar is a "Progress Bar" (shown at approximately half completion in the example above) that is updated in real time to show the relative progress of the current acquisition.

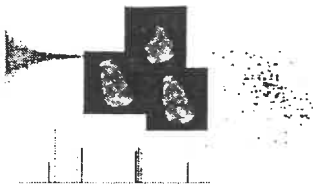
- At the far right of the Status Bar is the acquisition counter information. Counters will appear for each dimension in the currently running experiment in the format *current acq./total acqs. for dimension.*

Tool Tips

Many of the tools and buttons in NTNMR (especially on toolbars and in control swap areas) will pop up a Windows style "Tool Tip" when the mouse pointer is passed over them.



The example above shows the Tool Tip for the ZG button on the Acquisition Toolbar.



2 - Document Window

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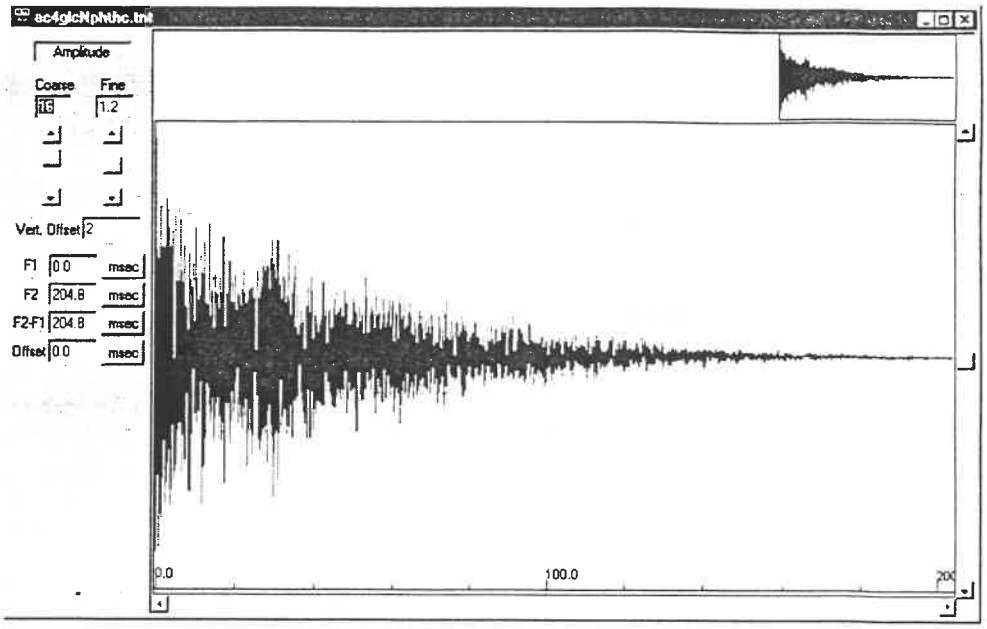
General Information

When NTNMR is launched, the last data file that was saved is opened in an NTNMR Document window. An example of a 1D data set is shown below.

> *The terms "Document Window" and "Data Window" are synonymous and are used interchangeably throughout the NTNMR manuals.*



The Document Window, at launch time, has the following components:

LEFT

- Control Swap Area (initially the Amplitude/Zoom Area)
- Record Selection Scroll Bar and Edit Box (for multi-dimensional data)

UPPER RIGHT

- Mini Display of NTNMR data

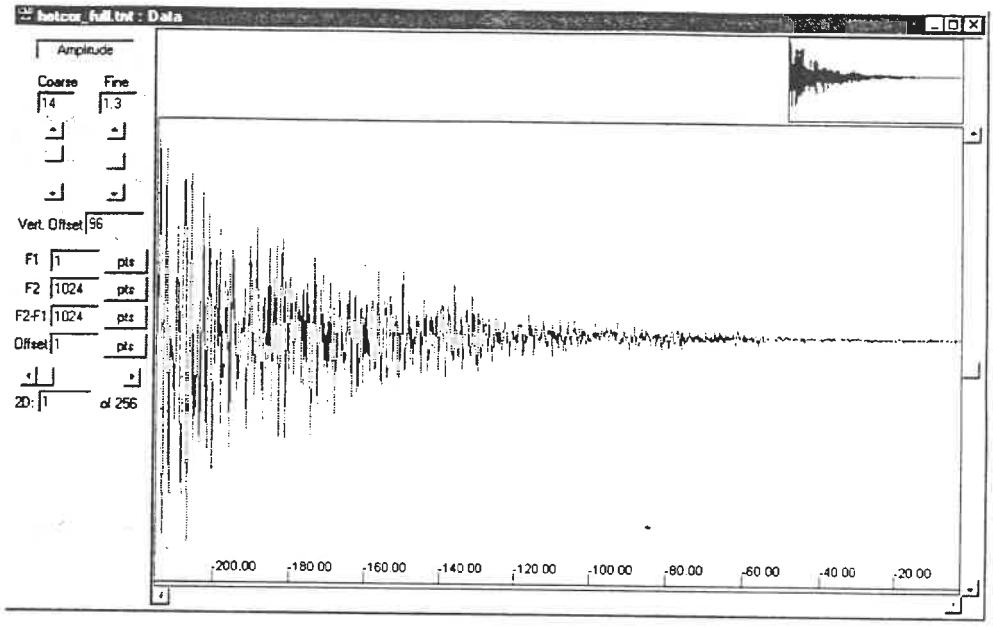
CENTER

- NTNMR Data Area

Another Document window component, the Data Point Information Box, will appear to the left of the Mini Display Area when a data point is selected with the cursor by left-clicking anywhere in the Data portion of the window.

A 2D data set in a Document Window is shown below. The first record is shown.

> *The term "Record" is used in NTNMR to refer to a 2D, 3D, or 4D point or block of data. This term is also applied to pseudo-2D data such as that from T1 experiments.*



To resize the NTNMR Document window, use the size box in the lower right corner of the screen or click the "Maximize" button in the upper right corner of the window. Alternatively, the window can be stretched horizontally or vertically by placing the mouse pointer at the edge of the window, and drag (double-headed cursor will appear). When the window is made smaller, the contents in the lower portion of the Control/Swap Area may not be visible. Windows can also be "minimized" by clicking the "Minimize" button in the upper right corner of the window.

Multiple Windows

NTNMR can open multiple document windows. File|Open will open a NMR data file in a new Data window. The window will be given the same name as the data file, and the window name will be added to the Windows menu list. Multiple copies of the same data file cannot be opened simultaneously. If the application requires that the same data set be opened in two separate windows simply copy rename the data. Available memory is the only limitation on the number of windows that can be opened.

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NTNMR Document Window Components

NTNMR Data Area

The Data Area displays NTNMR data for FIDs or Spectra. The Data area is resized automatically with the Data window.

Cursor and Data Point Information Box

Select a cursor position by single clicking the left mouse button in the Data Display Area. This causes a small rectangle, the Data Point Information Box, to appear above the Data Display Area to the left of the Mini Display Area. This box contains the following information about the selected cursor position:

- point position
- time, ppm, or frequency position
- amplitude of the real, imaginary and magnitude data

The cursor position can also be changed using the right and left arrow keys. If the [SHIFT] key is held down while using the right and left arrow keys the cursor position will jump by 10 points, otherwise the cursor position will change by one point. The data point information in the data box will automatically be updated to reflect the newly selected point.

Points display can be selected in the **View** menu to display the individual points.

ZOOM

Zooming is activated by a left mouse button "click and drag" operation over the region of interest in the Data Display Area. When the mouse key is released, a highlighted area in a contrasting color appears, and an area that corresponds to this selection is highlighted in a contrasting color in the Mini Display Area.

Click the left mouse button in the highlighted region in the Data Display Area to activate the zoom. The Mini Display Area will be updated with a highlighted region corresponding to the current zoom region displayed in the data display area.

Click the left mouse button in the highlighted region of the Mini Display Area and drag to scroll to another area in the data with the same zoom width.

Single clicking at any point within the zoom activates the cursor and causes the Data Point Information Box to appear. The cursor functions identically in the Zoom as in the Data Display Area described above.

If a zoom area was selected in the NTNMR Data Area, but not activated, click outside the highlighted area to cancel the zoom.

To deactivate the zoom, double-click the left mouse button in the Mini Display Area.

To set exact ppm or Hz limits for the zoom parameters, see **Zoom Area** in the Control/Swap Area section.

Zooming within a zoom is possible by the same procedure. To exit the zoom mode and restore the data display to full scale, double-click the left mouse button in the Mini Display Area.

Control Swap Area

The Control Swap Area is used to adjust the display parameters for the NTNMR Data Display Area. When NTNMR is launched, this area contains **Amplitude/Zoom** controls. The Control Swap Area will change when the various modes from the **Option** menu are selected.

The Control Swap are can be turn off completely in order to maximize the viewable data area. The behavior of the control swap area is as follows:

The Control Swap Area will be cleared when:

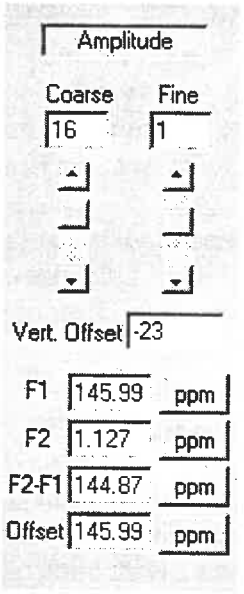
- any mode is selected from the Option menu WHILE another mode is active AND the new mode is exited by de-activating it from the Option menu
- any mode is de-activated through the **Option** menu

The Control Swap Area will default to the Amplitude Control mode when:

- a new mode is selected from the **Option** menu WHILE another mode is active AND the new mode is exited by clicking its Exit, Cancel or Okay buttons

- a file is opened
- a new file is created

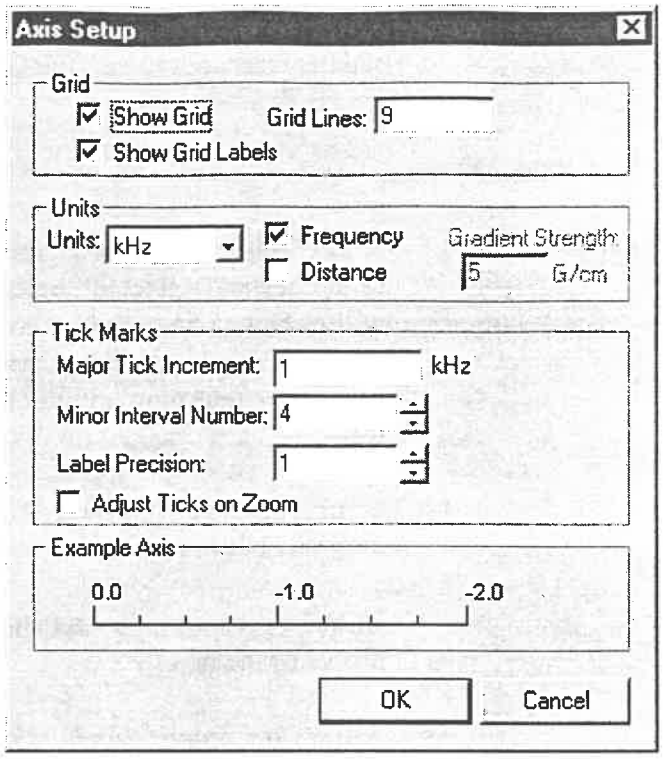
The figure below shows the Amplitude/Zoom area for a single 1D data file when no options are selected from the **Options** menu.



If the file is a 2D file or has multiple 1D records, as in a T1 experiment, a horizontal scroll bar appears at the bottom of the Amplitude/Zoom area. Use this bar to scroll through the records. The box below the bar indicates your current position in the 2D data. Instead of scrolling, you can also type the exact record you wish to advance to into the record box followed by [RETURN] or [ENTER].

Data Axis

The Data Axis (displayed below the data in the Data window) can be toggled on and off by selecting View|Axis. The Axis Setup dialog is activated by double left-clicking on the axis in the data display area.



Axis Setup Controls

Grid

- **Show Grid:** enables the grid drawing under the spectral display window.
- **Show Grid Labels:** enables grid labels
- **Grid Lines:** sets the number of grid lines to e drawn

Units

- **Units:** pop-up to allow the axis units to be set. Axis units track throughout a data window. Thus, if the units are changed in the Axis Setup dialog, they will also be changed in the Amplitude Control Swap area.
- **Frequency** and **Distance**: allows units to be set to frequency or distance. Active only when the data is in the frequency domain.

- **Gradient Strength**: text field for entering the gradient strength in units of G/cm for calibrating the axis is distance units

Tick Marks

- **Major Tick Increment:** Increment (set according to the currently selected units) at which major ticks will be drawn on the axis. The value at a high zoom factor which will automatically be re-adjusted to the limit upon returning to the full spectrum display mode.

- **Minor Interval Number:** this sets the number of intervals between labels.

- **Label Precision:** this sets the number of decimal places of the label.

- **Adjust on Zoom:** this check box enables a scaling of the axis display when the zoom region is selected.

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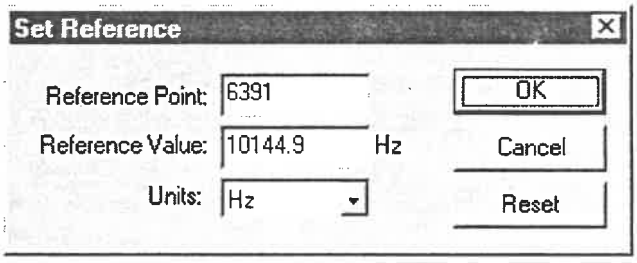
2.3
>>> NEXT >>>

Set Reference Dialog

The Set Reference Dialog is displayed when **Reference|Set Reference** is selected from the **View** menu.

Set Reference Dialog Controls

- **Reference Point:** the data point in the spectrum to which the new frequency or PPM value is to be applied
- **Reference Value:** the new value to be assigned to the **Reference Point** entered
- **Units:** the units for the Reference Value
- **OK** will reference the current data set at the Reference Point to the Reference Value. The current cursor position and its value for the currently selected units are loaded by default. These values can be changed directly by typing in the associated text fields. The units can be selected from the Units pop-up.
- **Cancel** will remove the dialog with no change in reference
- **Reset** will re-position zero Hertz in the center of the frequency axis



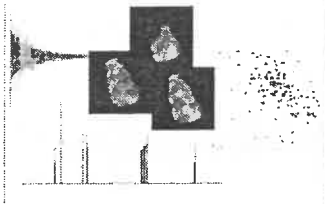
Setting the Spectrum Reference

When the Set Reference dialog is open, the current cursor position is displayed in the **Reference Point** window. A new **Reference Points** can be entered directly. Entering a new **Reference Value** will assign the value entered to the point in the spectrum indicated by the **Reference Point**.

An option for setting an absolute reference that will be available to other windows is also available. This option is discussed in the section on the **View** menu.

Hardware related considerations

The appearance of a NMR Spectrum and the direction of carrier frequency offsets are determined by spectrometer hardware. Channel A and B input positions to the ADC for quadrature detection affect the absolute sign of the spectral peaks with respect to the carrier, and the upper or lower IF side-band used for detection determines the direction of the carrier offset needed to center the spectra.



3 - NTNMR Menus

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3.1
>>> NEXT >>>

File Menu

Menu Item	Description
New (Crtl+N)	Creates a new blank data window and a blank sequence.
Open (Ctrl+O)	Opens a Data file and its associated Parameters in a new window. NTNMR will also open MacNMR files directly if the files are saved with the '*.mn5' file extension.
Close	Closes the currently active window and disposes of the parameters and data.
Import	Allows data in the NMR Pipe format to be imported. Note that the data file will be placed in the currently active window.
Save (Ctrl+S)	Saves the current Data and Parameters, overwriting any other Data previously saved under the same file name. The Sequence and Sequence Parameters are also saved. The user is not queried.
Save As...	Saves the current Data and Parameters in a user selected file name. The Sequence and Sequence Parameters are also saved. The window name is changed to the new name.
Revert to Saved	Re-opens the last saved copy of the current data file.
Export...	The user is prompted for a filename in which to save the current data set. Export file types available are Text (*.txt) and MacNMR (*.mn5). If the file is a 2D data set, all of the records will be saved.
Save Parameters...	Saves the current experiment parameters into a text file. The text file can be viewed and printed with any text editor. Sequence parameters are also saved.
Load Parameters...	Loads a set of experiment parameters from disk, including sequence parameters.
Print Setup...	Selects the page setup for the printer. (See the section on printing)
Print	Print the current data set.
Recent Files List	NTNMR keeps track of the most recently saved files allowing direct access to the files in the Recent Files List. (See example menu above)
Exit	Quits the NTNMR application.

When a Sequence window is active the following options are added to the File menu:

New Sequence	Replace the current sequence with a blank sequence.
Open Sequence	Select and load a new Sequence and its Parameters from disk.
Save Sequence	Save the current Sequence and its Parameters to disk.
Save Sequence As	Save the current Sequence and its Parameters to disk under a new file name.

<<< PREV <<<

3.2

>>> NEXT >>>

Edit Menu

Menu Item	Description
Select All	Selects all of the current data (functional for the NTNMR Document Window).
SetuplAxis	Opens the axis setup dialog shown below.
Preferences	Sets defaults for the user. See the Preferences section at the end of this chapter.

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3.3
>>> NEXT >>>

View Menu

Menu Item	Description
Toolbar	Activates/deactivates the standard NTNMR toolbar.
Status Bar	Activates/deactivates the status bar at the bottom of the NTNMR Main window.
Acquisition Toolbar	Activates/deactivates the Acquisition toolbar.
Console Toolbar	Activates/deactivates the Console toolbar. (Hardware dependent)
Lock Display	Activates the floating window for the lock display (hardware dependent).
Data|Real (Ctrl + R)	Displays the real part of complex data.
Data|Imaginary (Ctrl + I)	Displays the imaginary part of complex data. If real and imaginary are displayed simultaneously, the Data Point Information Box shows the real amplitude only.
Data|Magnitude (Ctrl + I)	Displays the power spectrum of complex data. If real and magnitude are displayed simultaneously, the Data Point Information Box shows the real amplitude only.

Turning off all three Data Display modes will cause only the grid and axes to appear in the display area. If you turn off the grid and axes displays, the program will not appear to be functioning.

Reference|Set Reference	Opens the Set Reference Dialog.
Reference|Get Absolute Reference	Sets the reference mark for the current spectrum to the Absolute Reference that was saved with Set Absolute Reference.
Reference|Set Absolute Reference	Saves the current reference mark for later use. This function allows a reference mark to be applied to another data window.
Axis	Draws a time or frequency axis in the NTNMR Data Area.
Grid	Activates the grid lines in the data window.
Points	Draws the data as discrete points when checked
Shim Units	Causes the Shim Units to appear in the upper right of the Data Display Area.
Auto Scale	Adjusts the Display Window parameters to center the displayed data in the NTNMR Data Area. You may toggle the on/off check mark by re-selecting the menu bar. Once the proper display range is determined, the auto scaling may be de-activated to improve display speed. Same as the Toolbar Auto Scale button.
Fit to Window	Performs a single Auto-Scale operation on the data in the current window.
Integrals	Toggles on and off the integral display.

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>>> NEXT >>>

Option Menu

Each of the selections in the **Options** menu activates a different processing mode for NTNMR data. See the chapter on Options for more information about the available modes.

Menu Item	Description
Amplitude Adjustment	Activates/deactivates the amplitude adjust mode. (Default mode)
Phase Adjustment	Activates the Phase area and allows you to perform zero order and first order phase corrections on the spectrum. Auto phase is also available.
Peak Pick	Enters the Peak Picking mode.
Integrals	Activates the integral display control icon and allows integrals to be defined in the NTNMR data display area.

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>>> NEXT >>>

Commands Menu

The **Commands** menu contains a list of data acquisition, data processing and file I/O instructions that can be executed by the NTNMR program. The menu is organized in a hierarchical fashion. Consult the **Commands** chapter for a complete description of each command available.

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>>> NEXT >>>

Window Menu

The **Window** menu provides items for activating/deactivating various windows as well as a list of currently active windows.

Menu Item	Description
New Window	Creates a new window containing a copy of the current data and parameters. (Different than File|New)
Cascade	Re-sizes and staggers all active windows.
Tile Horizontally	Horizontally tiles all open windows into the main window.
Tile Vertically	Vertically tiles all open windows into the main window.
Arrange Icons	Organizes all minimized windows at the bottom of the main window.
Comment	Opens the comment window. Same as the comment button.
Peak Listing	Opens a text window that contains the peak listing resulting from a Peak Pick.
Integral Listing	Opens a text window that contains the integral listing resulting from an integration operation.
Pulse Program	Activates the Pulse Sequence window. Same as the Pulse Sequence button.
Active Filenames	A listing of all of the open data and sequence windows.

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3.7
<<< PREV <<<

Script Menu

The **Script Menu** allows scripts to be activated from within NTNMR.

Menu Item	Description
Run Script	Execute a script by selecting a script to run through a standard File Open dialog.
Stop Script	Stop the currently running script.
Script name list	A list of scripts that are in the scripts folder in the NTNMR folder.

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Preferences Dialog

Certain preferences can be set which affect the operation of various aspects of NTNMR. Selecting Edit|Preferences activates a tabbed dialog box that has several settings for the general behavior of NTNMR. The description below outlines the available settings.

Acquisition/Console

Console settings are sent to hardware:

- Immediately
- Only when acquisition is started

These settings determine whether or not changes in the console display will be immediate or set only when a new acquisition is started. Items such as frequency change, pre-amplifier selection, etc. will be effected.

1D

Commands

- Zero out points with left shift

If selected the left shift and right shift commands will zero the data point(s) that is (are) shifted. If unchecked, the data points will be circularly shifted, appending the shifted point(s) to the end of start of the current data.

Auto Phase

- Analytical
- Iterative
- Max iterations

Selects the default auto phase mode and the default maximum number of iterations for the iterative auto phase mode. See the chapter that discusses the Option modes for more information on auto phasing.

2D

Basic Options

- Horizontal data inverted
- Vertical data inverted
- Horizontal axis visible
- Vertical axis visible

Vertical axis information from...

- Horizontal Axis
- 2D dashboard settings

If Horizontal Axis is selected, the vertical axis will be an exact copy of the horizontal axis. If 2D dashboard settings is selected, the vertical axis will be calculated from the 2D dashboard settings.

Spectral Component:

- Real
- Imaginary
- Magnitude
- Phase

Selects the data to be shown by default when the 2D data display mode is initially activated.

Data Shown Using

- Contours
- Gradients
- Stack Plot
- Multiple

Selects the default drawing mode.

Sequence

Not used in the current version of NTNMR.

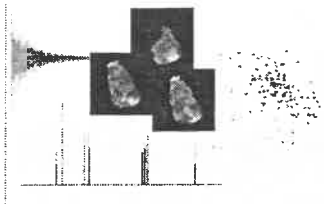
General

Default Units

- Time -sets the default units for time for 1D and 2D displays.
- Frequency -sets the default units for frequency for 1D and 2D displays.
- Distance -sets the default units for distance for 1D and 2D displays.

Directories

- Scripts - indicates the current directory used for scripts.
- Data - indicates the current default data directory.



4 - Commands

<<< PREV <<<
4.1
>>> NEXT >>>

Introduction

All data processing commands are listed in the Commands menu, which is organized in a hierarchical fashion. Other functions such as Set Reference (**View** menu), Auto Phase (**Option** menu), and Integration (**Option** menu) are accessed through other parts of the software.

Each of the main menu items is expanded in the following sections:

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Acquisition Commands

Compile Sequence	Compiles the sequence from the current window.
Zero Memory	Zeros the acquisition memory in hardware.
Go (Crtl + G)	Starts a new acquisition using the sequence and parameters from the current window without zeroing the acquisition memory.
Zero and Go (Crtl + Z)	Zeros acquisition memory and starts a new acquisition in the current window.
Repeat Scan (Crtl + R)	Starts the 'repetitive scan' mode. The current number of scans specified is run continuously without adding data to the signal averager.
Get Data (Crtl + U)	Uploads the data and parameters from the acquisition memory and replaces the data in the front-most window.
Get ADC Data	Uploads the current data and parameters from the digitizer (not the averaged data) and replaces the data in the front-most window.
Stop	Stops the current acquisition.
Abort	Stops the current acquisition.
Real Time Display	Toggles on and off the real time data display.

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4.3 Configuration Commands

>>> NEXT >>>

Reload Init files ... (Ctrl + Shift +R)	Presents a standard File Open dialog allowing selection of a 'config.con" file and other initialization files. Opening a new config.con will not affect the currently loaded data windows or sequences. However, any new sequences that are opened will use the information from the new config.con. Reload config.con also executes a Reset Hardware command. See the Pulse Sequence chapter for more information on the config.con file.
Reset Hardware (Ctrl + Alt +R)	Resets all Tecmag related hardware. (Hardware dependent)
Hardware Status	Queries all modules installed and return to the operational status. This command writes out a text file to the NTNMR temp directory that contains version information for all installed resources.
Load Grad. Pre-em. ...	Presents a File Open dialog for opening a set of gradient pre-emphasis parameters.
Save Grad. Pre-em. ...	Saves the current gradient pre-emphasis parameters from the Dashboard to a file and sets them as the default.

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4.4 Baseline Commands

>>> NEXT >>>

Baseline Correction (Crtl + B)	Removes the dc level of the signal by calculating the mean over the last 12% of the data (Commonly applied before Fourier Transform is performed. Note that the NTNMR Fourier Transform does not apply any DC correction).
Baseline Tilt	Corrects for slope and offset of the baseline. (Commonly used before Auto Integrate.)

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4.5 Zero Fill Commands

>>> NEXT >>>

Zero Fill	Doubles the number of data points (Points 1D) in memory and fills with zeros. This command is valid only for 1D data sets.
Echo Zero Fill	Doubles the number of data points (Points 1D) in memory and fills with zeros, but takes into account that the data is in echo format by zero filling around the point specified by the Dashboard parameter "Echo Center." This command is valid only for 1D data sets.

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>>> NEXT >>>

Apodization Commands

Exponential Multiplication (Crtl + E)	Performs an exponential multiplication on the 1D data set with a function defined by: f(t) = exp - [t * π * (LB 1D)] (LB 1D from Dashboard).
Gaussian Multiplication	Performs a Gaussian multiplication on a 1D data set with a function defined by: f(t) = exp - [(t * π * (GB 1D)) / (1.6651)] exp. 2 (GM 1D from Dashboard)
Double Exponential	Performs Gaussian/exponential weighting using the value in DM 1D. (DM 1D from Dashboard)
Sin Bell	Performs multiplication by a sin bell shaped function on a 1D data set with parameters SB Shift, SB Width and SB Skew from the Dashboard.
Sin Bell Squared	Performs multiplication by a sin bell squared shaped function on a 1D data set with parameters SB Shift, SB Width and SB Skew from the Dashboard.
Trapezoid	Performs weighting using 4 data points (TZ 1 1D, TZ 2 1D, TZ 3 1D and TZ 4 1D) as the trapezoid shape delimiters.
Traf Window	Performs Traficante Ziessow weighting using the parameter Traf 1D - see J. Mag. Res., 66, 182-186 (1986).
Blackman-Harris	Performs Blackman Harris weighting using the values of SB Shift and SB Width.
Echo Exponential Multiplication	Performs an echo exponential multiplication on a 1D data set with a function defined by: f(t) = exp - [t * π * (LB 1D)]. The center of the echo, which does not have to be half the number of points, is specified by the Dashboard parameter "Echo Center."

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>>> NEXT >>>

Transforms

Fourier Transform (Crtl + F)	Performs a one-dimensional fast Fourier transform on a 1D data set.
Inverse FFT	Performs a one-dimensional inverse Fourier transform on a 1D data set.
Real FFT	Calculates the one-sided Fourier transform where the imaginary part is set to zero. After the transform of n complex points, to get n/2 complex points back, use the Read 1st Half command. The transform is one-sided, 0 -> +SW, with the first point at zero frequency, so the axis will have to be redefined.
Echo FFT	Performs a one dimensional fast Fourier Transform on a 1D data set, assuming that the FID starts in the approximate center of the data at the point specified by the Dashboard Parameter "Echo Center."
NDFT (Alt + `)	Performs a pre-defined set of processing commands that can include baseline correction, zero filling, apodization, transformation and phasing. The command can be configured to process 1 to 3 dimensions with a single click. [SHIFT]-select the NDFT command to configure options for each dimension. This command can also be called by clicking on the NDFT toolbar button and configured by [shift]-clicking on the NDFT toolbar button.

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>>> NEXT >>>

Phasing Commands

Phase Correction (Crtl + J)	Applies the zero and first order phase correction in the Dashboard to the current data set.
Auto Phase 0	Uses the DISPA method (an analytical method) of auto phase correction to determine and apply the zero order phase correction. (See the chapter on Options for more information on phasing)
Auto Phase 0 and 1 (Crtl + H)	Uses the DISPA method or an iterative method of auto phase correction to determine and apply the zero and first order phase correction. Select [SHIFT] Auto Phase 0 and 1 to select and configure the two auto phase modes. (See the chapter on Options for more information on phasing.)

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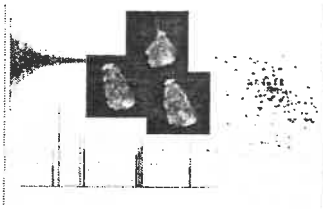
Data Manipulation

Reverse Spectrum	Reverses the spectrum in the current data window.
Read First Half	Extracts the first half of a data record. The Points 1D parameter on the dashboard is halved.
Read Second Half	Extracts the second half of a data record. The Points 1D parameter on the dashboard is halved.
Left Shift	Moves the complex data "Shift # Pts." left and fills the extra space with zeros. See the 1D Preferences for the option to circularly shift data points.
Right Shift	Moves the complex data "Shift # Pts." right and fills extra space with zeros. See the 1D Preferences for the option to circularly shift data points.
Transpose I Complex	Transposes the X and Y dimensions of a 2D data set.
Transpose I Hyper Complex	Performs a hyper complex transpose the X and Y dimensions of a 2D data set.
Separate Records	Allows separation or joining of multi-echo data sets. When selected, a dialog prompts the user to select Separate or Join and the number of 'echoes' to separate or join into. For example, executing "Separate 1 record into 2 segments" on a 256 x 256 data set would create a 128 x 512 data set where the second record would contain the data from the points 129 - 256 of the first record. Similarly, executing "Join 2 records into 1" on a 256 x 256 data set would create a 512 x 128 data set where the first record would contain the data from the original second record appended to the original first record.
Extract Planes	Extracts planes from a 3D data set into separate 2D data sets. A dialog prompts the user to select XY, XZ, or YZ planes. The data files are saved with the names 'basefilename.plane.index_number.tnt' into the directory specified. Use the Browse button to specify the destination directory for the data.
Extract Record	Extracts the active record of a nD data set and saves it to disk in the same directory as the current data set.
Pre-Process Digital Data	Applies a correction for digital acquisition points at the beginning of a FID. This command should only be used if the system is equipped with a digital receiver and if the 'Process Digital Data on Upload' flag is turned off in the preferences dialog.



5 - Options

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5.1
>>> NEXT >>>

Introduction

This chapter of the NTNMR Reference manual covers the various modes that are available from the **Options** menu. The Option modes utilize the 'Control Swap Area' which appears to the left of the NMR data. The Control Swap Area can be completely de-activated by de-selecting the current mode from the Options menu. See the Chapter on the NTNMR Document Window for a detailed discussion on the behavior of the Control Swap Area display.

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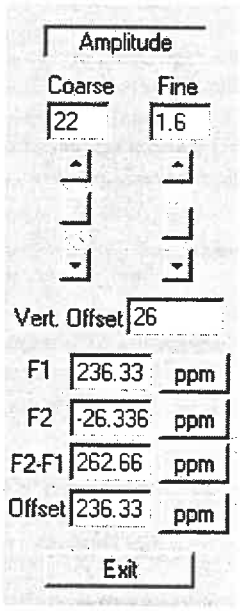
5.2
>>> NEXT >>>

Amplitude Adjustment

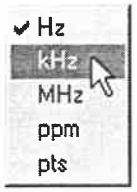


The amplitude adjustment control provides for precise scaling of the 1D data display in both amplitude and in zoom. The vertical offset of the data can also be set directly. Note that the unit display is a click-able, pop-up menu that provides for changing the current units displayed. See the preferences section in the Menus chapter for information on setting the default units for time, frequency and distance.

The keyboard and mouse can also be used to scale and zoom on data. Left-click and drag in the 1D display area to select a zoom region; click the selected region to zoom. Using the up and down arrow keys with the [SHIFT] key held down to adjust the offset of the data while the up and down arrow keys without the [SHIFT] will scale the data. The left and right arrow keys move the cursor. The Intellimouse wheel with and without the [CTRL] can also be used to adjust the scale and offset of the data display.

Amplitude Summary	
Coarse (value and slider)	Number of bits displayed. Adjustable in real time from the slider or by direct input into the text field.
Fine (value and slider)	Multiplying factor of coarse (normal range is 0.5 to 2.0). Adjustable in real time from the slider or by direct input into the text field.
Vertical Offset	Adjusts the vertical offset. Enter a value directly or use [SHIFT], up arrow and [SHIFT], down arrow on the keyboard.
F1	Sets the left edge of the zoom limit.
F2	Sets the right edge of the zoom limit.
F2-F1	Sets the width of the displayed frequency interval.
Offset	Sets the offset (left/right) of the current zoom.
Units Pop-up	Select the units to display on the axis. (See below)
2D and 3D Record	If a 2D or 3D data set is open, additional controls will appear that allow the navigation through multi-dimensional data sets.

Three axis units, msec, sec and points, are available for time domain. To change the axis units, left-click on the current units to reveal a pop-up menu with the current unit checked. All parameters will be updated for the current selection including the current axis labels displayed in the main data window.



Five axis units are available for frequency domain. To change the axis units from Hz to kHz, MHz, ppm or points, left-click and select the desired unit on the popup menu. All the parameters will be updated for the current selection.

The amplitude adjustment option appears as the default control swap area and allows the overall scaling and zooming of the data to be displayed.

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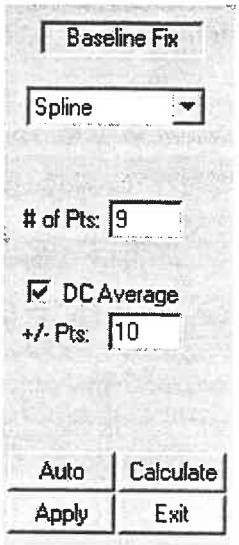
5.3

>>> NEXT >>>

Baseline Fix



The Baseline Fix mode (different from Baseline Correction command) is activated by selecting **Baseline Fix** from the **Option** menu. Baseline Fix provides the ability to apply Spline and Polynomial baseline functions to frequency domain data. Note that Baseline Fix often improves the quality of integration. The table below summarizes the various Baseline Fix functions.

Baseline Fix Summary	
Spine/Polynomial Selection	Allows selection of either a Spine fit or a least squares fit to an nth order Polynomial.
Order	Enter an integer between 1 and 12 for determining the order of the polynomial fit. *Only visible for Polynomial fits.*
# of Points	Enter an integer between 1 and 50 for the number of points to be used.
DC Average	Toggle on/off the DC averaging function. When on the number of points specified below in '+/-' points will be averaged about each point in the fit to calculate a baseline value.
Auto	Click to automatically calculate point placement for the current data set.
Calculate	Calculate the baseline function. The function will be drawn in the data display area.
Apply	Apply the current Baseline Fix to the active data set.
Exit	Exit Baseline Fix mode.

Working with Baseline Fix

Adding and Removing Points

To manually add and remove baseline points, right click and select add or remove from the right click menu. Right clicking on an existing point will activate the remove option from the menu.

Repositioning Baseline Points

Click and drag on any baseline point to move it to a new position.

Scaling the Display

As in the normal 1D data display the data can be scaled using the up and down arrow keys on the keyboard (as well as the Intellimouse, if equipped). *It may be necessary to adjust the scaling and offset of the data to see the calculated function on the display.

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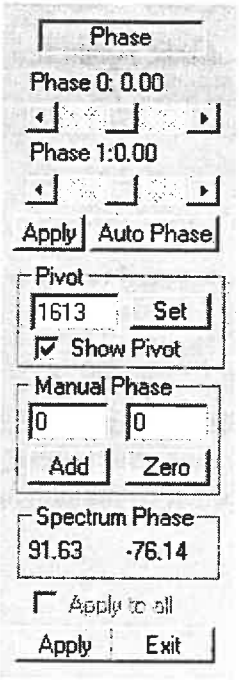
5.4
>>> NEXT >>>

Phase Adjustment



The Phase Adjustment allows you to perform manual zero and first order phase correction on the spectrum. Selecting **Option|Phase Adjustment** causes the Control Swap Area to change to the Phase Area, as shown in the figure to the left. Phase Adjustment mode is only available for frequency domain data. Each control item is discussed below.

Phase Adjustment Summary	
Phase 0 : Value	Slider to manually adjust the 0 order phase correction. The data display is updated in real time. Changes are not saved until the Apply or OK buttons are clicked.
Phase 1 : Value	Slider to manually adjust the 1st order phase correction. The data display is updated in real time. Changes are not saved until the Apply or OK buttons are clicked.
Apply	Applies the current Phase 0 and Phase 1 values set through the manual adjustment sliders and zeroes the Phase 0 and Phase 1 manual sliders.
Auto Phase	Executes the Auto Phase command. [SHIFT]-click to open the auto phase set up dialog. See below for a detailed description.
Pivot value	Displays the current phase pivot value. The phase pivot cursor position is displayed in the data window as a blue cursor. (see Show Pivot below.)
Pivot Reset	Resets the phase pivot point to the current cursor position.
Show Pivot	Toggles the display of the phase pivot cursor (shown in blue) in the data window.
Manual Phase	Two text entry fields for zero (left) and first (right) order phase parameters to be entered directly.
Add	Applies the current phase values displayed in the Manual Phase text boxes.
Zero	Zeroes the values in the Manual Phase text boxes. Does not undo previous phasing operations.
Spectrum Phase	Displays the phase 0 (left) and phase 1 (right) corrections that have been applied to the current data. Information only.
Apply to all	When checked, the phase corrections applied while in the phase adjustment mode apply to all records in a 2D set. For example, it is useful for applying uniform phase corrections to all records in a 2D experiment or a T1 experiment.
OK	Applies the current phase corrections to the data, exits the Phase Adjustment mode and updates the phase parameters in the Dashboard.
Cancel	Exits the Phase Adjustment mode leaving the data and Dashboard unchanged.

The **Phase** Adjustment area displays the total **Spectrum phase** applied at the bottom of the window, which may or may not be equivalent to the **System Phase** (the values used by the **Phase Correction** command in the **Commands** menu). To set the values that will be applied when you select **Phase Correction** from the **Commands** menu, edit the parameters "Sys. Phase 1D" and "Sys. Phase 2D" in the Dashboard.

The slider bars in the **Phase** area may be used to add or subtract zero and first order phase increments to the current phasing of a spectrum. The temporary view phasing display mode in the spectrum window draws the phasing changes

selected by the slide bar controls, but does not apply them to the data unless you hit the **Apply** button (or the **OK** button to exit the window). The pivot point used for the first order phasing is also displayed (in blue) in this area.

To manually input data, click on the desired edit box below the words **Manual Input**, enter the desired numeric value and click on **OK**. Cancel leaves the value unchanged. The **Add** button will apply these values to the data immediately without displaying the phasing in the temporary view mode first! **Zero** will reset the Manual input values to zero, but will not undo the changes to the spectrum.

The **Spectrum phase** section will normally display the same values as the values used to correct the spectrum, since the Spectrum phase is updated to reflect the total phase applied to that spectrum. Any additional incremental corrections or Manual input values is added to the **Spectrum phase.** These values are stored in the data file when the phased spectrum is saved. When a previously phased spectrum file is read, the Spectrum phase section is updated. In this case, the Spectrum phase displayed may be different from the System phase. The **OK** button will close the window and change the System phase to the new Spectrum phase values read from the file, and hence will change the values used by the **Phase Correction** command.

Selecting the **Cancel** button instead of the **OK** button will UNDO the Spectrum Phase Correction by the values applied from this window and close the window. The **Cancel** button does not change the previous System Phase Values. **Note that the value of the zeroth order Spectrum Phase (once OK is clicked) is re-calculated with a pivot point at the center of the spectrum to assure that the Phase Correction command is not dependent on a selection of a pivot point.**

Phasing Help

The two scroll bars, **Phase 0** and **Phase 1**, directly control the zero and first order phase correction parameters according to the formula: $\emptyset(i)$ = (Phase 0) + [(Phase 1) * (i -i_0) / #points in spectrum]. The correction is only previewed in the display window until the **OK** or **Apply** button is hit. Every time the **OK** button is pressed, the phase correction in the top two fields is applied to the spectrum. The bottom row of numbers (Spectrum Phase) is a record of the cumulative total phase applied to that spectrum.

Phasing in zoom mode is also possible, however non-linear (i.e. first order) changes in one part of the spectrum may not adequately represent non-linear phase changes across the entire spectrum. The Mini Display Area can be used as a guide, but does not provide adequate resolution to accurately judge phasing. You can return to the full spectrum display by double-clicking in the Mini

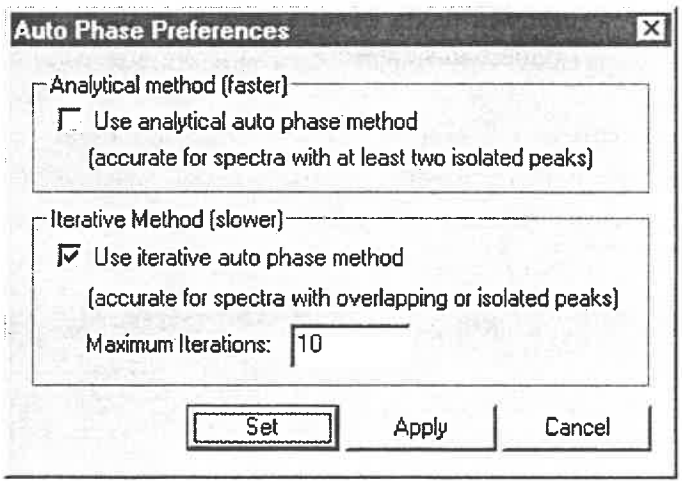
Display Area, or you can drag the highlighted zoom area in the mini-display window to move to another zoom region.

A productive approach to phasing is often to correct for Phase 0 errors in a Zoom region near the cursor and then to slide the Zoom region to another area of the spectrum far away from the Pivot Point and adjust for Phase 1 error. Iterating via this approach will often yield excellent results.

The **Real**, **Imaginary** and **Magnitude** parts of the spectrum can either be displayed together or separately during phasing by choosing the appropriate items from the **Display** menu.

Auto Phase

The **Auto Phase 0 and 1** command allows you to choose which auto-phasing algorithm is used for the automatic phase correction. Once you choose a method, that method will be used every time **Auto Phase 0 and 1** is chosen until the method is changed or when NTNMR is restarted. The default method when NTNMR is launched is the analytical DISPA method. To change the algorithm used, hold down the [SHIFT] key when you choose **Auto Phase 0 and 1** from the **Commands** menu or [SHIFT]-click on the **Auto Phase** button in the **Phase Adjustment** area. The Auto Phase setup dialog is shown below.



Analytical Method

When "Use Analytical Auto Phase Method" is chosen, the DISPA method is used. The DISPA method is described in the Journal of Magnetic Resonance (JMR 76, 458-478 (1988) by Edward C. Craig and Alan G. Marshall). This analytical method is reasonably accurate for zero and first order phasing when

there are 2 isolated peaks in the spectrum. This method is used for the Auto Phase 0 command and will work with only one peak in the spectrum. This method is the faster of the two available modes.

Iterative Method

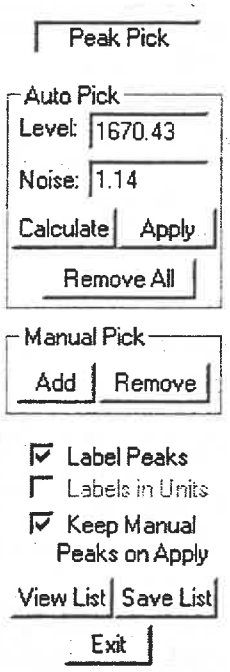
When "Use iterative auto phase method" is chosen, an iterative method of automatic phasing is used, which maximizes the number of points in the baseline and minimizes the width of the peak bases. This algorithm was developed at Abbott Laboratories of Chicago, IL, by Dr. Richard Stephens, and is used in NTNMR with the permission of Abbott Laboratories. This method is good for spectra with overlapping peaks, which do not phase well with the DISPA method. The default number of iterations is 10, which is the smallest number of iterations that yielded reasonably phased spectra in our test data sets. You may change the number of iterations, but any additional iterations will cause this method to take more time. Turn on "ignore auto phase errors" to have NTNMR disregard any errors returned from the auto phase routine. These errors usually occur when the maximum number of iterations has been reached; however, the spectrum is usually phased well enough after 10 iterations to be useful and so turning off the error reporting is usually safe.

Set, Apply and Cancel Buttons

Click “Set” to save the current settings, “Apply” to apply the current settings to the front data window and “Cancel” to leave the settings as they were before the dialog was entered.

<<< PREV <<<
5.5
>>> NEXT >>>

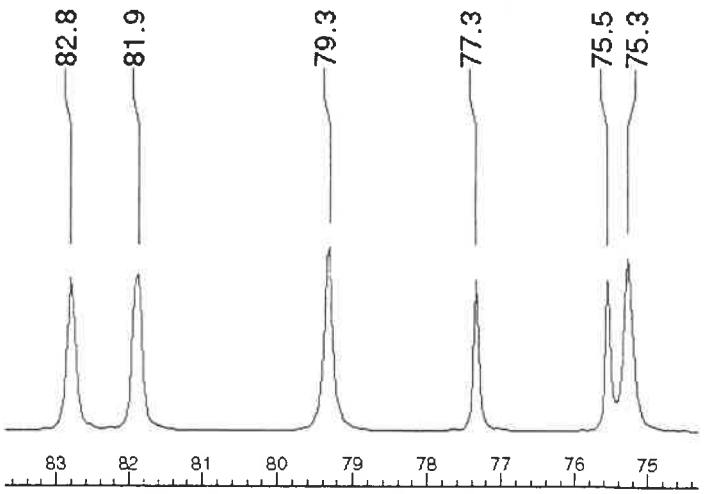
Peak Pick



The **Peak Pick** routine is entered by selecting the **Peak Pick** item under the **Option** menu. Choosing the Peak Pick option causes the Control/Swap Area to change from its current selection to Peak Pick, as shown in the figure.

The current Peak Picks, if any are present, can be displayed by selecting **Peak Picks** from the **Display** menu without the need for entering the peak Pick Option mode.

Note that in the NTNMR Data Window, Peak Pick are displayed only by label, i.e. a number assigned to each peak found ordered from left to right in the display. When printing, the user has the option to display either the peak pick labels or the chemical shift values directly on each peak.



Example of a printed PeakPick format.

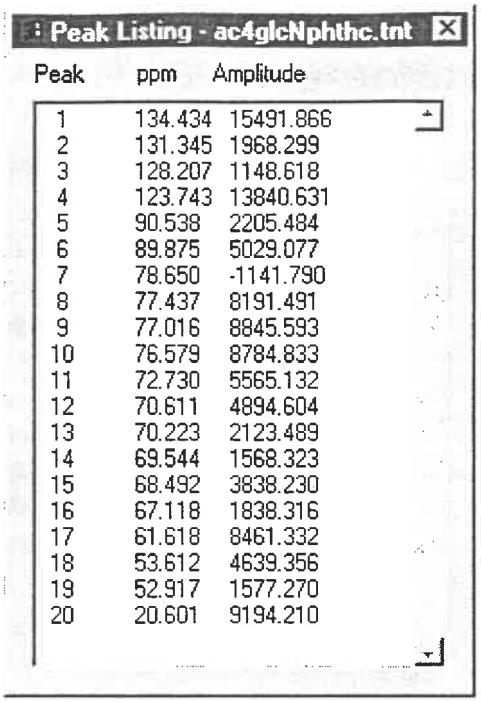
Peak Pick Summary	
Auto Pick: Level	Value above where peaks are detected. NTNMR calculates an initial level threshold.
Auto Pick: Noise	Value which data points must vary by to be considered a peak. NTNMR calculates an initial noise threshold.
Calculate	Calculates the Level and Noise Parameters for the current display area. If an area has been highlighted by a click-and-drag operation, the Level and Noise parameters are calculated for the highlighted region.
Apply	Executes an automatic peak pick using the current Level and Noise parameters.
Remove All	Removes all Peak Picks.
Manual Pick: Add	Adds a peak pick at the current cursor position. Manual picks appear in blue. If a region of the spectrum is highlighted, the Add button will execute an Auto Peak Pick for the highlighted region only using the current Level and Noise parameters.
Manual Pick: Remove	Removes the peak pick at the current cursor position regardless of whether it was generated automatically or manually. If a region of the spectrum is highlighted, all picks that fall inside the highlight will be removed.
Label Peaks	Turns on and off peak labeling on the Data Display Area.
Keep Manual Peak on Apply	If checked, all manual picks that have been made will remain after an auto pick has been executed. Otherwise, manual picks will be cleared when an auto pick is executed.
View List	Opens the Peak List window. (See below)
Save List	Saves the current peak list to a text file.
Exit	Exits the Peak Pick Mode.

General Information

The Peak Pick area provides two edit boxes: Level and Noise. The Level threshold sets a limit on the height of peaks selected. The Noise threshold tests for the difference between potential peaks when moving from point to point in the peak search.

NTNMR will calculate default values for Level and Noise if no values are saved with the data. To set a value for Level or Noise, enter a new value in the appropriate text box. The Level can also be adjusted by positioning the mouse pointer at the top of the level area on the display by dragging up or down.

The Peak Listing window is shown below. A list of currently picked peaks along with the associated chemical shift and amplitude are shown. The peak listing can be saved as a text file by clicking on the Save List button.

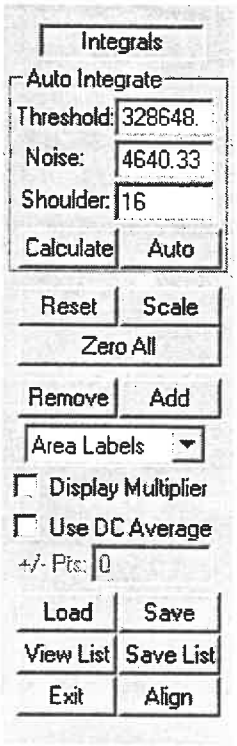


Peak Listing - ac4glcNphthc.tnt

Peak	ppm	Amplitude
1	134.434	15491.866
2	131.345	1968.299
3	128.207	1148.618
4	123.743	13840.631
5	90.538	2205.484
6	89.875	5029.077
7	78.650	-1141.790
8	77.437	8191.491
9	77.016	8845.593
10	76.579	8784.833
11	72.730	5565.132
12	70.611	4894.604
13	70.223	2123.489
14	69.544	1568.323
15	68.492	3838.230
16	67.118	1838.316
17	61.618	8461.332
18	53.612	4639.356
19	52.917	1577.270
20	20.601	9194.210

<<< PREV <<<
5.6
>>> NEXT >>>

Integrals



Choosing the **Integrals** option causes the Control/Swap Area to change from its current selection to **Integrals**, as shown in the figure below. The current integrals, if any are present, can be displayed by selecting **Integrals** from the **Display** menu without the need for entering the Integration Option mode.

The NTNMR Integration mode allows for a great deal of flexibility in adjusting individual integral parameters. It is essential that the user reviews and understands the various functions of the integration routine for optimal results.

Integrals Summary	
Auto Integrate: Threshold	A floating-point number determines if a peak is to be considered for integration. By default, it is 7% of the maximum peak in the spectrum.
Auto Integrate: Noise	A floating-point has value 1.5 times the average of all points that are not above the Peak Threshold. This value, in conjunction with the Shoulder Points, will determine where an integral begins and ends.
Auto Integrate: Shoulder	A long integer value that determines how many points will be averaged as Auto Integrate scans away from a peak.
Auto Integrate: Calculate	Calculates the Threshold, Noise and Shoulder values for an auto integration. Values are calculated for the current data region displayed, or if a region is highlighted for the highlighted region.
Auto Integrate: Auto	Executes an auto integrate command and draws the results on the data display window. Only the data region displayed is integrated. If a region of the spectrum is highlighted, only that region is integrated.
Reset	Resets the active integral to the default values assigned when the integral was originally added.
Scale	Automatically scales the active integral box to the display. Note that this does not effect the integrated value.
Zero All	Zeros the slope, offset and curvature values.
Add	Adds an integral box over the selected region of the spectrum. If there is no highlighted selection a single integral will be added from the entire spectrum.
Remove	Removes all integrals included in the selected region of the spectrum. If there is no highlighted selection all integrals will be removed from the spectrum.
Labels Pop-up	Determines what type of label will be drawn on each integral. 'No Labels' turns off the integral labels on the display. 'Area Labels' displays the area under each integral. 'Number Labels' displays an identification number for each integral.
Display Multiplier	The Display Multiplier button will cause the multipliers set in the Integral Information window to be shown on the Data Display area.
Use DC Average	Allows a user-selectable number of points around the starting point of the integral to be averaged together and used as a dc offset value. Note: if the DC Average button is off or the number of points to average is zero, the first point of the integral is used as a dc offset.
+/- Points	Number of points to be used in calculating the DC average when DC Average is selected.

Integrals Summary Continued	
Load	Loads and integral (*.int) template file from disk.
Save	Saves the current integrals as an integral template file (*.int).
View List	Opens the integral display list. (See below)
Save List	Saves the current integral list as a text file.
Exit	Exits the Integral mode.
Align	Aligns all of the integrals.

General Information

The **Auto Integrate** command scans the data set and chooses integrals based on characteristics of the data set. Auto Integrate is available from the **Commands** menu.

Integrals are calculated using the following formula:

data_buffer[n] - dc_offset + (curvature * n) + slope

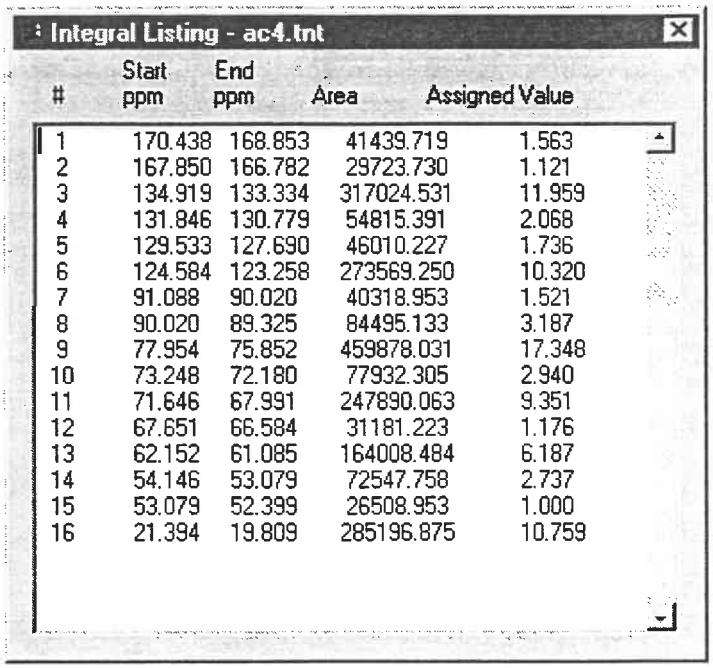
The **Baseline Tilt** command is a command that is used in conjunction with **Auto Integrate**. Choose **Baseline Tilt** from the **Commands** menu either before or after **Auto Integrate** has been applied. This command corrects for the slope and offset of the baseline. Using this command will level off the ends of the integrals created by **Auto Integrate**, since the baseline is corrected. If you have already corrected the baseline using a spline or polynomial fit via **Baseline Fix** from the **Options** menu, do not use this command.

The three characteristics or parameters associated with the **Auto Integrate** are the Peak Threshold, Noise Value and Shoulder Points. The Peak Threshold is a floating-point number that determines if a peak is to be considered for integration. By default, it is 7% of the maximum peak in the spectrum, and is calculated exactly the same way as in the **Peak Pick** mode. If a peak is above the threshold, it will be included in an integral. The Noise Value has a floating-point value 1.5 times the average of all points that are not above the Peak Threshold. This value in conjunction with the Shoulder Points, will determine where an integral begins and ends. The Shoulder Points is a long integer value that determines how many points will be averaged as Auto Integrate scans away from a peak. Once the average of this number of points is below the Noise Value, the integral is terminated.

The **Auto Integrate** parameters are re-calculated each time **Auto Integrate** is chosen from the **Commands** menu. This means that every time **Auto Integrate**

is chosen, the three parameters will be recalculated and then the integrals will be picked.

The Integral List window is shown below. Information about each integral in the current window is displayed and can be saved (**Save** button) as an integral template (*.int) file. Integral template files can be loaded from the **Load** button.



#	Start ppm	End ppm	Area	Assigned Value
1	170.438	168.853	41439.719	1.563
2	167.850	166.782	29723.730	1.121
3	134.919	133.334	317024.531	11.959
4	131.846	130.779	54815.391	2.068
5	129.533	127.690	46010.227	1.736
6	124.584	123.258	273569.250	10.320
7	91.088	90.020	40318.953	1.521
8	90.020	89.325	84495.133	3.187
9	77.954	75.852	459878.031	17.348
10	73.248	72.180	77932.305	2.940
11	71.646	67.991	247890.063	9.351
12	67.651	66.584	31181.223	1.176
13	62.152	61.085	164008.484	6.187
14	54.146	53.079	72547.758	2.737
15	53.079	52.399	26508.953	1.000
16	21.394	19.809	285196.875	10.759

Working With Integrals - Manual Integration

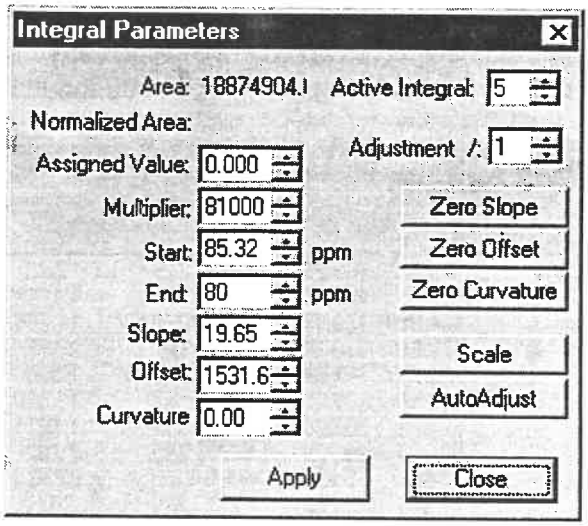
Adding Integrals

Add an integral to the spectrum by clicking and dragging to a select region of the spectrum and then either clicking on the 'Add' button or right clicking and selecting 'Add Integral'.

Removing Integrals

Remove a current integral by clicking and dragging to select the region of the spectrum that contains the integral and either click on the 'Remove' button or right-click and select 'Del Integral'.

Adjusting Integrals Using the Integral Parameters Dialog



Integrals can be adjusted by mouse or by parameter. Double-clicking on any integral will open the 'Integral Parameters' dialog which contains adjustments for all parameters for each individual integral in the spectrum. The table below outlines each parameter. See the next section for information on adjusting integrals by mouse.

Integral Parameters	
Area	Displays the area of the active integral in absolute units.
Normalized Area	Displayed the normalized area of the integral.
Active Integral	Selects the active integral. All parameters displayed are for the current active integral. The active integral will be highlighted in green.
Adjustment	Assigns a scaling value (i.e. sensitivity) to all adjustments made in the Integral Parameters dialog as well as by mouse.
Assigned Value	Allows assignment of an assigned value to a particular integral in the spectrum. When a value is assigned to a particular integral all other integrals are given new assigned values. This is used to normalize all integrals in a spectrum.
Multiplier	A scaling value for an integral display. Note that this parameter does not change the integration values.
Start	The start position of the integral is the left-hand side.
End	The end position of the integral is the right-hand side.
Slope	Adjusts the integral slope. (See the General Information section for details)
Offset	Adjusts the integral offset. (See the General Information section for details)
Curvature	Adjusts the integral curvature (see the General Information section for details).
Zero Slope	Zero the active integrals slope.
Zero Offset	Zero the active integrals offset.
Zero Curvature	Zeroes the active integral curvature.
Scale	Automatically scale the active integral.
Auto-Adjust	Auto adjusts all parameters for the active integral.
Apply	Apply the changes made in the Integral Parameters dialog.
Close	Close the Integral Parameters dialog.

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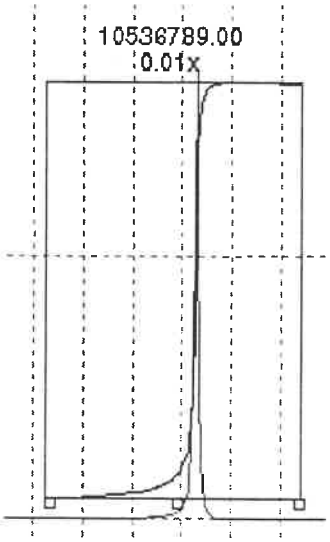
these parameters can be set by "Integrate" Automation fctn in VBscript

Adjusting Integrals Using the Mouse

Each individual integral can be adjusted using the mouse in 5 different ways:



- Position the mouse pointer at either the left or right edge to adjust the start or end position of the integral
- Position the mouse pointer at the top of the integral box to adjust the scaling of the integral
- Position the mouse point at the bottom right hand corner to adjust the integral slope
- Position the mouse pointer at the bottom middle adjustment box to adjust the integral curvature
- Position the mouse pointer at the bottom left hand corner to adjust the integral offset

Note - Holding down the[Shift] key while adjusting an integral by mouse will increase the sensitivity of the adjustment.

Working with Integrals - Automatic Integration

The integration routine allows for automatic integration of an entire spectrum or a selected region. The 'Calculate' button will automatically scan the spectrum (or selected region) and adjust the threshold, noise and shoulder parameters. Clicking the Auto button will then apply the integrals. Note that it is sometimes advantageous to allow NTNMR to automatically calculate the threshold, noise and shoulder parameters for selected regions of the spectrum rather than a total calculation.

Using the Auto Integrate function is a quick way to place integrals on the spectrum, and many times will yield acceptable results for routine integration. If the results are not satisfactory, individual integrals can be adjusted, removed or added as discussed in the sections above.

See the General Information section above for detailed information about the Level, Noise and Shoulder parameters.

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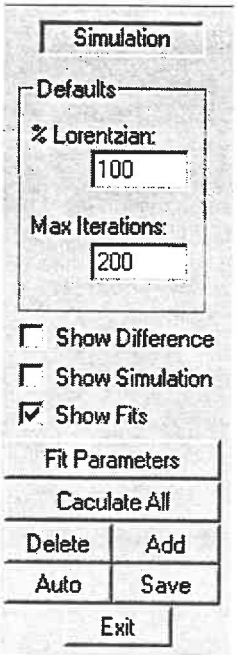
>>> NEXT >>>

Line Fits



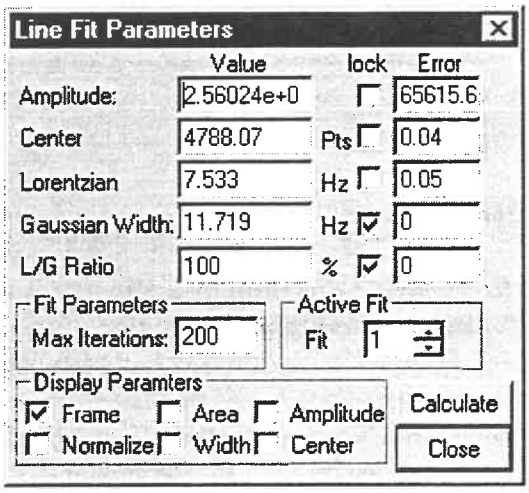
Line fit mode allows for multiple 'Simulation Boxes' to be added to the active spectrum. The line fit toolbar (shown to the left) controls the general behavior of line fits and the display. Individual line fits parameters are modified by mouse and/or by the Line Fit Parameters dialog discussed below.

Click and drag to highlight a region of the spectrum where a new line fit is to be added and click the 'Add' button to create a new 'Simulation Box'.

The table below outlines the various parameters in the master line fit toolbar.

Master Line Fit Parameters	
% Lorentzian	Define the default Lorentzian/Gaussian character of new line fits added. This setting will not override settings in the Line Fit Parameters dialog.
Max Iterations	Sets the maximum number of iteration that will be used when a line fit calculation is executed.
Show Difference	Toggles the display of the difference (in blue) between the real points of the active data set and all line fits.
Show Simulation	Toggles the display of the simulated spectrum (in black) resulting from the sum of all line fits.
Show Fits	Toggles the display of the individual line fits.
Fit Parameters	Opens the Line Fit Parameters dialog. (See below for more information)
Calculate All	Iterates on all line fits.
Delete	The Delete command will remove any line fits that are completed highlighted by a click and drag operation.
Add	The Add command will add a new line fit simulation box over the currently highlight region of the spectrum.
Auto	Attempts to automatically locate all peaks in the spectrum and add simulation boxes for each peak found.
Save	Saves the line fit information for all line fits in the spectrum to a text file.
Exit	Exit the simulation (line fit) mode.

Line Fit Parameters Dialog



The line fit parameters dialog is used to adjust parameters for individual line fits in the spectrum. Each simulation box can be adjusted independently of all others. The table below summarizes all of the parameters in the Line Fit Parameters dialog.

Line Fit Parameters Dialog	
Amplitude	Reports the current amplitude of the active line fit. This value can be edited manually.
Center	Reports the current center point for the active line fit. This value can be edited manually.
Lorentzian	Reports the current Lorentzian width for the active line fit. This value can be edited manually.
Gaussian Width	Reports the current Gaussian width for the active line fit. This value can be edited manually.
L/G Ratio	Reports the current Lorentzian character (in %) for the active line fit. This value can be edited manually.
Max Iterations	Sets the maximum number of iterations allowed for a calculate operation on the active line fit.
Active Fit	A spin control that shows the ID number of the active line fit. Click on the up and down arrows to scroll through the parameters for all line fits without exiting the Line Fit Parameters dialog.
Frame	Turns on and off a frame around the active line fit.
Area	Turns on and off the area value display for the active line fit.
Amplitude	Turns on and off the amplitude value display for the active line fit.
Normalize	Automatically normalizes all values of the current line fit.
Width	Turns on and off the width value display for the active line fit.
Center	Turns on and off the center value display for the active line fit.
Calculate	Re-calculate the fit for the active line fit.
Close	Close the Line Fit Parameters dialog.
Lock	Each parameter value can be locked by clicking the Lock Check Box next to the value display. A parameter that is locked will not be changed by a re-calculation command.
Error	Reports the error estimated for each parameter by the calculation routine.

Working with Line Fits

Line fits are added to the active spectrum by adding individual "Simulation Boxes." Simply click and drag to highlight a region of the spectrum and then click the 'Add' button. Once a simulation box has been added to the spectrum, its characteristics can be modified through the Line Fit Parameter dialog as described above or by mouse. In general, the mouse should only be used to make coarse adjustments while the Line Fit Parameter dialog should be used for fine tuning individual line fits.

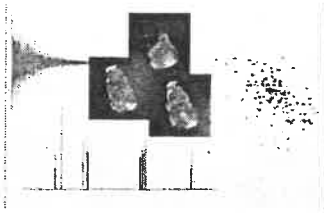
Manipulating a Simulation Box by Mouse
An individual line fit (Simulation Box) can be modified by mouse by clicking and dragging at various points on the simulation box.

- Position the mouse pointer on the left or right hand side of the simulation box to expand the overall width of the simulation box
- Position the mouse pointer on the top or bottom of the simulation box to increase or decrease the overall height of the simulation box
- Position the mouse pointer over the small box on the simulated line to increase the line width of the simulation
- Position the mouse anywhere inside the simulation box to move the entire simulation box left or right

Once the line fit has been positioned, use the Line Fit Parameters dialog to perform final adjustments.

General Notes

- It is often helpful to zoom in on a region of the spectrum when manipulating line fits
- Multiple line fits may overlap
- Using the 'Show Difference' and 'Show Simulation' displays helps give a qualitative picture of the quality of individual line fits



6 - nD Display & Analysis

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6.1
>>> NEXT >>>

Introduction

NTNMR has facilities for viewing multi-dimensional data in a variety of ways. Understanding the various view options and which are most appropriate to your data will ensure that you use NTNMR to its fullest. There are 4 view modes, each mode having several options. Each mode has a main toolbar which controls many of the features. In addition to the main toolbar, auxiliary toolbars may be present. As with all toolbars in NTNMR, the various toolbars specific to multi-dimensional display are dockable and movable and can also be turned off to maximize the display area. Options and controls for the various modes are discussed in detail in the following sections.

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6.2
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Activating nD Display Mode

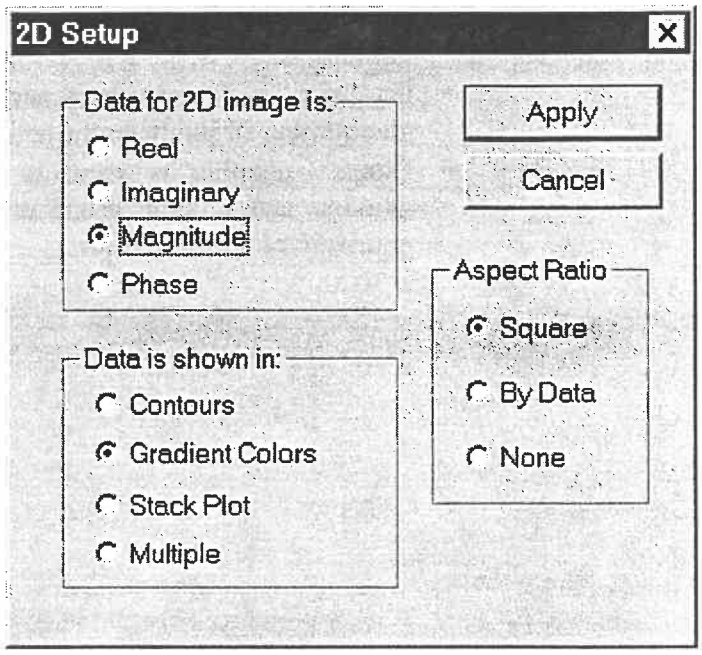
The multi-dimensional display mode is activated by clicking on the nD display button in the toolbar (show graphic) in an analogous fashion to the way the Pulse Sequence edit window is activated. Also analogous to the pulse sequence editor, each data file can have its own nD display window - the only restriction is available memory. Once activated, an nD display window will appear in the list of open windows in the 'Window' menu. Note that the various views associated with a data file such as Pulse Sequence, nD Display, Print Preview, etc. will appear in the Window menu list by the data file name and appended with a number indicating the order in which they were opened. For example, if a data set named 'GRE.tnt' was opened and then an nD Display window was activated followed by the opening this file's Pulse Sequence window, the Widow menu would have the following entries: GRE.tnt:Data, GRE.tnt:2 and GRE.tnt:3. GRE.tnt:Data (or GRE.tnt:1) would apply to the data file, GRE.tnt:2 would apply to the nD display and the GRE.tnt:3 would apply to the Pulse Sequence window. The order of the menu listing depends on the order the various windows were opened.

nD Display Button: 

Clicking on the nD display button will open the nD Display window in the mode that it was last used. That is to say the various options to be discussed

below will be set according to the last file that was used. Multi-dimensional display options are not saved with the data file.

Options can be set prior to opening the nD Display window by holding down the [SHIFT] key on the keyboard, while clicking on the nD display button. The 2D Setup dialog will be displayed (show graphic):



The following options can be selected:

Data type - selects the spectral component to be displayed

- Real - uses the real data points
- Imaginary - uses the imaginary data points
- Magnitude - performs a magnitude calculation:
  Sqr. Rt.(R^2 + I^2)
- Phase - calculates the phase map:
  arctan (I/R)

View Type - selects the type of display

- Contours - calculates a contour plot of the current data
- Gradient Colors - shows the data in continuous color or grayscale mode
- Stack Plot - draws a stack plot of the data
- Multiple Panes - technically a subset of the Gradient Colors mode. This mode allows up to 25 planes of

a 3D or pseudo-3D data set to be displayed simultaneously in a gray scale or continuous color mode.

Aspect Ratio -sets the display aspect ratio (Note - the data is not altered, only the display)

- Square - forces the data to be drawn as a square, regardless of the actual number of points in each dimension.
- By Data - maintains the aspect ratio as dictated by the number of points in the actual data set.
- None - display is sized to the current display window size without regard to the actual number of points in either dimension.

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>>> NEXT >>>

General Applications Guidelines

Depending on the particular application, most users are likely to find that by using a particular subset of the view modes and options. Below is a brief discussion of the various modes and their general applicability to various applications. Of course, the following are only typical examples and are not meant to be inclusive.

2D Imaging data

- Data type: Magnitude
- View Mode: Gradient Colors
- Aspect Ratio: Square

3D or Multi-Slice Imaging data:

It is usually most useful to first view the data as indicated above for 2D Imaging data, examining individual planes by using the 'Plane' spin control and then activating the following settings:

- Data type: Magnitude
- View Mode: Multi-Pane
- Aspect Ratio: Square

Spectroscopy data:

- Data type:
  -Non-phase sensitive experiments: Magnitude
  -Phase sensitive experiments: Real
- View Mode: Contours
- Aspect Ratio: Square or None

T1 data, kinetics data and variable temperature data acquired as pseduo-2D:

- Data type: Real
- View Mode: Stack Plot
- Aspect Ratio: Does not apply

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>>> NEXT >>>

nD Display Mode Menus

Only menu items specific to the nD Display mode are covered here. For information on other menu items, consult the **NTNMR Menus** chapter.

File Menu

Save 2D As...	Saves the current 2D view as a bitmap (*.bmp) file.
Print Setup	See chapter on printing.
Page Setup	See chapter on printing.
Print Preview	See chapter on printing.
Print	See chapter on printing.

Edit Menu

See NTNMR Menus chapter.

View Menu

Palette	Toggles on/off the color palette.
Gradient Toolbar	Toggles on/off the gradient toolbar.
Contour Toolbar	Toggles on/off the contour toolbar.
Slice Toolbar	Toggles on/off the slice toolbar.
Cursor | Crosshair	Activates a full screen crosshair cursor.
Cursor | Vertical Ruler	Activates a vertical ruler cursor. The size of the ruler cursor is determine by the currently active vertical axis unit.
Cursor | Horizontal Ruler	Activates a horizontal ruler cursor. The size of the ruler cursor is determine by the currently active horizontal axis unit.
Cursor | Small Crosshair	Activates a small crosshair cursor.
Data Type Displayed | Real	Uses the real spectral component for image/contour rendering.
Data Type Displayed | Imaginary	Uses the imaginary spectral component for image/contour rendering.
Data Type Displayed | Imaginary	Calculates the magnitude (Sqr. Rt. (R ^ 2 + I ^ 2))of each complex data point and uses this component for image/contour rendering.
Data Type Displayed | Phase Map	Uses the (arctan (I/R)) of each point for image rendering.
Aspect Ratio | Force Square	Forces the 2D display to be drawn square, regardless of the number of data points in either dimension.
Aspect Ratio | By Data	Uses the number of data points in each dimension to define the aspect ratio for display.
Aspect Ratio | None	Uses the maximum available screen space to display the data without regard to the actual number of points in either dimension.
Set Reference...	Activates the 2D Set Reference dialog. See the section below on setting the 2D reference.
2D Settings...	Activates the 2D Settings dialog. See the section below on 2D Settings.
Re-Calculate Levels on Plane	Toggles on/off a mode when the Plane spin control is used to scroll through the 2D planes in a 3D or pseudo-3D data set, the Color Lookup Table for active plane is automatically re-calculated. If this options is off, the Color Lookup Table for the currently displayed 2D plane will be applied to all subsequently displayed planes in the active data set.

Commands Menu

Integrate Selection	Performs a simple integration over the currently selected region. See the section on 2D zooming for details on how to select a region.
Slice | Horizontal	Activates the horizontal slice display mode. (Slice Toolbar will be activated)
Slice | Vertical	Activates the vertical slice display mode. (Slice Toolbar will be activated)
Label | Insert	Prompts the user with a text box for adding a text label at the current cursor position.
Label | Erase	Removes the label (if any) at the current cursor position.
Reverse | Horizontal	Reverses the data display in the horizontal direction. (This command is display only, the data is not altered)
Reverse | Vertical	Reverses the data display in the vertical direction. (This command is display only, the data is not altered).
Reset View	Resets the 2D display area to full display.
Previous Zoom	Sets the 2D display area to the previous user defined zoom.

Scripts Menu

See NTNMR Menus chapter.

Window Menu

See NTNMR Menus chapter.

Help Menu

See NTNMR Menus chapter.

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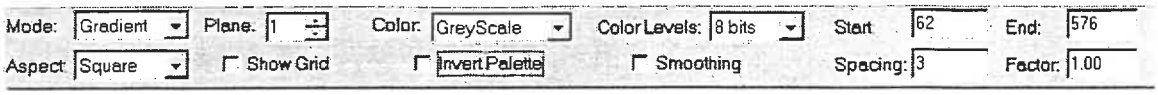
Gradient Color Display Mode

Main Toolbar Controls



- Mode: All nD Display modes have the mode control active. This allows the View Mode to be changed at anytime without the need to exit and re-enter the nD Display. Available options are:

  Gradient - i.e. continuous colors
  Contour
  Stack Plot
  Multiple

- Plane: This spin control allows viewing of all planes in a 3D or pseudo-3D (such as multi-slice data) data set in succession. The number shown corresponds to the currently display plane and can be changed by directly entering a value or by using the up and down arrows.

- Color: Allows selection of either Gray Scale or Color display mode. Color mode uses a rainbow style lookup table.

- Color Levels: This control allows user selection of the color depth. The setting from 8 bits to 2 bits are available.

- Start: Sets the level in the data in arbitrary units at which the first color/gray level will be rendered. (See 'Windowing and Leveling' below).

- End: Sets the level in the data in arbitrary units at which the last color/gray level will be rendered. (See 'Windowing and Leveling' below)

- Spacing: Sets the spacing between the first and second levels drawn. (See 'Windowing and Leveling' below)

- Factor: Sets the multiplier factor used to calculate the spacing for levels 2 through N. (See 'Windowing and Leveling' below)

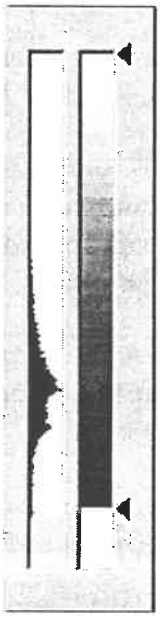
- Aspect: Options for selecting the aspect ratio for drawing the data. 'Square' forces the data to be drawn square regardless of the number of actual points in each dimension. 'By Data' draws the data on the screen in an aspect ratio calculated by the number of points in each dimension. 'None' uses the maximum available space in the nD display window without regard to the actual number of points in the data.

- Show Grid: Toggles on and off a grid that is drawn according the to major tick marks chosen for the horizontal and vertical axes.

- Invert Palette: Flips the color/grayscale palette that is used to render the data.

- Smoothing: Toggles a mode that applies a smoothing algorithm to the data for display purposes only. The raw data is not altered.

Color Lookup Table Toolbar



The Color Lookup Table toolbar allows graphical control over the Start, End and Spacing parameters as well as a visual histogram display of the data.

Histogram: The histogram display gives a visual cue to the relative amount of data at any particular level. The histogram threshold can be set in the 2D Settings dialog as a percentage of the maximum data value.

Windowing and Leveling

The Color Lookup Table has handles that can be manipulated graphically to set the windowing and leveling for a data set. Click, hold and drag the top arrow to move the end level and the bottom arrow to move the start level. Click, hold and drag anywhere on the color bar to move the window over the data.

Double-click on the color bar to reset the color distribution to the default values - i.e. start at 1 and end at the maximum data.

The Color Lookup Table can also be manipulated by the Start/End/Spacing/ and Factor parameters discussed above. Notice that as the graphical tools are used to window and level the data, the Start/End/Spacing and Factor values are adjusted and vice versa.

An extra degree of flexibility is added by using the Factor parameter value. The Factor parameter allows one to apply a non-linear lookup table to the data. A Factor value of '1.00' applies a strictly linear mapping of the color/grayscale levels to the data, meaning that the spacing between each level is identical and is equal to the value in the parameter Spacing. A Factor value of greater than or less than one will apply a non-linear mapping of the color lookup table onto the data according the following:

Level 1 = Start
Level 2 = Start + Spacing
Level N = Start + (Spacing * Factor ^ (N - 2))

Where N = the total number of levels specified

This allows look-up tables to be constructed that emphasize the lower portions of the data by increasing the spacing between levels as the level number increases, or to emphasize the upper portions of the data by decreasing the spacing as the level number increases. This effectively compresses the Color Lookup Table on either end.

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Multi-Pane Display Mode

The Multi-Pane display mode is a sub set of the Gradient display mode which allows the simultaneous display of up to 25 planes of a 3D or pseudo-3D data set. This mode is most often used for viewing multiple slices from a multi-slice data set of for view planes from a diffusion weighted data set. This mode is restricted to displaying data in the continuous color or gray scale mode.

Main Toolbar Controls

Most of the toolbar controls for the Multi-Pane display mode are identical to those in the Gradient display mode. Those controls that are unique to the Multi-Pane display are described below, for others consult the section above on **Gradient Color Display Mode**.

- Plane: The plane control in Multi-Image mode moves the focus (indicated by a red outline) to the specified plane. If the layout specified is smaller than the total number of planes, the plane control with "rotate in" the next plane to the display. In other words, if planes one through four of a sixteen plane data set are displayed, when the Plane control counter reaches five, the image display will be re-drawn with images two through five (two at the upper left and five at the lower right).

- Border: This spin control sets the number of points to use a border between all panes displayed.

- Layout: The Layout combo box allows selection of 2x2, 3x3, 4x4 and 5x5 modes. NTNMR will attempt to fill the available screen space regardless of the total number of planes displayed.

Windowing and Leveling

Windowing and leveling of the data is accomplished as described in the section above on the Gradient Display Mode. The same windowing and leveling parameters are applied to all planes in the data set. If the Mode control is used

to exit Multi-Image mode, the current windowing and leveling parameters are carried over into the new mode.

Zooming

All zooming functions as discussed in the section on zooming below are available in Multi-Image mode. As with windowing and leveling, all planes will have the same zoom parameters applied to them. Therefore, any image displayed can be used to define a zoom region. When the zoom operation is executed all images will update with new boundaries.

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Contour Display Mode

Main Toolbar Controls

- Mode: All nD Display modes have the mode control active. This allows the View Mode to be changed at anytime without the need to exit and re-enter the nD Display. Available options are:

  Gradient - i.e. continuous colors
  Contour
  Stack Plot
  Multi Pane

- Plane: This spin control allows viewing of all planes in a 3D or pseudo-3D data set in succession. The number shown corresponds to the currently display plane and can be changed by directly entering a value or by using the up and down arrows.

- Color: Allows selection of "Black and White," "+/-" or "Ramped Color" display modes. The mode selected determines the colors that will be used to draw the contours. "Black and White" draws all contours in black and therefore lends no distinction to positive or negative contours in the data. The "+/-" mode draws all positive contours in blue and all negative colors in red. "Ramped Color" (the default mode) uses a color ramp to define the color assigned to positive and negative contours. Positive contours are drawn starting with light blue and ending at dark blue so that levels that are closer to "Start" are drawn lighter and the level color darkens as the level increases. For example, more intense data is drawn with a darker shade of blue. Similarly, negative data closest to "Start" are drawn in a light shade of red, whereas negative data closer to "End" are drawn with an increasingly darker shade of red For ex.ample, more intense negative data is drawn in a darker shade of red. See also the "Invert Palette" selection below.

- Positive # Levels: This text box controls the number of positive contours that will be drawn. The check box allows positive contour levels to be turned off.

- Negative # Levels: This text box controls the number of negative contours that will be drawn. The check box allows negative contour levels to be turned off.

- Start: Sets the level in the data in arbitrary units at which the first contour level will be drawn.

- End: Sets the level in the data in arbitrary units at which the last contour level will be drawn.

- Spacing: Sets the spacing between the first and second levels drawn.

- Factor: The Factor parameter allows one to apply a non-linear lookup table to the data. A Factor value of '1.00' applies a strictly linear mapping of contour levels on the data, meaning that the spacing between each level is identical and is equal to the value in the parameter Spacing. A Factor value of greater than or less than one will apply a non-linear mapping of the color lookup table onto the data according the following:

  Level 1 = Start
  Level 2 = Start + Spacing
  Level N = Start + (Spacing * Factor ^ (N - 2))

  Where N = the total number of levels specified.

- Aspect: Options for selecting the aspect ratio for drawing the data. 'Square' forces the data to be drawn square regardless of the number of actual points in each dimension. 'By Data' draws the data on the screen in an aspect ratio calculated by the number of points in each dimension. 'None' uses the maximum available space in the nD display

window without regard to the actual number of points in the data.

- Show Grid: Toggles on and off a grid that is drawn according the to major tick marks chosen for the horizontal and vertical axes.

- Invert Palette: Flips the ramped color palette used to assign colors to contour levels. This selection inverts the "positive" palette and the "negative" palette independently. When selected positive and negative levels will be drawn from dark to light instead of the default light to dark. The base color (blue for positive and red for negative) is not inverted. See the description of the "Color" parameter above for more information.

Color Lookup Table Toolbar

The Color Lookup Table toolbar allows graphical control over the Start, End and Spacing parameters as well as a visual histogram display of the data.

The histogram display gives a visual cue to the relative amount of data at any particular level. The histogram threshold can be set in the 2D Settings dialog as a percentage of the maximum data value.

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Stack Plot Display Mode

Main Toolbar Controls

- Plane: This spin control allows viewing of all planes in a 3D or pseudo-3D data set in succession. The number shown corresponds to the currently displayed plane and can be changed by directly entering a value or by using the up and down arrows.

- Whitewash: When selected, the data is drawn such that the front most peak of any overlapping peaks takes precedent.

- Scale: This spin control allows the overall scaling of the stack plot drawn to be adjusted. Values can be directly entered or the up and down arrows can be used for adjustment.

Manipulating a Stack Plot

There are three handles that can be used to manipulate the aspect ratio, position and overall size of stack plots. Click-hold-and-drag on any of the three handles to interactively manipulate the drawing. The speed that stack plots can be manipulated and can be increased by toggling off the "Whitewash" option.

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Zooming

The zoom feature is active in Contour, Gradient and Multi-Image display modes.

Defining a zoom region:

To define a zoom region left-click and drag. (Show step by step graphics here) Once the zoom region has been defined release the mouse button. The zoom box has handles in each corner and on all edges for manipulating the size of the box. Click-hold-and-drag on any of the handles to re-size the zoom region. Click-and-hold anywhere inside the defined zoom box to re-position it on the display. Right-click anywhere in the center of the zoom box to execute the zoom.

Note that the aspect ratio of the zoom box is constrained by the currently selected "Aspect." If the aspect ratio is set to "Force Square" only, square zoom regions are allowed. If the aspect ratio is set to none, any arbitrary rectangle can be used.

Clearing a zoom region:

Left-click anywhere outside of the defined zoom region to clear the current selection.

Returning to full scale:

"Reset View" in the Commands menu will reset the display to full scale.

Returning to the previous zoom:

"Previous Zoom" in the Commands menu will set the display to the previously defined zoom region.

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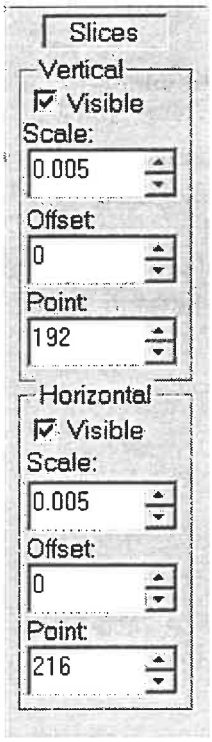
Data Slice Tool

In Gradient and Contour display modes NTNMR has facilities for viewing 1D slices through the 2D array in the horizontal and/or vertical directions.



Selecting Slice | Horizontal or Slice | Vertical from the Commands menu will activate the Slice toolbar. The Slice toolbar has two identical groupings of controls, one for vertical display and one for horizontal display.

- Visible: Toggles on/off the slice display for the vertical or horizontal direction appropriately.
- Scale: The scaling of all slices for each direction can be adjusted independently. Scale values can be entered directly or the up and down arrows can be used to scale the data.
- Offset: By default, the active slice is drawn at its corresponding point position in the data display. The offset parameter allows the slice that is drawn to be moved away from the its actual point position in the data.
- Point: The point parameter specifies the slice of the data that is drawn and is indicated by a slice position line drawn on the display. Entering a value directly or using the up and down arrow keys will cause the corresponding slice to be drawn.

Manipulating slices by Mouse:

Data slices can be moved in either direction by mouse. When the mouse pointer is positioned over the slice position line, a double-headed arrow appears. Click-hold-and-drag to move the slice position line to a new position.

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Cursor Options

Four nD cursors are available and can be selected from the "View" menu under the sub heading "Cursor."

Crosshair: Activates a full screen crosshair cursor.

Small Crosshair: Activates a small crosshair cursor.

Vertical Ruler: Activates a vertical ruler cursor. The size of the ruler cursor is determined by the currently active vertical axis unit.

Horizontal Ruler: Activates a horizontal ruler cursor. The size of the ruler cursor is determined by the currently active horizontal axis unit.

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Coordinate, Amplitude, and Distance Information

NTNMR displays spectral information along the top of the nD display area depending on the active display mode.

Contour Mode:

X and Y coordinate information is displayed for the current cursor position in both the current axis units and in points.

The raw data point amplitude is shown for the current cursor position.

Gradient Mode:

X and Y coordinate information is displayed for the current cursor position in both the current axis units and in points.

The raw data point amplitude is shown for the current cursor position.

The distance between the last two cursor positions defined by a mouse click is displayed in the units of the currently active axis.

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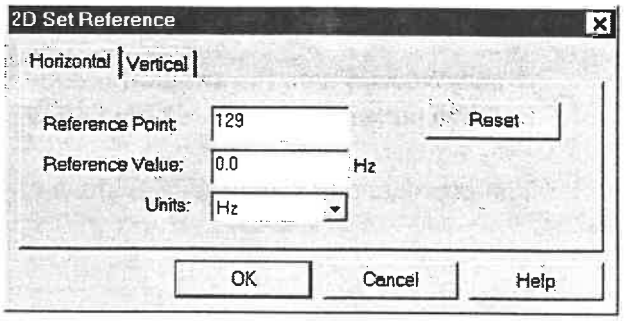
Setting the 2D Reference

The reference marks for the horizontal and vertical dimension are set through the 2D Set Reference dialog, which is activated by selecting "Set Reference" from the View menu. There tabs for activating the horizontal and the vertical settings; both function identically.



- **Reference Point**: By default, each time the 2D Set Reference dialog is opened, the current value for the center point in the specified dimension is indicated. This value can be edited so assign a new value to any point in the spectrum.

- **Reference Value**: By default, each time the 2D Set Reference dialog is opened, the current reference value for the center point in the specified dimension is displayed (the center point is indicated as the default entry for "Reference Point"). The value assigned to the point indicated by "Reference Point" can be entered directly.

- **Units**: Indicates the currently active axis units. The units can be changed and the units for the reference value will be updated appropriately.

- **Reset**: Clicking the Reset button for either dimension will set the reference value to zero (in the currently selected units) for the center point in the spectrum.

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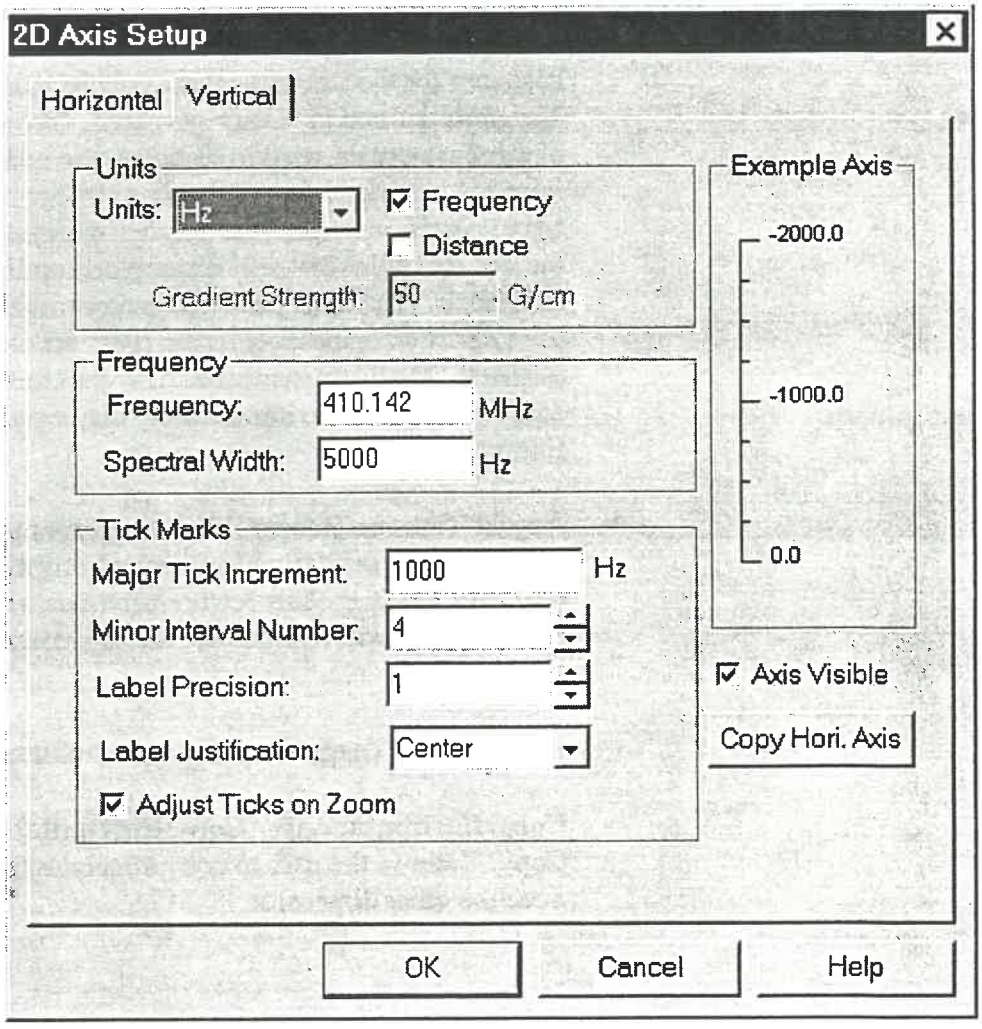
2D Axes

Horizontal and vertical axes are defined in the 2D Axis Setup dialog. The dialog is activated by selecting "Axis Setup..." from the View menu or by double-clicking on either axis (if no axis is visible double-clicking to in the axis display region will activate the Axis Setup dialog). There are tabs for setting up the horizontal and vertical axes independently.



- **Units**: Axes can be defined in frequency or distance units. Allowed frequency units are Hz, kHz, MHz, and ppm. Allowed distance units are um, mm, cm, and m. The gradient strength parameter must also be specified for correct calibration of a distance axis.

- **Frequency**: The frequency and spectral width are extracted from the dashboard and are used to calculate the axis. By default the frequency and the SW from the directly detected dimension are inserted into both the horizontal and the vertical axis dialogs. Both parameters can be edited directly by the user.

- **Tick Marks**: The major tick increment defines the base unit for the tick marks that will be labeled. The units defined in "Units" are used. The number of minor intervals, used to calculate the number of minor tick marks, is specified as an integer number. Label precision defines the number of digits after the decimal point that will be included on the major tick labels. The label justification control allows the major tick mark labels to be right, left or center justified. Modifications made to any of the Tick Mark parameters are immediately displayed in the Example Axis.

- **Adjust Ticks on Zoom**: Often when zooming, the tick marks for the defined axis may become too coarse or too fine. This feature activates a mode in NTNMR that will re-calculate the tick marks for the new zoom.

- **Axis Visible**: Toggles on/off the axis in the display.

- **Copy Horizontal Axis / Copy Horizontal Axis**: Copy... allows the user to copy all axis settings from the other dimension.

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>>> NEXT >>>

2D Preferences

The master NTNMR Preferences dialog is open when "Preferences" is selected from the Edit menu. It contains a tab for 2D display default settings.

- **Horizontal data inverted**: applies a spectrum reverse to the horizontal axis of the data before display. (display only, the actual data is not altered)
- **Vertical data inverted**: applies a spectrum reverse to the vertical axis of the data before display. (display only, the actual data is not altered)
- **Horizontal axis visible / Vertical axis visible**: Determine whether or not horizontal and vertical axes will be displayed as the default behavior. Regardless of this setting, the axes can be activated through the 2D Axis Setup dialog.
- **Data component**: Sets NTNMR to display Real, Imaginary, Magnitude or Phase data by default. The data component used to render the data can be changed on the fly in the 2D display mode through the View menu and the right-click menu.
- **Data shown**: Sets NTNMR to display contours or gradients as the default. The data rendering can be changed on the fly in the 2D display mode.

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2D Settings

The 2D Settings dialog (opened by selecting "2D Settings" from the "View" menu) contains master controls for many of the items that are available on the 2D Display Main Toolbars. Each tab is discussed in turn below.

Gradient Color Settings Tab

- **Gradient**: Color or Gray Scale can be selected.
- **Gray Scale Intensity**: Slider controls allow the starting and ending gray scale intensity that will be used to map the color palette. (Active for gray scale only)

General 2D Settings tab

- **Histogram Threshold**: Settings are to control the appearance of the histogram in the Color Lookup Table Toolbar. The value entered is the percentage of the maximum data value; all data above the percentage of the maximum value specified will be included in the histogram count.
- **Multi-Pane Display**: When the Multi-Pane display mode (i.e. "Multiple") is active, this parameter sets the number of pixels that will be used as blank space in between panes in the display window.

Contour Level Setting Tab

- **Positive Levels / Negative Levels**: These toggles turn on and off the positive and negative contours respectively.
- **Start**: Sets the level in the data at which the first contour will be drawn.
- **# Positive Levels**: Sets the number of positive levels that will be drawn.
- **# Negative Levels**: Set the number of negative levels that will be drawn.

- **Spacing**: Parameter used to determine the separation of contour levels. See the section above on Contour display mode for details on how contour levels are calculated.

- **Factor**: Parameter used to determine the separation of contour levels drawn. See the section above on Contour display mode for details on how contour levels are calculated.

- **Pen Width**: The pen width (in points) that is used to draw the contours to the screen.

- **Data Range - Data Minimum**: The minimum data amplitude is calculated and displayed. This parameter is informational only and cannot be edited.

- **Data Range - Data Maximum**: The maximum data amplitude is calculated and displayed. This parameter is informational only and cannot be edited.

- Contour Color Settings Tab

- **Contour Palettes**: Choices for Black and White, Two color (red and blue) and Ramped Color are available for contour rendering.

Gradient Level Settings Tab

- **Levels** - Number of Colors: Parameter that determines the number of colors that will be used to render the data display (active for Gradient and Multiple modes only). This number corresponds to the Color Levels parameter in the toolbar.

- **Range - Data Minimum**: The minimum data amplitude is calculated and displayed. This parameter is informational only and cannot be edited.

- **Range - Data Maximum**: The maximum data amplitude is calculated and displayed. This

parameter is informational only and cannot be edited.

- **Show Data**: Sets the start level for the data display.
- **To**: Sets the end level for the data display.

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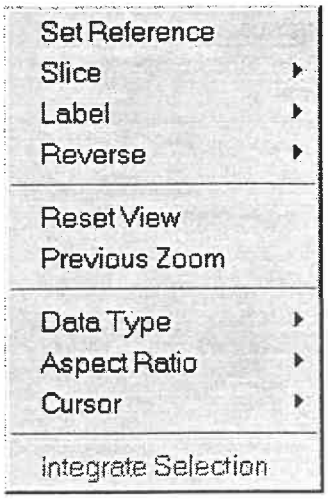
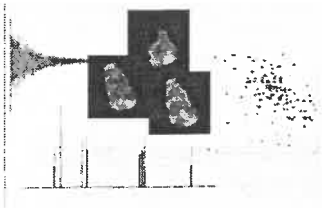
nD Display Right Click Menu

Right-clicking anywhere in the nD display area will open the "right-click" menu. Many of the commonly used features of the nD Display mode can be accessed from this menu and is usually the quickest way to work with the display.



- **Set Reference**: Activates the Set Reference dialog. (See section above for details on setting the reference mark)
- **Slice / Horizontal**: Displays a horizontal slice at the current cursor position and activates the slice toolbar. (See Data Slice Tool above)
- **Slice / Vertical**: Displays a horizontal slice at the current cursor position and activates the slice toolbar. (See Data Slice Tool above)
- **Reverse / Horizontal**: Reverses the orientation of the 2D display about the horizontal direction. (Display only, the data is not altered)
- **Reverse / Vertical**: Reverses the orientation of the 2D display about the vertical direction. (Display only, the data is not altered)
- **Reset View**: Resets the zoom to full
- **Previous Zoom**: Resets the display to the previous zoom region chosen.
- **Data Type**: Selects the spectral component that is used to rendering the display. Choices are Real, Imaginary, Magnitude and Phase.

- **Aspect Ratio**: Allows the aspect ratio of the display to be set to "force square", "by data" and "none."
- **Cursor**: See Cursor Options above.
- **Integrate Selection**: When a zoom box is defined, Integrate Selection performs a simple integration over the selected region.



7 - Printing

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Introduction

NTNMR supports printing of 1D, multiple 1D and 2D data sets. Printouts can be sent to any available printing device or saved to postscript using any available printer driver. Note also that both 1D and 2D data sets can be saved as bitmap or jpeg format using the Export command from the file menu available in the 1D display and 2D display modes but *not in print preview mode.*

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1D Printing

1D Print Commands

All printing functions are accessed from the File menu in the Print section (see below). Four 1D printing commands are available: Print Setup, Print Preview, Add to Print Preview and Print (Ctrl + P).

Print Setup	Opens the setup dialog for the currently active Windows printer. Depending on the printer driver, items such as paper source, page orientation, color management, etc. are set in this dialog.
Print Preview	Activates the NTNMR Print Preview mode. See the Print Preview section for an overview of the various controls for manipulating printouts.
Add to Print Preview	Adds the currently displayed data to the Print Preview window.
Print (Ctrl + P)	The Print command bypasses the Print Preview mode and send the current data directly to the printer. The default print template will be used to format the print out (if a default print template has been saved).

Default Print Template

1D Print outs can be made more consistent by creating and saving a default print template. Print templates are saved using the 1D Print Preview mode (see the next section). Once a default print template has been saved, NTNMR will apply the default template to all print outs that are executed by selecting 'Print' from the file menu or by clicking the 'Print' button on the main toolbar. The default print template will also be applied upon entering 1D Print Preview mode.

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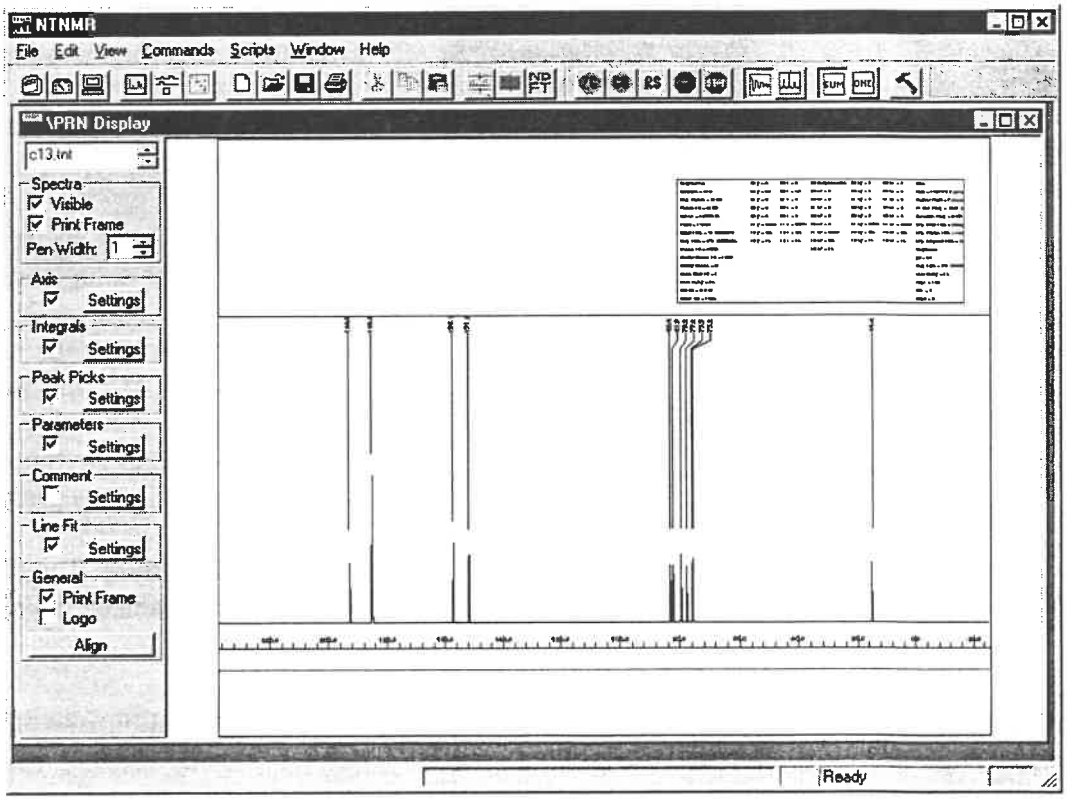
1D Print Preview

Select 'Print Preview' from the File menu when in any 1D view to add the current data set to the Print Preview and open the Print Preview mode.

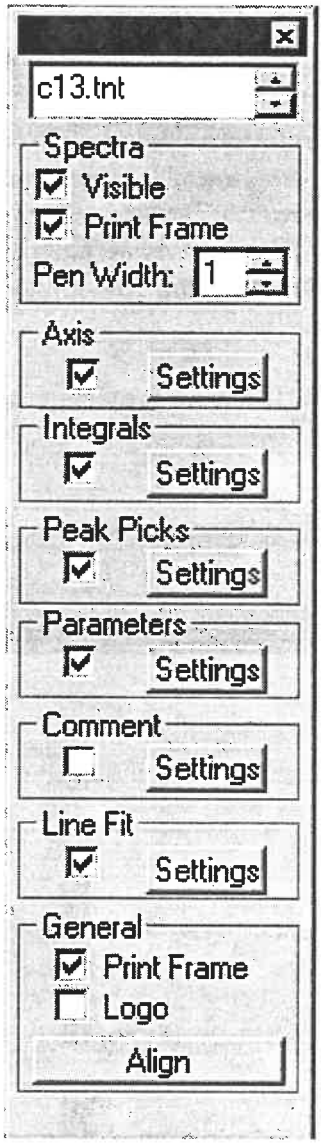
> *Note: NTNMR has two print preview modes: 1D (including multiple 1D, register plots, etc.) and 2D. These two modes are independent and do not interact. 1D plots (as projections, as 1D slices, or from separate 1D files) can be included in 2D plots along the top and left sides. See the 2D Print Preview section for information on 2D printing.*

Shown below is an example of the 1D print preview window.



Customizing 1D Printouts

1D Print Preview Toolbar



Data Set Selection Box: The text box at the top of the window shows the filenames for the data sets that have been added to the 1D Print Preview. All other settings except for those in the 'General' section apply only to the data set that is currently active in the Data Set Selection box.

Spectra / Visible: Determines whether or not the selected spectrum will be printed.

Spectra / Print Frame: Determines whether or not NTNMR will draw a frame around the active spectrum.

Spectra / Pen Width: Allows selection of the pen width to be used to draw the active data set.

Axis Checkbox: Toggle on/off the axis for the selected data set.

Axis Settings: Opens the Print Preview Settings dialog to the Axis setup item.

> **Pen:** Determines the pen width that is used to draw the axis for the active data set.
>
> **Axis:** Selects the font size to be used for the axis labels for the active data set.

Integrals Checkbox: Toggle on/off the integrals for the selected data set.

Integral Settings: Opens the Print Preview Settings dialog to the Integrals setup item.

> **Font:** Sets the font size for displayed integral information.
>
> **Pen:** Selects the pen width used for the integrals for the active data set.

Other Options: Show Assigned Value, Show Frequency Limits, Show Multiplier, Show Slope/Offset/Curvature

Peak Picks Checkbox: Toggle on/off the peak picks (if any) for the selected data set.

Peak Picks Settings: Opens the Print Preview Settings dialog to the Peak Picks setup item.

Font: Selects the font size to be used for the peak picks for the active data set.

Pen: Selects the pen width used for the peak picks for the active data set.

Label Combo Box: Choose whether peaks picks are labeled by number or by chemical shift. The current axis units will be used for label by chemical shift.

Parameters Checkbox: Toggle on/off the parameters display for the selected data set.

Parameters Settings: Opens the Print Preview Settings dialog to the Parameters setup item.

Font: Selects the font size to be used for the parameters for the active data set.

Comment Checkbox: Toggle on/off the comment display for the selected data set.

Comment Settings: Opens the Print Preview Settings dialog to the Comment setup item.

Font: Selects the font size to be used for the comment (if any) for the active data set.

Line Fits Checkbox: Toggle on/off the line fits (if any) display for the selected data set.

Line Fits Settings: Opens the Print Preview Settings dialog to the Line Fits setup item.

Pen: Selects the pen width to be used for the line fits (if any) for the active data set.

General / Print Frame: When selected, a frame will be printed around the entire plot *(this is a global setting for the entire plot).*

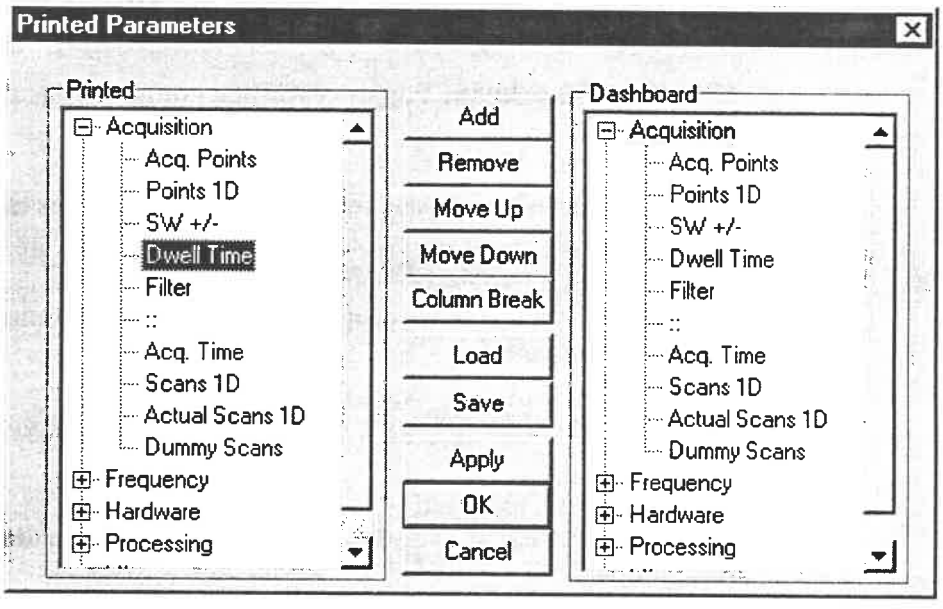
General / Logo: When selected, a logo will be added to the plot *(this is a global setting for the entire plot).*

Align: Snaps all print preview elements to the invisible grid.

Data Parameters

By default, all parameters from the dashboard are included in the parameter section of the printout. Furthermore, each data set added to the print preview has its own set of parameters. The specific parameters that are included in the printout can be customized for each data set in the print preview window.

To customize the parameters that are printed, double-click anywhere on the parameters in the Print Preview Window. The Printed Preview Parameters window (shown below) can be used to select the parameters that will appear on the printout. The current Dashboard parameters appear in the right hand pane and the currently selected parameters to print are in the left-hand pane. Printed parameters can be added, removed or repositioned using the 'Add', 'Remove', 'Move Up' and 'Move Down' buttons.



Column breaks for the printed parameters can also be added.

The Load and Save buttons allow 'Par' files to be read from and saved to disk.

By default, all parameters in the current dashboard are used for all printouts.

Manipulating Spectra in the 1D Print Preview

In addition to adjusting the various parameters discussed in the two sections above, visible components can be re-positioned and re-sized by mouse.

- Selecting a Visible Component: Click anywhere on the item. When selected, the item will be highlighted with a red outline box.

- Re-sizing an Item: Position the mouse cursor at any edge of a highlighted item. When the mouse is positioned, the cursor will change to a double-headed arrow. When the new cursor appears, click and drag to re-size the item. Note that data axes cannot be independently re-sized. Data axes are automatically re-sized to match the associated spectrum.

- Moving an Item: When the mouse cursor is positioned over an item in the print preview window, the cursor changes to a four-headed arrow. Once the four headed arrow is visible, click and drag to reposition the item.

- Positioning a Data Axis: Each individual data set may have its own data axis. Data axes, however, cannot be arbitrarily position on the printed page. Left and right movement of a data axis is linked to the position of the actual data. The axis can be positioned vertically by clicking and dragging up or down in the window.

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2D Printing

2D Print Commands

When an nD display window is open and front most, the following print selections are available from the File menu: Print Setup..., Page Setup... and Print Preview.

Print Setup	Opens the setup dialog for the currently active Windows printer. Depending on the printer driver, items such as paper source, page orientation, color management, etc. are set in this dialog.
Page setup	Opens the NTNMR Page Setup dialog for 2D printouts. (See below)
Print Preview	Activates the 2D Print Preview window.

Page Setup

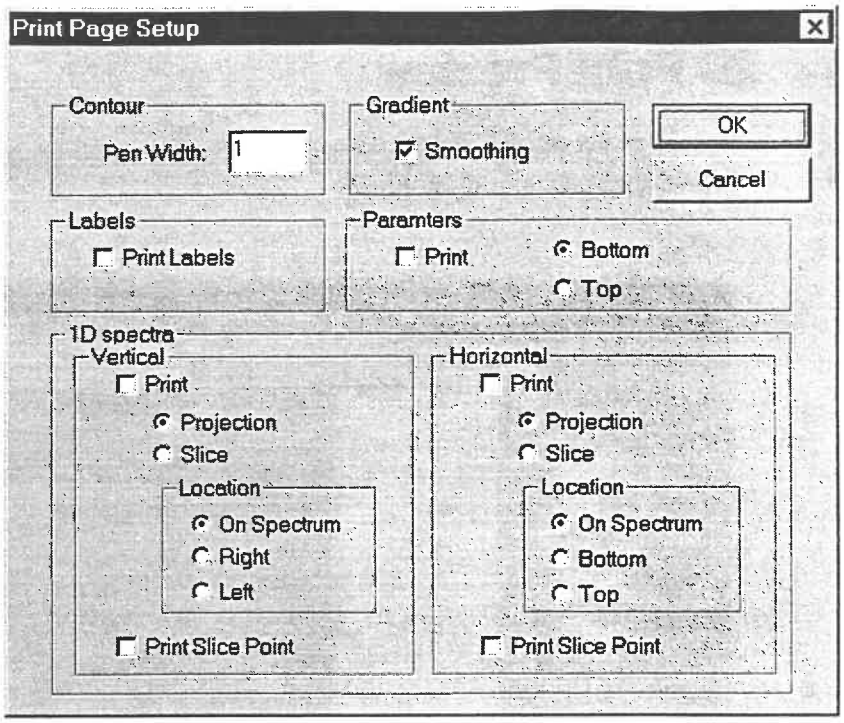
The 'Page Setup...' menu item opens the Page Setup dialog (shown below).

> *Note: Note all 2D Page Setup features are implemented in NTNMR versions 1.1 or earlier.*

Contour / Pen Width: Adjusts the pen width that is used for drawing contour plots for printing.

Gradient / Smoothing: Activates a smoothing algorithm to improve the appearance of gradient style 2D plots. The algorithm applied is the same one that is used in the nD display window; consult the chapter on nD display for details.

Labels / Print Labels: Toggles on / off the display of labels that were added to the data in the nD display mode.



Parameters / Print: When checked, the parameters for the data set in the 2D Print Preview will be added to the printout.

Parameters / Bottom (Top): Selects whether the parameters will be printed above or below the data on the page.

1D Spectra / Vertical:

Print: When checked, the 1D data (if any) for the vertical dimension will be printed.

Projection (Slice): Selects between printing a 1D projection or a 1D slice.

Location / On Spectrum (Right) (Left): Select the location, with respect to the 2D plot, where the 1D spectrum will appear.

Print Slice Point: When checked, NTNMR will print a slice point identification number on the 2d plot indicating the position of the 1D slice (if any) that is selected.

1D Spectra / Horizontal:

See '1D Spectra / Vertical'

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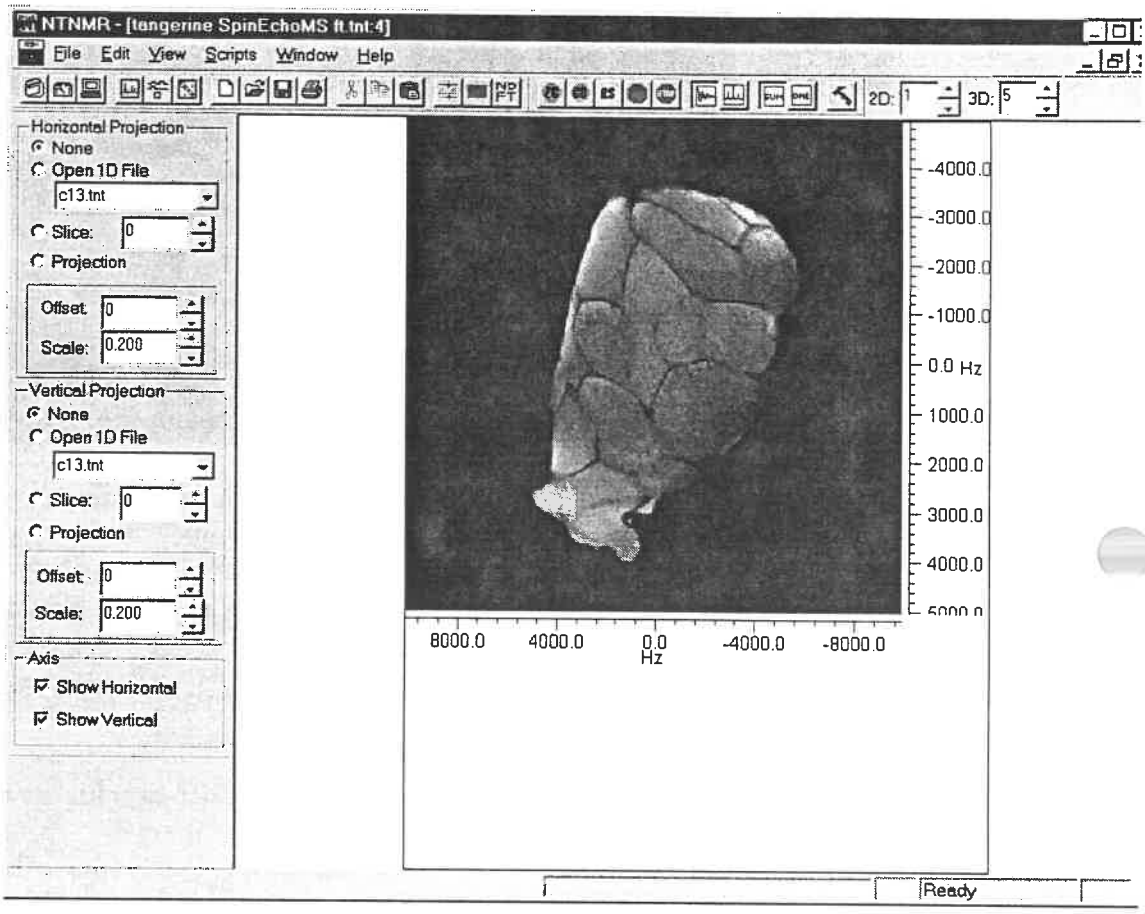
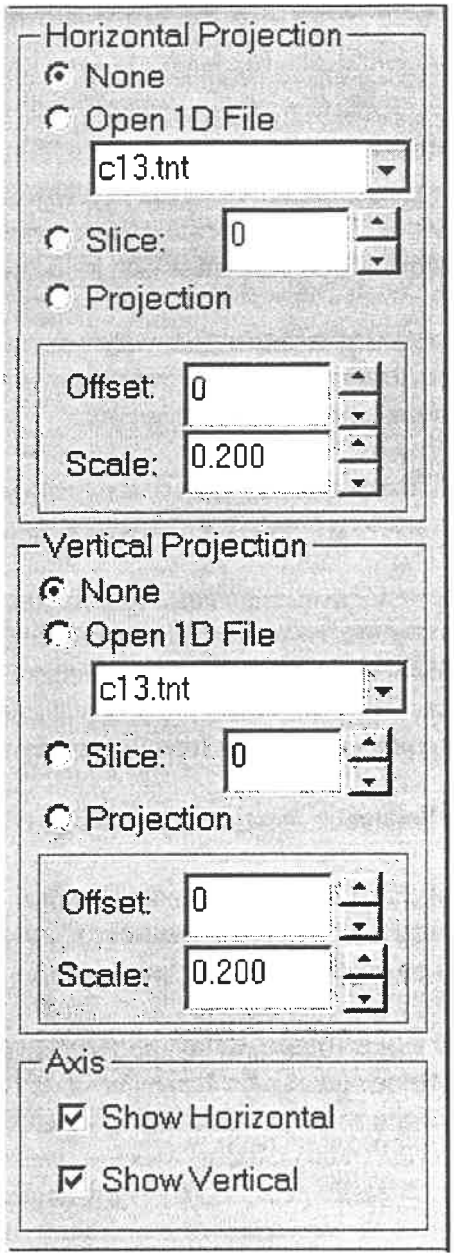
2D Print Preview

Select 'Print Preview' when in any nD display mode to activate the 2D Print Preview mode (shown below).



Customizing 2D Printouts

2D Print preview toolbar



Horizontal Projection

None: No 1D file will be displayed for the horizontal dimension.

Open 1D File: Select this radio button and choose a filename from the combo box below it to use a 1D data file from any 1D data set currently open in NTNMR.

Slice: When a slice selected, corresponding to the number that is displayed to the right, it will be displayed as the horizontal projection.

Projection: will be calculated and displayed by summing all of the data in the horizontal direction.

Offset: Adjusts the offset, in points, for the 1D data displayed from the 2D plot.

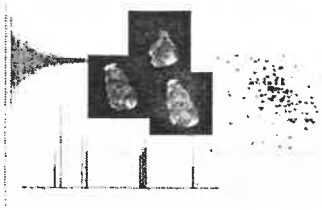
Scale: Adjusts the scale factor for the 1D data that is displayed on the horizontal axis.

Vertical Projection

Controls for the vertical 1D data projection are analogous to the horizontal controls described above.

Axis / Show Horizontal: Toggles on and off the display of the horizontal axis for the 2D plot.

Axis / Show Vertical: Toggles on and off the display of the vertical axis for the 2D plot.



8 - Pulse Sequences

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8.1 Introduction

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This chapter discusses the general features of the NTNMR sequence editor common to all hardware types. This chapter does not cover hardware specific information such as the purpose of a particular line in the sequence.

When the user transfers to the **Pulse Sequence** window via the **Pulse Sequence Button** on the NTNMR document window, a new window appears for defining a pulse sequence or displaying a pre-defined sequence.

Pulse Sequences in NTNMR are created, edited and displayed in a graphical format analogous to that used to represent sequences in the literature.

Each horizontal line of the pulse sequence corresponds to a function in the spectrometer as defined in the hardware configuration file 'config.con'. Various icon libraries are available for assigning different functions to a line without using complex mnemonics. The columns of the Pulse Sequence Window represent the events in a sequence, ordered from left to right.

General features of Pulse Sequence creation and editing in NTNMR are:

- Sequences are always saved with the data file (*.tnt), but can also be saved separately (*.tps) so that they can be used with other data files.

- All sequence tables (phase, delay, etc.) are saved with the sequence and can be created with text edit tools inside of the sequence Edit Table dialog window. The Edit Table dialog window, with built-in text editor, is easily accessed by right clicking on any table icon in the sequence or by clicking on the Edit Tables button in the Sequence Toolbar.

- Cut, Copy and Paste commands provide convenient event-level editing within a sequence or between sequences.

- Multi-dimensional tables are segmented into a separate section of the graphical window.
- Tables can be viewed as icons or as table names.
- Unlimited user defined variables can be used. User defined variables appear in the sequence tab of the dashboard.

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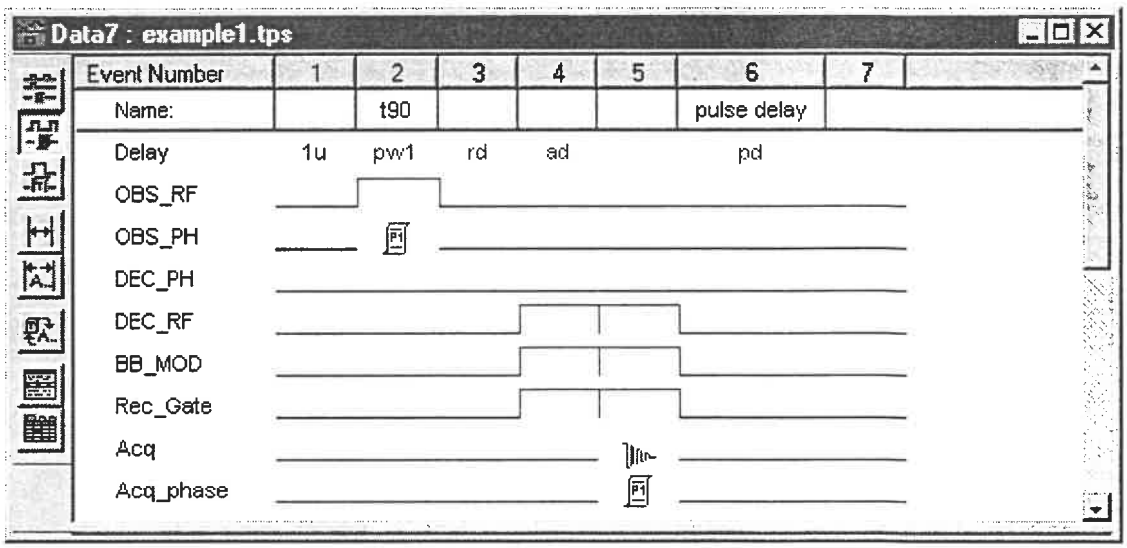
Pulse Sequence Window

The Pulse Sequence Window is accessed via the **Pulse Sequence Button** on the Main Toolbar in the Main NTNMR Window. Only one Pulse Sequence Window can be associated with a Document Window (i.e. data file); however, each open data file can have a different sequence window associated with it. The following figure shows a typical Pulse Sequence Window:



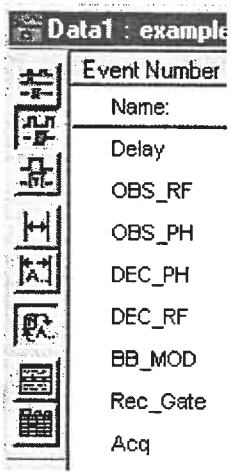
The Pulse Sequence Window has the following components:

- Sequence Toolbar (left side of window).

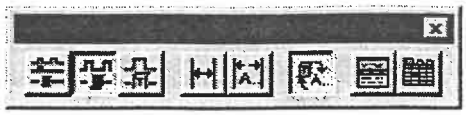
- Line labels (i.e. "OBS_RF", "OBS_PH", etc.) associated with the hardware configuration (installation dependent).
- Event numbers (from left to right across the top of the window).
- Event names (user definable, i.e. "t90", "pulse delay") are for information only.
- Delay line defines the duration of each event in the sequence.

Pulse Sequence Toolbar

The Pulse Sequence Toolbar contains several buttons that are used for controlling the appearance of the pulse sequence and for editing the pulse sequence. By default the Sequence Toolbar is "docked" at the left side of the Sequence Window. The Sequence Toolbar can be "undocked" and moved in the same way that other toolbars in NTNMR are manipulated.



Shown below is the Sequence Toolbar "undocked." Note that the toolbar defaults to a horizontal orientation when it is undocked. The toolbar can be positioned anywhere on the desktop and can be docked at any edge of the Sequence Window.



Each of the Sequence Toolbar Buttons is discussed in turn below.

Pulse Sequence Size 

Three sequence display sizes are available (small, medium, and large from left to right). Clicking on a sequence size button will cause the sequence to be re-drawn using the new size.

Default Column Width 

This button resets the column width to the NTNMR default size. See below for information regarding resizing columns.

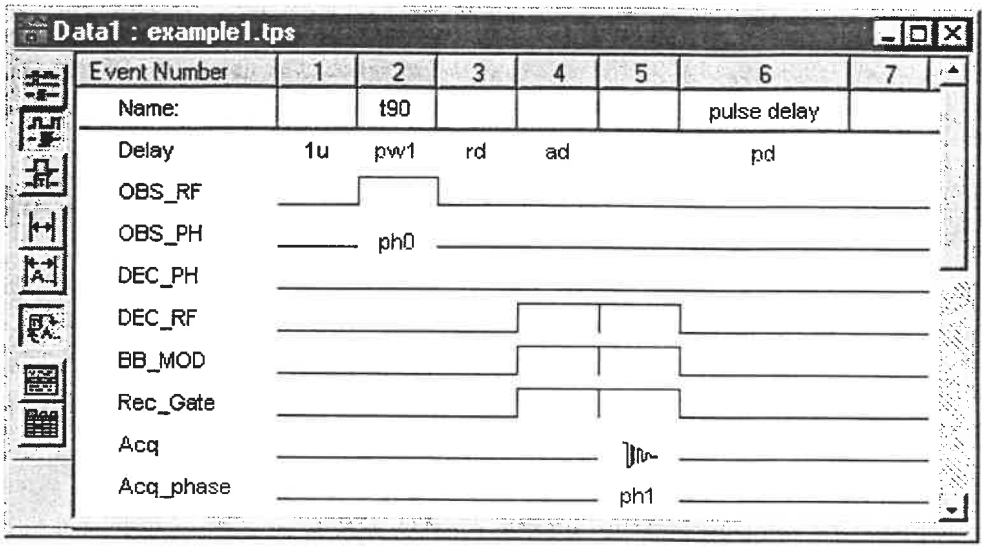
Expand Column Width 

The Expand Column Width button automatically resizes all columns so that the complete text name is displayed. In the sequence window example above the columns have been expanded so that the name of Event 6 ("pulse delay") is fully displayed. If the columns are not expanded some user defined event names may be truncated. See the next section for information on resizing individual columns.

Table Name/ Table Icon Toggle 

Tables can be displayed as icons or as text. This button toggles between the two modes. In text mode, the table name is displayed. Note that in either mode, pausing the Mouse over a table for about 1 second will pop up a "Table Tip" containing the table name, a partial list of the table entries (truncated to 16 entries) and the total number of entries in a Tool Tip style box.

The Pulse Sequence Window below shows the Table Name display mode. This represents the same pulse sequence shown in the Table Icon mode in the Pulse Sequence Window above.



Edit Tables

The 'Edit Table' window can be opened by clicking the 'Edit Tables' button. This is the same as right-clicking on any table in the sequence.

Edit Variables

Clicking on the 'Edit Variables' button opens the Dashboard to the Sequence tab. This allows quick access to all of the sequence variables that have been assigned for editing. Also note that, similar to tables, pausing the Mouse over a variable name in the sequence will pop up a Tool Tip window that displays the variable name and its current value.

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Pulse Sequence Menus

File Menu

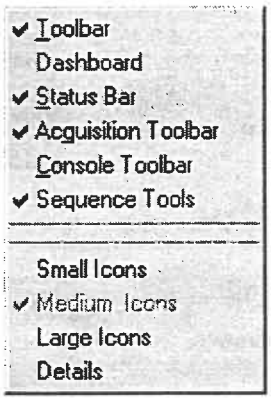
The **File** Menu for the Sequence window is identical to the **File** Menu for the Document window with the addition of four Pulse Sequence related items.

New Sequence	Replace the current sequence with a blank sequence.
Open Sequence...	Select and load a new sequence from disk.
Save Sequence	Save the current sequence to disk.
Save Sequence As...	Save the current sequence to disk under a new file name.

Edit Menu

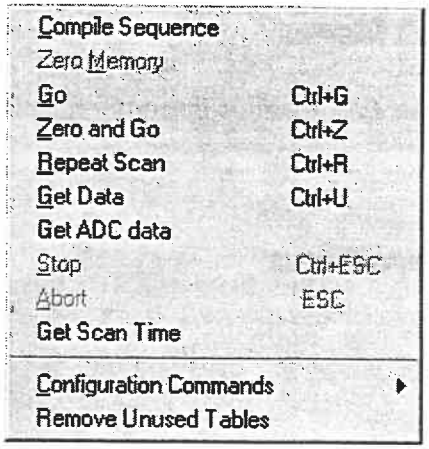
The Edit menu is currently inactive in the sequence window.

View Menu



Toolbar	Toggles on and off the Sequence Toolbar.
Dashboard	Toggles on and off the Dashboard.
Status Bar	Toggles on and off the Status Bar.
Acquisition Toolbar	Toggles on and off the Acquisition Toolbar.
Console Toolbar	Toggles on and off the Console toolbar (Shims, etc.).
Sequence Tools	
Small, Medium, Large Icons	Selects the Sequence Size display. Same as the Pulse Sequence Size buttons on the toolbar.
Details	Activates an alternate text only display of the pulse sequence.

Commands Menu



Compile Sequence	Compiles the active pulse sequence. *Not required before ZG.
Zero Memory	*Inactive.*
Go	Start an acquisition without overwriting the data in the signal averager memory.
Zero and Go	Start an acquisition, overwriting the data in the signal averager memory.
Repeat Scan	Start the repetitive scan mode. NTNMR runs the current sequence repeatedly until the user issues a stop command.
Get Data	Upload the current data from the signal averager to the host PC RAM and displays the data in the active window.
Get ADC Data	Upload the current ADC data to the host PC RAM and displays the data in the active window.
Stop	Executes a 'soft-stop' at the smallest common multiple of all 1D phase tables. *Same as the yellow stop button on the acquisition toolbar.*
Abort	Executes an immediate stop, regardless of the current phase cycle or acquisition status. *Same as the red stop button on the acquisition toolbar and the ESC key on the keyboard.*
Get Scan Time	Reports an *estimate* of the duration of the current experiment.
Configuration Commands	See the Commands chapter.
Remove Unused Tables	Removes unused tables from the current pulse sequence.

Window Menu

The Window Menu in the Sequence Window has the same functionality as the Window Menu in the Document Window. See the chapter on Document Windows for more information.

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Defining and Editing Pulse Sequences

Sequence Components

Terminology

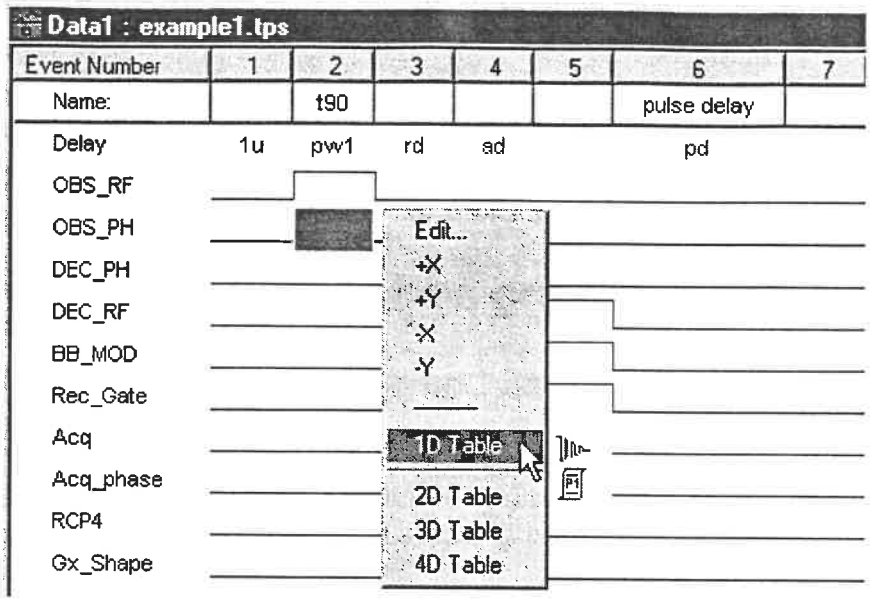
Each position (**Event**) in an NTNMR pulse sequence can be thought of as a "cell" in a spreadsheet representation of a pulse sequence with its own unique X, Y position. An Events location is determined by its **Event Number** (X position in the "spreadsheet") and its **Line Label,** referred as simply as the **Line** (Y position in the "spreadsheet"). The pulse sequence progresses from left to right, executing all commands in a "column" (i.e. **Event Column**) simultaneously for the duration defined by the **Delay** for that column.

Any particular X, Y position in the sequence is usually referred to simply as an **Event**. This terminology is used throughout this manual. When an entire column in the pulse sequence is referred to, the term **Event Column** is applied.

> *Consult the hardware documentation for your system for a description of the specific sequence lines and their functionality.*

Working with the Graphical Display

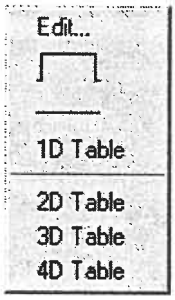
To define a sequence of events, select a spectrometer function by left-clicking on an **Event** in the Pulse Sequence, and choose an icon item from the pop up menu list, as shown:



According to the configuration of the particular line in the sequence, a different pop-up menu will appear. Specific information on the types of icon libraries and configuring lines in the sequence is given at the end of this chapter. In general, however, NTNMR will have been pre-configured and editing any system wide configuration files will not be necessary.

The type of pop-up menus that are available and the individual selections are discussed here.

Transmitter Type (TX, GR, ET)



The transmitter type pop up menu is generally used for lines that control the transmitter gates (i.e. On/Off) of RF channels on the spectrometer ("Observe" channel, "Decoupler" channel, "F1" channel, "F3" channel, etc.) This pop up may also be used to control the Gain or Attenuation of an RF channel, to activate other spectrometer controls that behave in an "on/off" manner such as the receiver gate, or even to control devices external to the spectrometer such as

switches. In some cases, the TX icon may be used to control functions that allow entries of 0 to 100 (floating point), 0-63 in steps of 0.5, etc.

The transmitter type pop-up menu is also used for controlling gradient amplitude lines.

Edit... : The edit selection temporarily converts the display for the current sequence position to a text entry display. The **Edit...** selection has three functions, depending on the current state of the sequence position.

1. If an "**Off**" (see below) gate is assigned to the position being edited, a number can be entered directly. After entering a value and pressing the [ENTER] key, an "**On**" (see below) gate will appear at that position. Note that the number entered must correspond logically to the number of bits that have been assigned for that particular control. For example, if the command that is activated is an RF attenuator that has 8 bit control, the valid entries would be from 0 to 255. Conversely, if the command being edited controls the RF transmitter controlled by 1 bit, then only values of 1 and 0 would be allowed (i.e. "on/off").

2. Choosing **Edit...**: When an "**On**" gate is already active for a position, it will allow editing of the current value for the command.

3. Choosing **Edit...** : When a table is active for that event, the table name will be allowed to be changed. In all cases, choosing **Edit...** is the same a double left-clicking on an **Event** in the sequence.

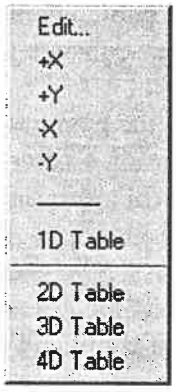
The "**On**" gate:  This command is the equivalent of choosing **Edit...** and assigning a value of 1. This is the common representation of an active event ("on") in a sequence diagram and has the same meaning in NTNMR. Note that for commands that allow greater than one bit control the same "**On**" gate icon is displayed.

The "**Off**" icon:  This is the default display for all **Events** in a sequence that are inactive. Selecting the off icon from a the pop-up menu of an active position in a sequence will de-activate that **Event** and clear any value that was stored with that **Event**.

1D Table, 2D Table, 3D Table and **4D Table**: The 4 table selections will activate a table icon for the current position in the sequence. The 1D table will appear in place as the TX table icon  . For 2D - 4D tables, the icon will appear in a separate section at the bottom of the sequence. See the section on

multi-dimensional sequences for detailed information. TX tables can contain lists of any valid data for a particular control. The table editor is discussed in the next section. Regardless of the type of table that is selected, a text entry field will be displayed for assigning a name to the table.

Phase Type (PH)



The Phase pop-up menu is used for lines in the sequence that control the phase of the various RF channels and of the signal averager.

Edit...: The edit selection temporarily converts the display for the current sequence position to a text entry display. Similar to the **Transmitter** pop-up discussed above, the behavior of the **Edit...** selection is context sensitive. There are two possibilities:

1. If there is no active command for the position, or if there is a fixed phase designated (i.e. +X, +Y, ...), a text edit field will appear that allows the user to enter an integer number. This number should be logical with respect to the number of bits that are assigned to the control. A common case would be 2-bit phase control. This typically corresponds to 0, 90, 180, 270 (+X, +Y, -X, -Y) and the control values would be 0, 1, 2 and 3, respectively. Note that the numbers entered are not phase numbers, such as 90 or 180, but rather integer numbers that correspond to the number of bits that need to be set for a given phase. While phases of 0, 1, 2 and 3 are common place on many spectrometers. There is also the possibility to have an arbitrary number of bits assigned to the control of a phase shifter. In this case, it is not always intuitive what integer value corresponds to a given phase. See the section on Tables for information on handling these more complex cases.

2. If a table has previously been assigned to the command that is being edited, a text entry field will appear that allows the name of the table to be edited.

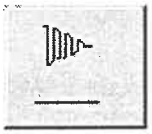
In all cases, choosing **Edit...** is the same as double left-clicking on a position in the sequence.

Fixed Phase Selections (+X, +Y, -X, -Y): These selections will assign a fixed phase to a particular event in the sequence. This simply means that no phase cycling will occur for that event in the first dimension. +X equals a value of 0, +Y equals a value of 1, -X equals a value of 2 and -Y equals a value of 3 regardless of how many bits are assigned to that particular line.

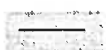
The "**Off**" icon:  This is the default display for all **Events** in a sequence that are inactive. Selecting the off icon from a the pop-up menu of an active position in a sequence will de-activate that position and clear any value that was stored with that **Event**.

1D Table, 2D Table, 3D Table and **4D Table**: The 4 table selections will activate a table icon for the current position in the sequence. Phase tables are used to program phase cycling schemes for pulse sequences. The 1D table will appear in place as the PH table icon  . For 2D - 4D tables, the icon will appear in a separate section at the bottom of the sequence. See the section on multi-dimensional sequences for detailed information. PH tables can contain lists of any valid data based on the number of bits assigned. The table editor is discussed in the next section. Regardless of the type of table that is selected, a text entry field will be displayed for assigning a name to the table.

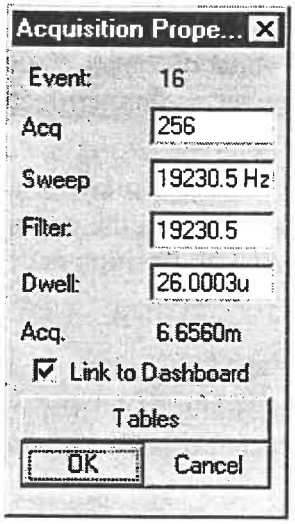
Acquisition Type (ACQ)



Acquisition icon: The Acquisition icon (represented by an FID symbol) tells the system to begin acquiring data at that event in the sequence. The number of points to be acquired is determined by the "Acq. Points" parameter in the Dashboard. When the Acquisition icon is chosen, the Dashboard parameter "Acq. Time" will automatically be inserted into the **Delay** field for that event, indicating that the duration for that event is determined by "Acq Points" * "Dwell 1D."

The "**Off**" icon:  This is the default display for all positions in a sequence that are inactive. Selecting the off icon from a the pop-up menu of an active position in a sequence will de-activate that position and clear any value that was stored with that position.

If an acquisition icon has already been added to a sequence, left-clicking on the acquisition icon will reveal a pop-menu with the "**Off**" option discussed above, as well as the "**Properties**" option. Selecting properties will open the Acquisition Properties window.



The Acquisition Properties window allows the user to set the number of points *(all systems)*, sweep width, filter and dwell time *(digital receiver systems only)* for each acquisition event independently. By default, all acquisition events are assigned the number of points, sweep width, dwell and filter settings from the dashboard. Using the Acquisition Properties window allows these parameters to be set on a individual basis. There is also a "Link to Dashboard" check box the can be used to indicate which acquisition events should be connected to the dashboard.

Some systems with digital receivers can also specify a sweep width table for any dimension through the acquisition properties 'Table" button.

Shape Type (SH, PS, RM, AT)

Edit...: The **Edit** selection temporarily converts the display for the selected **Event** to a text entry display enabling an existing shape table to be re-named. In all cases, choosing **Edit...** is the same a double left-clicking on a position in the sequence.

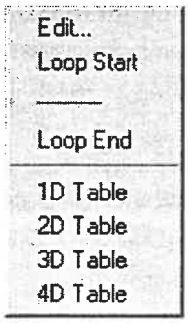
Shape Table: The Shape Table selection activates a shape table and assigns the  icon to that event. Shape tables are primarily for use when generating waveforms for the Tecmag Gradient Module or for the Tecmag RF Transmitter Module. See the section on tables for more information. The **Delay** for the event that contains a Shape Table dictates the length of the event. The shape will be automatically scale to the duration ("Delay") of the event where it appears. So, if the Shape Table has 512 entries and the **Delay** for that event is set to 500 msec, then the table will be clocked out at a rate of (500/512) msec per point. (See below for the alternate "continuation" mode for gradient waveforms)

The "**Off**" icon:  This is the default display for all positions in a sequence that are in-active. Selecting the off icon from a the pop-up menu of an active position in a sequence will de-activate that position and clear any value that was stored with that position.

When using the shape icon to specify a gradient waveform, the "**continuation**" mode is also active. As stated above, all default shapes, including gradients, are played out during the event in which they are specified with a table time per point defined by the duration of the event divided by the number of entries in the table. However, one a shape (*gradient only*) has been defined the continuation icon can be placed in subsequent contiguous events to force the waver form to be played out over multiple events. Left-clicking in subsequent order will reveal the "Continue Table" option. When selected, the  icon will appear in the sequence. In the case the time per point for the waveform will be determined by the sum of the delays for the waveform event and all continuation events divided by the number of points in the table.

Loop Type

> *Important note regarding loops: The number of loops that can be executed in a sequence is unlimited. However, the number of loops that can be nested is limited to 4.*



Edit...: The **Edit** selection temporarily converts the display for the current sequence position to a text entry display. The behavior of the **Edit...** selection is context sensitive with several possibilities.

1. If there is no active loop or loop table for the position, the text entry will be used as the number of times the loop is to be executed. After a value has been entered and the [ENTER] key has been pressed, the ↳ (**Loop Start**) icon will appear.

2. If a Start Loop command has been assigned to the current position, **Edit...** will allow the user to enter the number of times that the loop should be executed.

3. If a Loop Table has previously been assigned to the command that is being edited, a text entry field will appear that allows the name of the table to be edited.

4. If a **Loop End** command has previously been assigned to a position, **Edit...**is selected and a value greater than 1 is entered, the command will be converted to a **Loop Start** instruction. In all cases, choosing **Edit...** is the same a double left-clicking on an **Event** in the sequence.

Loop Start: This selection defines the event as the start of a loop. By default, a value of 1 is entered for the number of times to execute the loop. Once a Loop Start instruction has been entered in the sequence, select **Edit...** or double left-click on the Loop Start instruction to change the value for the number of times to execute the loop.

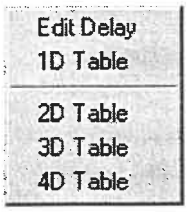
The "**Off**" icon: — This is the default display for all **Events** in a sequence that are in-active. Selecting the off icon from a the pop up menu of an active position in a sequence will de-activate that position and clear any value that was stored with that position.

Loop End: This defines the end of a Loop. No data value is needed. Loops are executed exactly the same way that parentheses are in mathematics. Thus, the inner most loop will be completed first and the outer most loop will be executed last.

1D Table, 2D Table, 3D Table and 4D Table: There are options for loop tables for each dimension up to 4. Loop tables can be used *only* in place of the **Loop Start** instruction and require a **Loop End** instruction. See the section on tables for information on defining and editing tables.

Delay Line

The duration for each event in a pulse sequence is defined in the **Delay Line** that appears as the top line in the sequence window. This line is not dependent on the hardware configuration and will always be present. When a new event is created, either by activating a command for a given position or by using the "Insert" command in NTNMR, a default value of 1u is entered for the new event. The **Delay Line**, similar to the other types of sequence commands, has a unique pop-up menu that it activated when the mouse is single left-clicked on a **Delay** position.



Edit Delay: The **Edit Delay** selection is context sensitive with two possible options.

1. If an event has a time or a variable name associated with it (as opposed to a table), this selection will allow direct editing of the time value or the variable name for that event.

2. If an event in the **Delay Line** has a table associated with it, the **Edit Delay** selection allows the table name to be edited. In all cases, choosing **Edit...** is the same a double left-clicking on a position in the sequence.

1D Table, 2D Table, 3D Table and 4D Table: These selections activate delay tables. Tables up to 4 dimensions are allowed. 1D tables are created in place and multi-dimension tables are created in a separate location in the sequence window. See the sections on tables and multi-dimensional sequences for more information.

> *All entries in delay tables must have units associated with them (n, u, m, s). Note that "0n", "0u", "0m" and "0s" are invalid entries and will cause fatal errors in sequences.*

Cut, Copy, and Paste Functions

Sequence **Event Columns** can be manipulated by common Windows-style techniques. When any **Event Number** is left-clicked, the entire column corresponding to that event is highlighted. Highlighted events can be cut (Ctrl-

X) or copied (Ctrl-C) using the common Windows keyboard commands or by selecting "Cut" or "Copy" from the Edit menu. A cut or copied sequence event can be pasted into the sequence at any position by highlighting an event and selecting "Edit / Paste" (or by typing "Ctrl-V"). Note that Paste inserts the copied event(s) *after* the currently highlighted event.

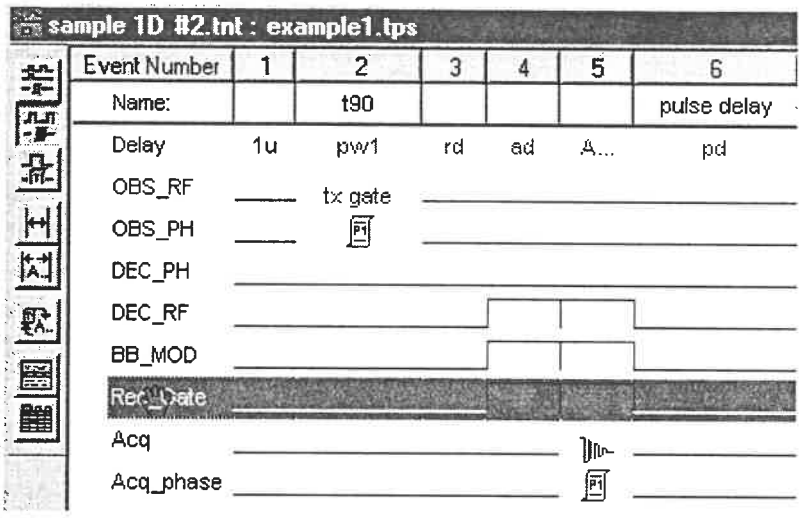
Multiple events can be selected by first clicking on an event number and then shift clicking on another event. All events in a contiguous block will then be selected. The same cut, copy and paste techniques described above apply when dealing with multiple events.

Changing the Order of the Line Labels

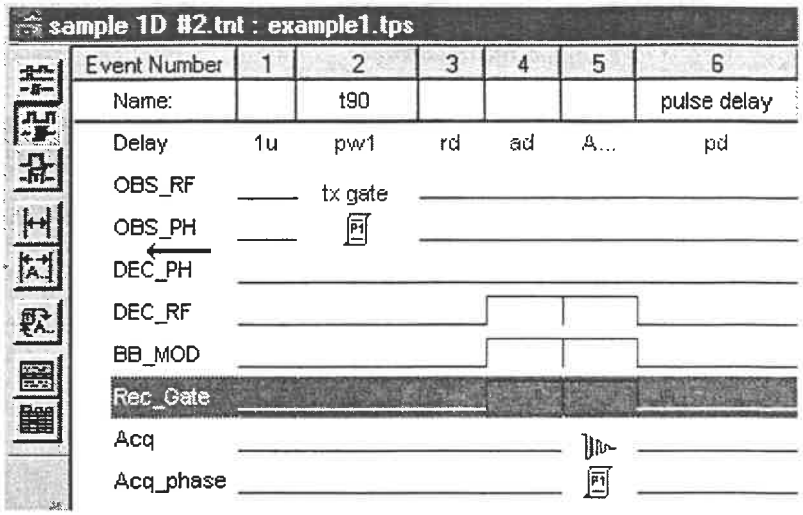
The default order lines that appear in the pulse sequence is defined by the configuration file "config.con." The order can, however, be changed on a per sequence basis. When the lie order is changed, the result is cosmetic only and is meant to be an aid in visualizing and editing sequences; the "config.con" file is *not* altered. The new line order is saved with the sequence file.

An example of moving two lines is shown below:

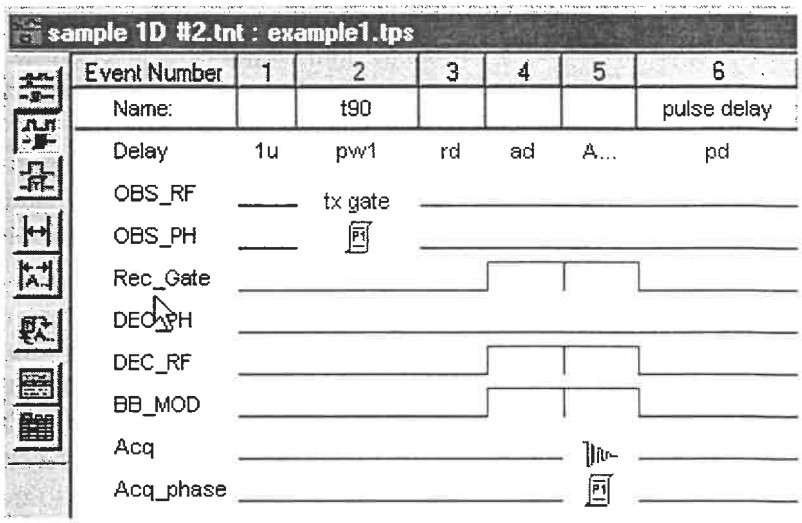
1. Click on a line label. When the mouse is over a highlighted line, label the pointer changes to the "hand" icon.



2. Click, hold the left mouse button and drag away from the highlighted line. The cursor display changes to an arrow (as shown below).



3. Move the arrow to the position in the sequence where you want the new line positioned and release. In this example, the line "Rec_Gate" was moved from being positioned just above the "Acq" line to just above the "DEC_PH" line.



<<< PREV <<<

Tables

8.5

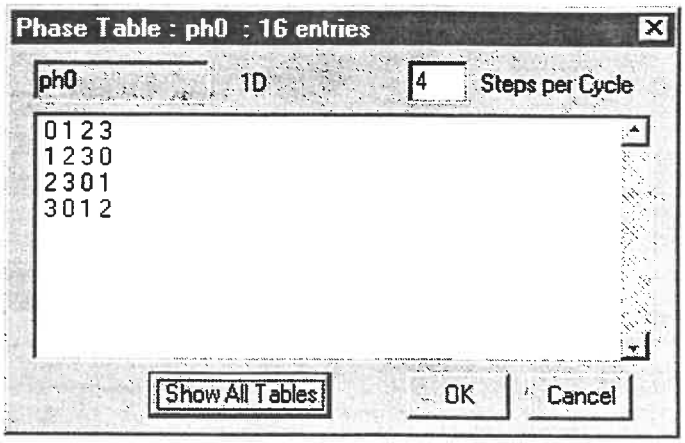
>>> NEXT >>>

Using the Table Edit Window

Common Features

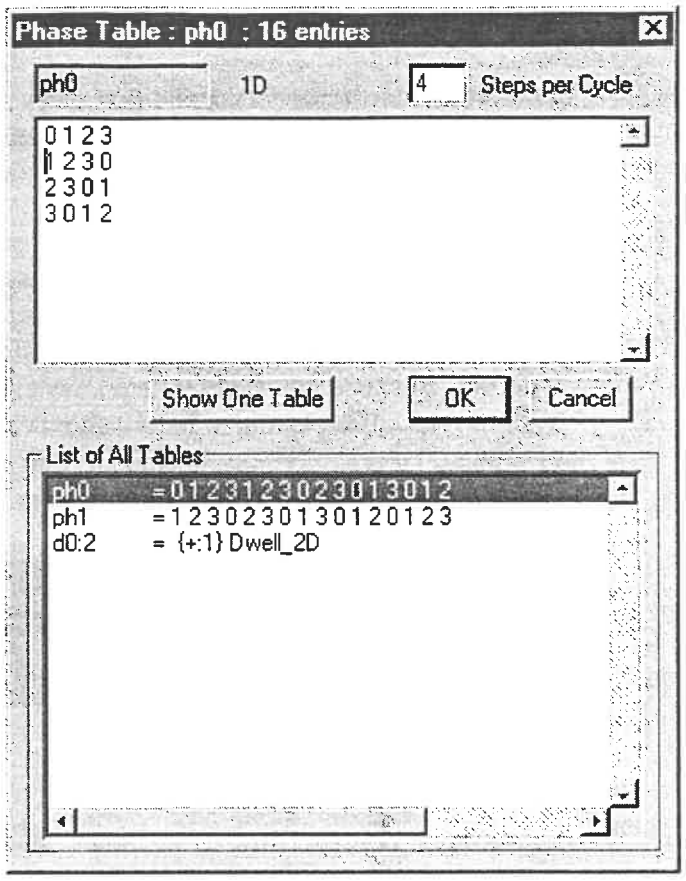
The Edit Table dialog window is accessed by right-clicking on any table icon in the Pulse Sequence Window or by clicking on the Edit Tables button on the

Sequence Toolbar. An example of the Table Edit window is shown below with a phase table active.



A single edit table window is used to edit all types of tables: Phase, Delay, Shape, Gradient, Transmitter and Loop. The type of table is detected upon creation by NTNMR through the module type code for the pulses sequence line. When a table is created, the user may assign it any name. By default, phase tables are named as ph0, ph1, ph2... phN, in the order they were created. Similarly, Delay tables are give the "d" prefix, shape tables are give the "shape" prefix, loop tables are give the "lp" prefix, and transmitter tables are give the "TX" prefix. Again, these prefixes are not mandatory, although they do provide a reasonable scheme for naming tables in a sequence. Also note that, by default, all 2D, 3D and 4D table names are appended with "*:dimension_number*" (i.e. "ph0:2").

Clicking on the **Show All Tables** button will expand the table edit window to display a list of all tables for the current sequence (**List of All Tables** display). Note that the table name and contents are shown in the **List of All Tables** display. However, tables with greater than 16 entries are truncated. The **Show One Table** button toggles the display back to the default.



When the Table Edit window is in the **Show All** mode, as in the example above, a left-click on any table in the **List of All Tables** window will update the **Edit** window to allow the table selected to be viewed in full and/or edited.

The Title Bar of the **Edit Tables Window** shows the type, name and number of entries in the currently selected table in the format *table_type* : *table_name* : *number_of_entries*.

The table name is displayed in the upper left corner of the window and the dimension of the selected table is displayed to the right of the name.

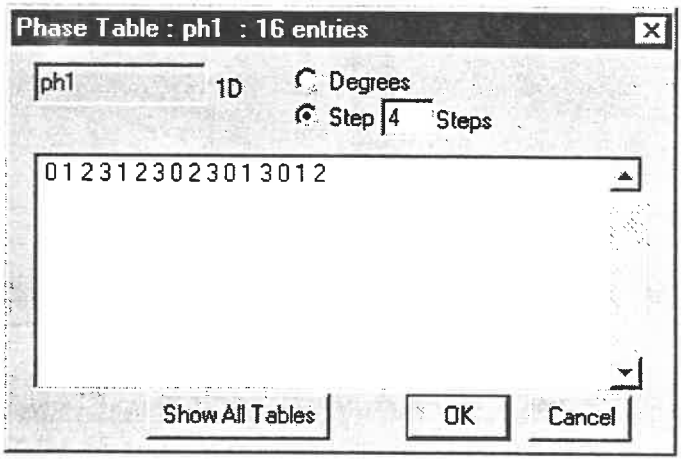
The **OK** button saves all changes that have been made and exits the **Edit Tables** window.

The **Cancel** button exits the **Edit Tables** window, leaving all tables unchanged.

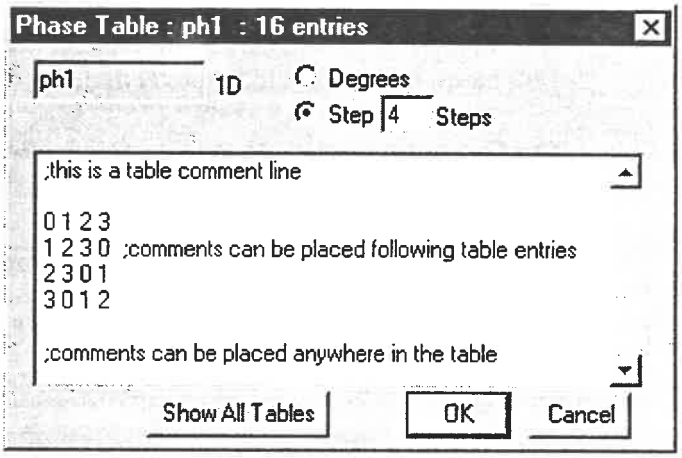
Editing Tables

The Edit window allows normal text entry similar to a text editor. The mouse can be used to position the cursor and to select text. Windows standard cut, copy and paste operations are available by the "Ctrl + X", "Ctrl + C", and "Ctrl + V" keystrokes, respectively.

Table items *must* be de-limited by either a space ([SPACE]) or a carriage return ([ENTER]). The space and the carriage return are interpreted in exactly the same way when the sequence is compiled. In the example above, the table is formatted using a carriage return after every fourth entry making the table easier to read. The example below shows the same table entered with spaces in between all entries. The two tables are functionally identical. No other characters can be used to delimit entries in a table.



Tables can also contain comments. The ";" character (semi-colon) is used to indicate a comment. All text *following* a semi-colon *on a line* is ignored by the compiler. The example below shows the use of the comment character in a table.



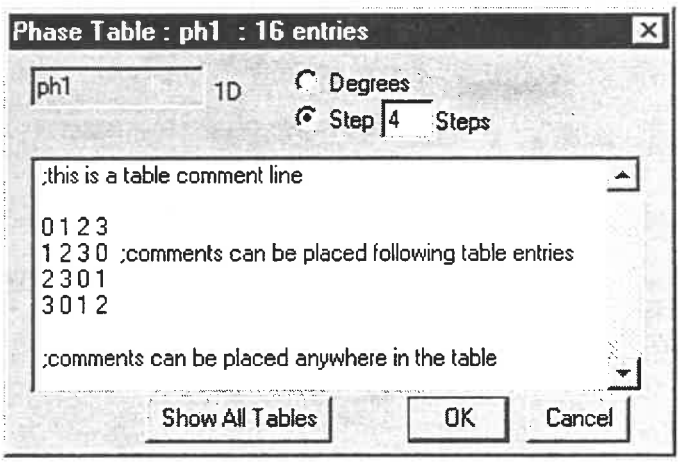
Context Sensitive Features

Depending on the type of table that is selected from the **List of All Tables**, the Table Edit window will display different features. Each type of table is discussed below.

Phase Tables

The Phase Table edit display (shown below) contains a Text Edit window where the table is created/edited as well as the "**Step**" and "**Degrees**" options. The Text Edit window has all of the general features discussed above.

Step mode: The entries in a phase table are *unit-less* numbers that represent a phase (see below for "Degree" mode).



For the most common case where the phases 0, 90, 180 and 270 are available, the numbers 0, 1, 2 and 3 will most often correspond to these values. This is common notation for phase tables. For cases where a greater degree of resolution is available, and the hardware has been configured appropriately, numbers greater than 3 may be used. For example, if 3 bits of phase resolution is available then number from 0 to 7 are valid.

The **Step Per Cycle** field allows simplified table creation when greater than 2 bits (i.e. 0, 90, 180, 270) control is available. The formula (360/**Steps per Cycle**) is applied to the entire table. So, if the value of **Steps per Cycle** is set to 8, the maximum resolution would be 45 degrees and if **Steps per Cycle** is set to 4, the maximum resolution would be 90 degrees. This allows simplified table creation in cases where, for example, a 90-degree resolution is required, regardless of the number of real bits of resolution available. Note that this value

applies on a *per table* basis, not to an entire sequence. The following examples illustrate this:

Example 1

Hardware phase resolution = 12 bits
Table Steps per Cycle = 4
Phase table = 0 1 2 3

In this case, the values of 0, 1, 2, and 3 would correspond to 0, 90, 180 and 270 degrees, respectively.

Example 2

Hardware phase resolution = 12 bits
Table Steps per Cycle = 8
Phase table = 0 2 4 6

In this case, values 0, 2, 4 and 6 corresponds to 0, 90, 180 and 270 degrees, respectively.

Example 3

Hardware phase resolution = 12 bits
Table Steps per Cycle = 8
Phase table = 0 1 2 3 4 5 6 7

The actual phases generated by the hardware are:

0 = 0
1 = 45
2 = 90
3 = 135
4 = 180
5 = 225
6 = 270
7 = 315

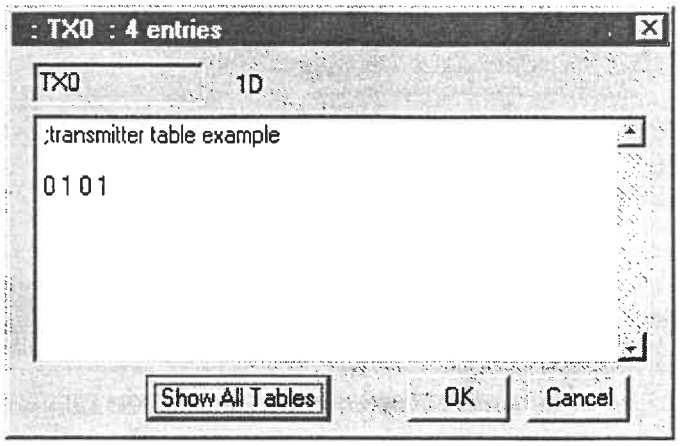
Degree mode: When the degree mode option is selected, phase tables can be entered in units of degrees from 0 to 360. NTNMR will attempt to choose the closest possible phase value that the hardware is capable of producing.

> *NTNMR does not have built in functionality for converting phase values in degrees to the proper logic output for PTS phase synthesizers with the phase rotation option. NTNMR can be used to control the phase rotation feature of the PTS. However, values that are sent to the PTS must be sent as straight 12 bit (or however many bits are being used) number to the PTS.*

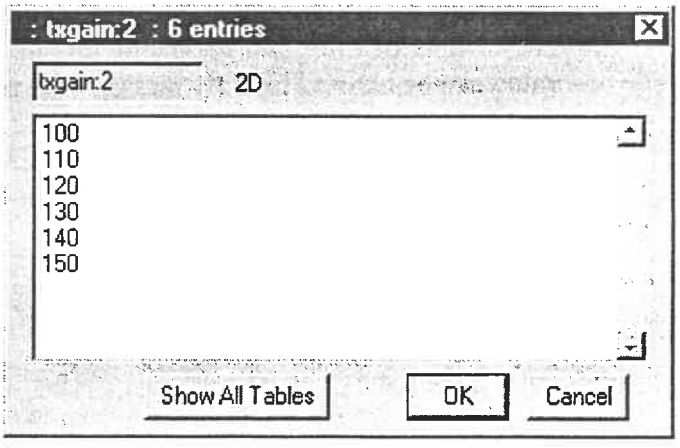
Transmitter Tables

Tables can be used in any dimension on transmitter (TX) type events to specify complex transmitter behavior. Common uses for this type of table are for alternately turning on and off a transmitter pulse in a sequence, or if the TX line in the sequence is controlling and attenuator to vary the amplitude of an RF pulse with respect to any dimension. Sample tables are shown below.

The following example shows a 1D TX table that controls the Observe RF pulse in a sequence. In this example, the RF pulse for this event is off in the first scan, on in the second, off in the third, etc.



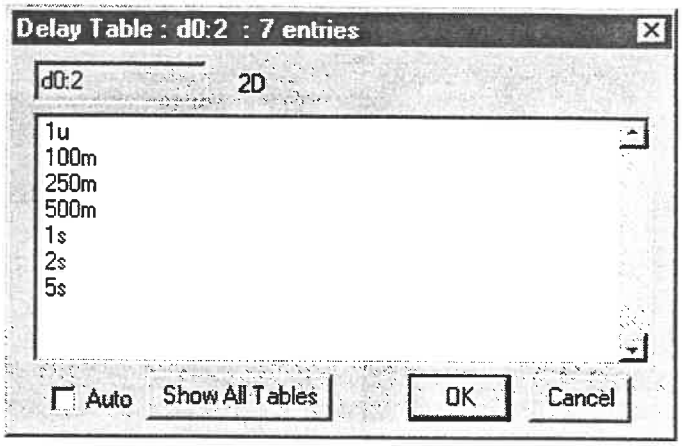
This example shows the use of a 2D transmitter table that is controlling the transmitter gain. In this case, each 2D scan would use the next transmitter gain on the list. A common application for this type of table would be a pulse sequence for determining the 90-degree pulse width.



Delay Tables

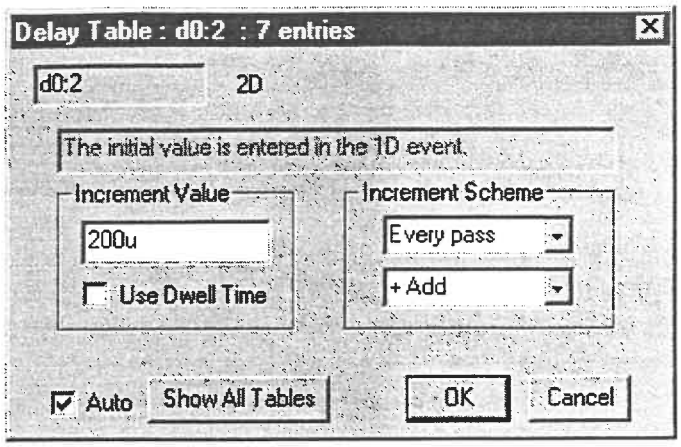
> *All entries in Delay Ttables must have units associated with them (n, u, m, s). Note that "0n", "0u", "0m" and "0s" are invalid entries and will cause fatal errors in sequences.*

Two types of Delay Tables are available: manual and auto. The manual table is most commonly used for pseudo-2D type experiments such as T1 relaxation measurements. In this case, a list of delays is explicitly created, along with units, in the Edit window. An example is shown below.

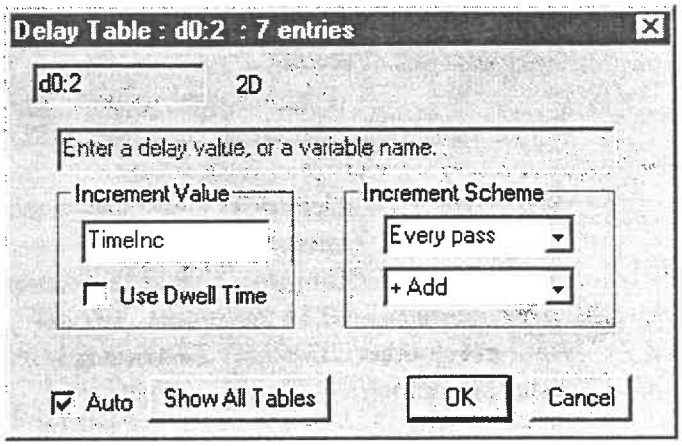


When the **Auto** box is checked, the Edit window display is changed to allow automatic incrementation of a delay table with respect to the dimension of the table. The most common use for a table of this type of for multi-dimensional dwell tables (i.e. t1, t2, etc.).

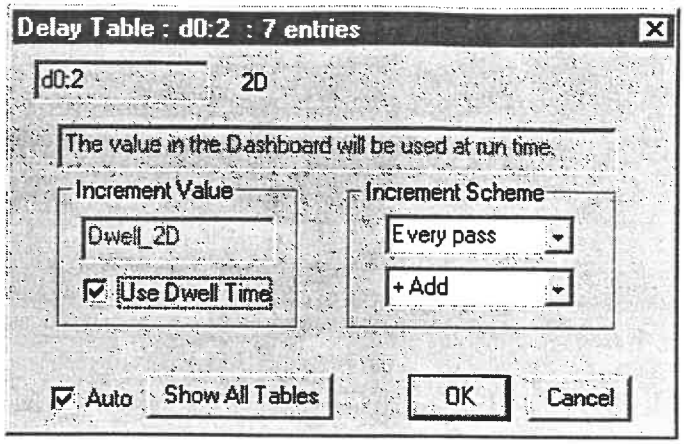
When in **Auto** mode, the value for the first increment, the first 2D or t1 point in the case of a 2D table, is given by the delay entered for the 1D event in the sequence. Each subsequent 't1' point is incremented by the increment value. The increment value can be specified in one of three ways. First, the increment value can be entered directly into the **Increment Value field**. For the case of the table shown below, the Increment Value has been set to 200u. If the 1D Event Delay time corresponds with this 2D table, set to 1u, then time for that event for the first 2D point would be 1u, for the second it would be 201u, for the third 401u, and so on.



Instead of entering a specific time in the **Increment Value** field, a variable name can be supplied. In this case, (see example below where the variable "TimeInc" is used for the Increment Value) the increment value will be specified by a user defined sequence variable in the Dashboard. See the section below on Sequence Variables for more information on creating and editing variables.



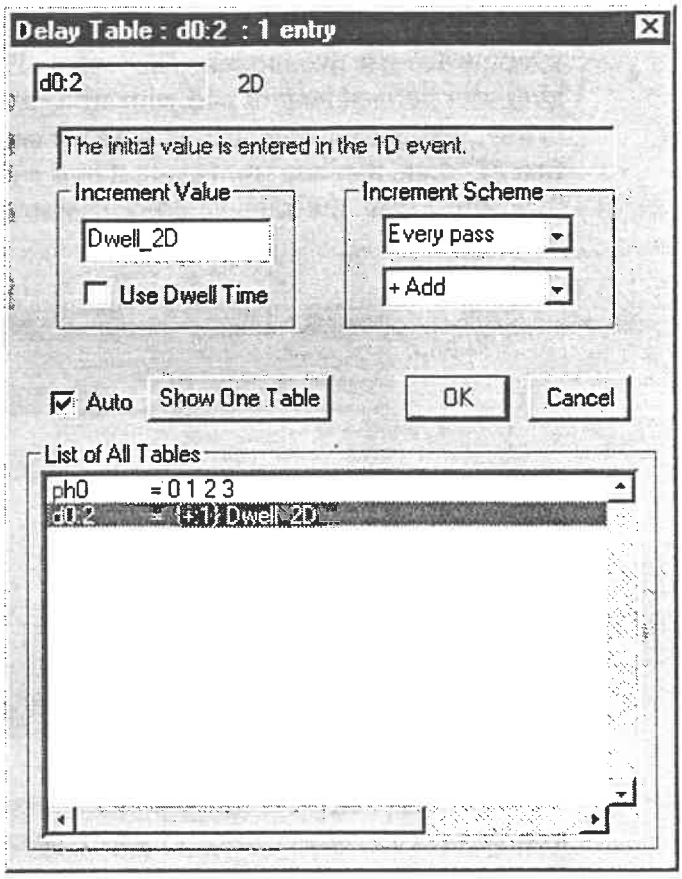
Finally, checking the **Use Dwell Time** option will force the table to use the Dashboard Parameter Dwell_2D for 2D tables, Dwell_3D for 3D tables and Dwell_4D for 4D tables.



Also available in the Auto mode is the ability to define when the table will be incremented. The **Increment Scheme** provides controls for this purpose. The top selection, by default set to **Every Pass**, has the additional choice **Every 2 Passes**. The choice determines when the table will be incremented. If **Every Pass** is chosen, the table will be auto-incremented after *every* 2D point. If **Every 2 Passes** is chosen, the table will be auto-incremented on *every other* 2D point. This is particularly useful in setting up phase sensitive experiment using the States-TPPI method.

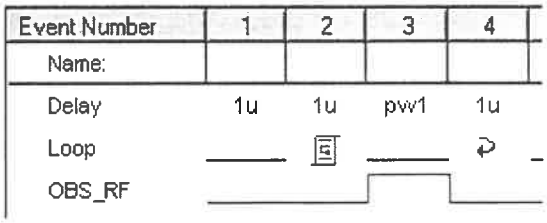
The second field, which appears as **+ Add** by default, is not currently used.

When the Auto selection is chosen for a table the following notation is used in the **List of All Tables** to represent the table: *table_name* = {+:1} *increment _variable_name* for tables that are incremented with every 2D point and *table_name* = {+:0,1} *increment _variable_name* for tables that are incremented with every other 2D point. The notation for tables in Auto mode is shown in the example below.



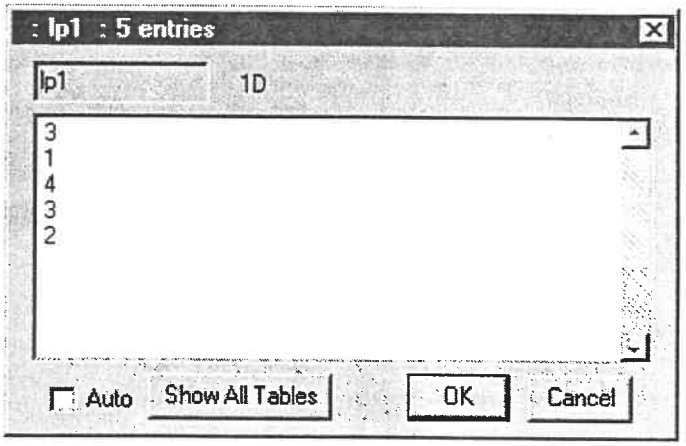
Loop Tables

The Start Loop instruction can be replaced with a Loop Table of any dimension. Loop tables allow the number of times that a loop will be executed within a given scan to be set to any arbitrary number with respect to any dimension. An example of the appearance of a Loop table in a sequence is displayed below.

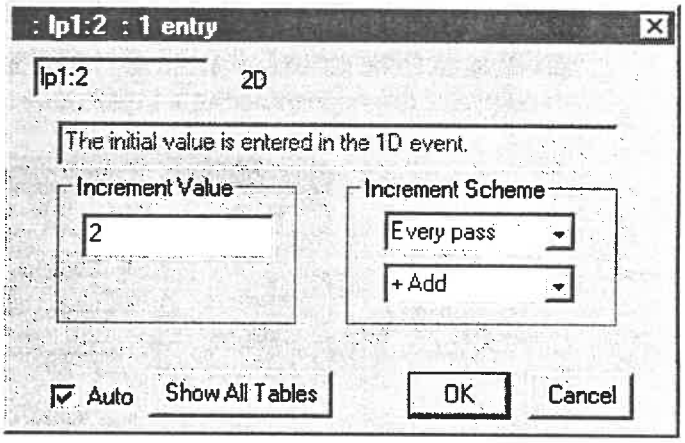


In this example, a 1D Loop table has been used as the start loop instruction in Event 2. When sequence execution reaches event 4, the pulse programmer will return to event 2 and repeat the number of times that is indicated in the Loop table for the current scan.

The Table Edit window for Loop Tables is very similar to the Delay Table edit window and has two modes. The "manual" mode allows tables to be created with user defined lengths and with arbitrary order. If the loop table, shown below, was used in conjunction with the sequence example above, during the first 1D scan, the loop from event 2 to 4 would be repeated 3 times. During the second 1D scan, the loop would be repeated 1 time, during the third 1D scan 4 times, etc.



If the **Auto** box is checked, options analogous to those for Delay Tables become available. This mode allows a Loop Table to be auto-incremented according to the scan counter for the dimension of the table. The **Increment Value** field will be the number that is added to the loop counter for each incrementation. The **Increment Scheme** controls allow the table to be incremented after **Every Pass** or after **Every 2 Passes**. The **+Add** field is currently in-active.



DMOD Tables

A special table type is available for clocking out data tables one entry at a time. Contiguous pulse programmer lines assigned in the 'config.con' file (see the section "Pulse Sequence Configuration File") using the icon library "LD" are classified as "DMOD" (Dedicated MODulator) lines. DMOD is only a description of the line functionality. The actual name assigned to the line in the pulse sequence can be any text string (as "MOD_1" in the example below).

Consider the follow entry in the 'config.con' file:

```
MOD_1          ES1  11 12  1  0  0  LD  1 0 ;
```

Lines 0 through 11 (i.e. LP11, LP10, LP9 ... LP0) of the module ES1 are defined as DMOD lines.

Any DMOD line in a pulse sequence is controlled, first loading a table and then by activating an "On" gate (same icon as a TX type) to clock the first entry. Each subsequent instance of the "On" gate in the DMOD line will clock the next value in the table until the end of scan, at which time the table will be reset to the first entry.

A DMOD table is loaded by selecting the "**Stepped Table**" choice from the pop-up menu on the DMOD line. The most common application of the DMOD line would involve loading a table in an early event in the sequence, and then toggling the 'On' gate in later events, each time sending the data for the next table entry.

Note that the data output of any lines defined as DMOD lines is *not* latched. However, the data from the DMOD line will be active for the all contiguous "On" events and during the event immediately following the last contiguous on event.

DMOD Sequence Example

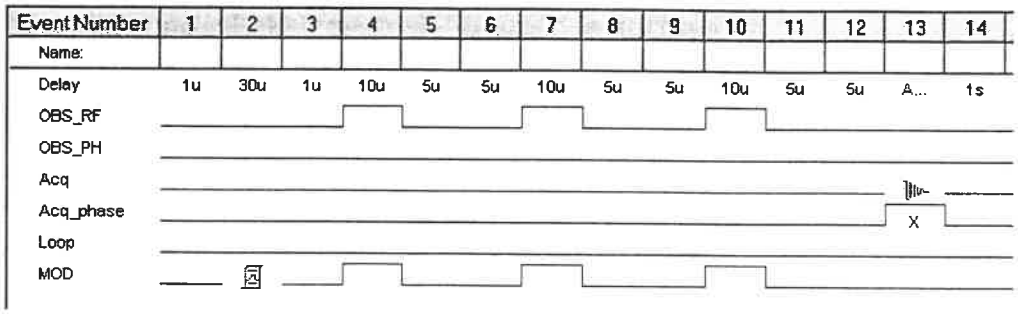
In the example sequence shown below, a "Stepped Table" was added in Event 2 of the "MOD" line. For the case of this example, assume that the "MOD" line has 2 bits assigned to it in the 'config.con' file.

Consider the following table entries for the Stepped Table in Event 2:

```
0 1 2 3 0 1 2 3
```

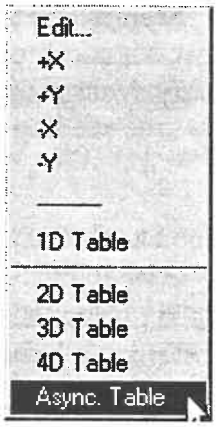
The first table entry is clocked out in Event 4 and stays active during Event 5 for a total duration of 15u. In Event 7, the second table value 1, is clocked out

and remains active for Event 8. The third table entry, 2, is active for Events 10 and 11. When the scan counter is incremented, after the completion of the last Event (Event 14), the table pointer is reset to the beginning and the first entry is again active for Events 4 and 5.

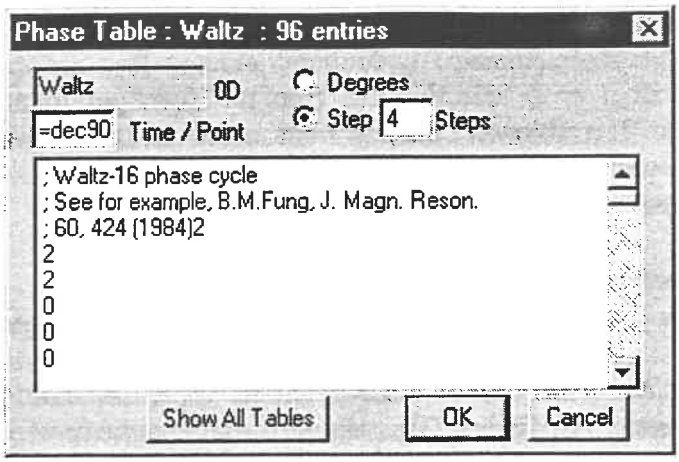


Async Tables

Sequence lines that are defined using the "DP" icon library also have the option of being run asynchronously with respect to the other events in the sequence. When defining the table in the sequence, select the option "Async. Table"



The Async Table option will activate the table edit window shown below:



This is the standard phase table edit dialog with the addition of the Time/Point option. This specifies the duration of each table entry (the 90 pulse in the case of Waltz, for example).

Once the asynchronous table has been defined the "Continue Table" selection can be used to continue the table in contiguous, subsequent events.

General Table Information

Table Size

There is no *software* limit on the number of tables of any type or on the number of entries in any given table. There are, however, hardware limits on the length of tables. Please consult the "Hardware Topics: Pulse Programming" guide for more information.

Multiple Instances

Tables can be re-used an unlimited number of times in the sequence. If, for example, a phase table is created and named "ph1", subsequent events can also use the table "ph1". Double-click on the new (or existing) Event, select Edit from the Event pop-up menu, or select a table of the correct dimension from the Event pop-up and enter the name "ph1".

Table Formats & Units

As mentioned earlier, table entries must be de-limited by a space or a carriage return. Also, a ";" character (semi-colon) can be used to comment lines in tables.

Time units *must* be included with each entry in Delay tables. The following symbols are valid: n = nanoseconds, u = microseconds, m = milliseconds, and s = seconds.

Renaming Tables
Tables can be renamed by double-clicking on the table name and entering the new name, or by selecting Edit from the Event pop-up menu and typing the new name. If a table with the new name exists, the existing table will be used for that event. If a table with the new name does not exist, a new blank table will be created.

Removing Tables
Tables can be turned off in the sequence (as can any other active Event) by selecting the "off icon" from the pop-up menu. Tables that have been removed or renamed will remain available in the Table Edit dialog and will still appear in the List of All Tables. This allows the table to be re-used or to be re-activated later if needed. Table can be permanently removed from the List of All Tables by selecting the table in the list and pressing the [DELETE] key.

Selecting "Remove unused tables" from the Sequence Window Commands menu will permanently remove any tables that are not in use in the active sequence.

Importing Tables
NTNMR does not currently have facilities for importing tables directly. However, tables can be copied from a text editor and pasted into the Table Edit window.

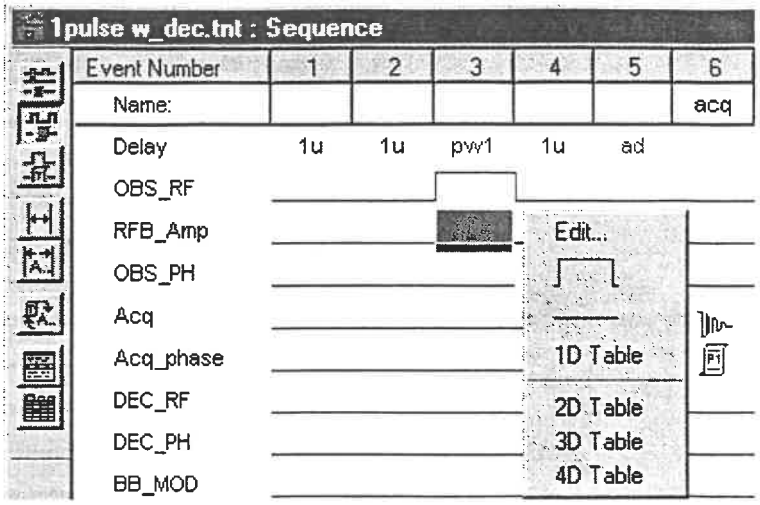
<<< PREV <<<

8.6 Sequence Variables

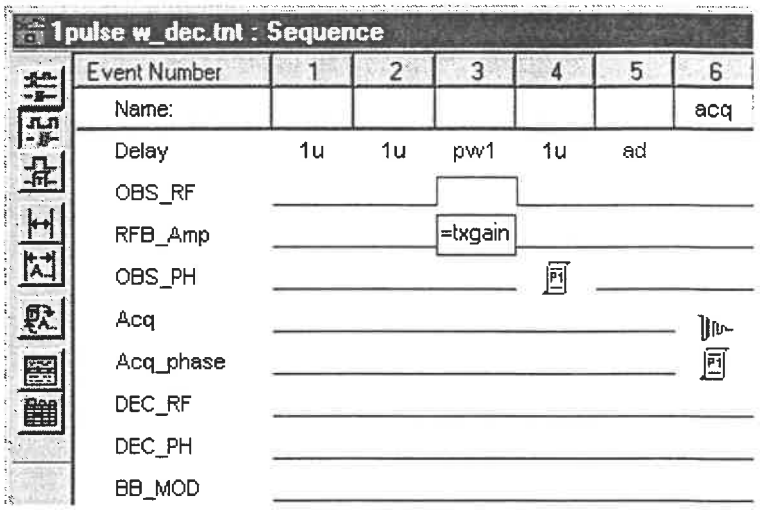
>>> NEXT >>>

NTNMR allows *unlimited* sequence variables to be defined. With the exception of the Acquisition line, any Event on any line in the sequence can have a variable assigned to it. To create and assign a variable to an Event, double-click the event (or select Edit... from the Event pop-up) and type "=*variable_name*". The "=" symbol (equal sign) indicates that the text that follows is a variable. The example below shows the steps to create a sequence variable. Sequence variables (displayed in green) appear in the Sequence tab in the Dashbaord. When viewing a sequence the Dashboard can be opened directly to the Sequence tab by clicking on the Edit Variables button on the Sequence toolbar or by right-clicking on any variable name.

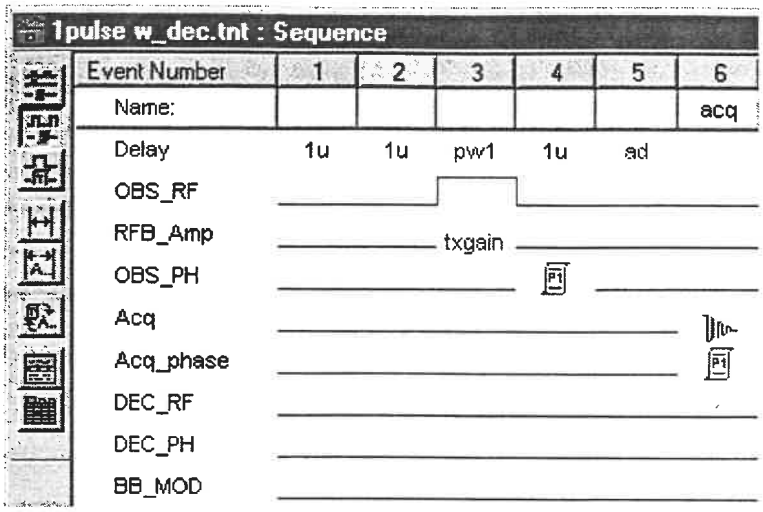
Click on the Event where the variable is to be inserted and select Edit... or double-click on the Event.



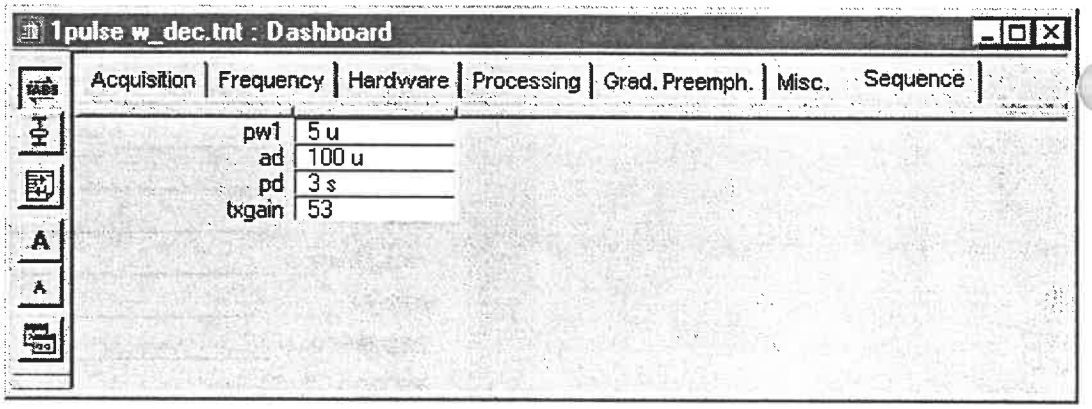
Type the "=" sign followed by the variable name ("txgain" in the example).



Press the [ENTER] key and the variable name will change to green.



The **Sequence** tab in the Dashboard will immediately be updated to include the newly created variable. Clicking on the **Sequence Variable** button will open the Dashboard and go directly to the **Sequence** tab as shown below.



This allows sequences to be written that can be completely controlled from the dashboard without the user having to edit the sequence directly. Sequence variables *and* values are saved with the **Data** file and the **Parameters** file. Sequence variables are also saved with the Sequence file.

Variables can be used multiple times in the sequence. Use the same method to assign a new variable outlined above. When the sequence encounters a variable name that has already been used the sequence assumes that the same variable is to be used for multiple events.

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8.7
>>> NEXT >>>

Acquisition

The **ACQ** and **ACQ Phase** labels in the timing diagram are always present, appearing by default after the last row defined in the timing diagram configuration file 'config.con' and before the loop counter line.

The **number of complex data points** collected during each acquisition event is set by the Dashboard parameter "Acq Points". Multiple acquisition events are allowed in a sequence. The number of points acquired in *all* Acquisition events is equal to "Acq. Points" set in the Dashboard. For special acquisition options see the Acquisition Properties section above.

Acquisition Phase

The acquisition phase for each acquisition is selected from the ACQ Phase line. The acquisition phase table format is exactly like other phase tables. Each acquisition can have a unique phase table, only phase values of 0, 1, 2, or 3 are allowed according to the table below:

ACQ	odd	even	Table value
+x	+A	+B	0
+y	-B	+A	1
-x	-A	-B	2
-y	+B	-A	3

If no ACQ Phase is selected, the default phase is set to 0.

For Quadrature Phase Detection, "ph1" might contain four entries 0, 1, 2 and 3. The phase of the transmitter would have a corresponding phase table with four entries to associate transmit pulse phase with acquisition phase. The phase cycle is complete when the scan count ends in a multiple of four. **Use "Soft" Stop to stop a pulse sequence after the next complete phase cycle.**

Acquisition Status

As discussed in the Chapter on the Main NTNMR Window, the acquisition status is reported in the **Status Bar** at the bottom of the Main Window (*not* the Data window). The number of scans completed for each dimension and a progress bar report the experiment status. The title bar of the Data window also indicates that an experiment is active and the time the experiment was started.

S.A. Dimension & S.A. Mode Parameters

The S.A. Dimension and S.A. Mode parameters are special dashboard parameters that control the order in which data is stored in the signal averager. Valid entries for S.A. Dimension are 0,1, 2, 3 or 4, while valid entries for S.A. mode are 0 or 1. Note that S.A. Mode is only active for S.A. Dimension = 0.

The S.A. Dimension parameter indicates in which order the data is acquired and stored. The following examples illustrate these parameters:

Example 1: Summation of individual acquisition events inside of a loop

S.A. Dimension = 0, S.A. Mode = 0

This is the default mode for S.A. Dimension = 1. In this mode, each acquisition within a loop will be added to itself each time through the loop. A sequence that contains two acquisition events inside of a loop, each with 512 points, will result in a final data set of 1024 points. The first 512 points will result from the summed data of the first acquisition and the second 512 points will result from the summed data of the second acquisition.

Example 2: Summation of all acquisition events inside of a loop

S.A. Dimension = 0, S.A. Mode = 1

In this mode, all acquisitions inside of a loop will be added. A sequence that contains two acquisitions inside of a loop, each with 512 points, will result in a final data set of 512 points.

Example 3: Block averaging of T1 relaxation data

S.A. Dimension = 2

When acquiring T1 relaxation data is often desirable to acquiring 1 (or several) scans per T1 time point instead of acquiring all averages for a single time point and then continuing on to the next time point. This approach evenly distributes instrumental artifacts over the whole data set.

The classical sequence (inversion recovery) for measuring T1 relaxation is the following pseudo-2D experiment:

180 - tau - 90 -acq

Where 'tau' is a suitable table of time values. Running this experiment in the non-block averaging mode would involve phase cycling the 180 and 90-degree

pulses as well as the acquisition in the "1st" dimension, and writing the 'tau' list as a 2D table. When the experiment is run, one 2D record would be created for each 'tau' value where each record would be the result of "Scans 1D" averages. The 2D record for the first 'tau' would be completed, then the second and so on.

To acquire this data in block average mode, simply write the phase tables for the 180 and 90-degree pulses. For the acquisition as 2D tables, write the 'tau' table as a 1D delay table, and set S.A. dimension to 2. In this case, when the experiment is run, one scan will be acquired for each 'tau' point in turn. Then NTNMR will loop back to the first 'tau' point and acquire a second average for each 'tau' point, etc.

Example 4: Multi-slice imaging

S.A. Dimension = 2

A common use for S.A. Dimension = 2 is a multi-slice imaging experiment. In this case, one average is acquired for each frequency slice indicated in the experiment. After 1 average of all frequencies has been acquired, a second average is then acquired at each frequency and so on.

The experiment then is written so that the frequency selection table is a 1D table and the phase tables for signal averaging are 2D tables. Then when S.A. Dimension is set to 2, NTNMR will acquire 1 scan for each frequency in the 1D table, storing the data in a serial fashion in the signal averager. (Note that if the signal averager was set to 1, the default mode, each of the frequency selected FIDs would be summed.) Once all entries of all 1D tables have been executed, NTNMR will increment the 2D tables and reset the signal averager memory pointer to the beginning, thus achieving signal averaging.

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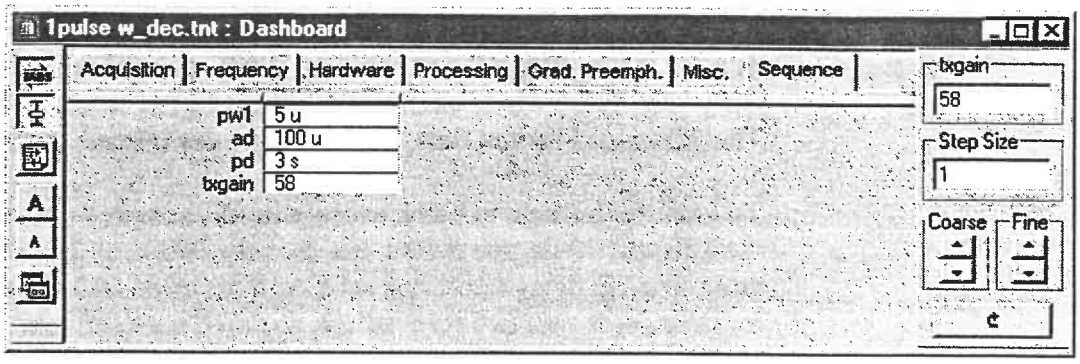
8.8
>>> NEXT >>>

Real Time Adjustment Mode

The Real Time Adjustment mode allows all user defined sequence parameters and virtually all Dashboard parameters to be interactively adjusted while acquiring data. Clicking on the  button in the Dashboard activates the real time adjustment mode. The Adjustment dialog is added to the Dashboard on the right hand side of the window as shown below.



To activate a parameter for adjustment, left-click in the desired parameter's text edit field. The adjustment dialog will be updated, inserting the new parameter name, it's current value and a default **Step Size** that is 10% of the current value. The **Step Size** can be manually edited as in the example above where it has been set to 1.

When a repetitive scan (**RS**) is activated, the Real Time Adjustment Mode is active. Clicking on the up and down arrows in the **Coarse** field will adjust the parameter by the amount indicated in the **Step Size** field. Clicking on the up and down arrows in the **Fine** field will adjust the parameter by (0.1 * **Step Size**). Once an adjustment has been made the Toggle button at the bottom of the window is updated to display the starting value. Clicking on the Toggle button will re-set the parameter to the starting value and update the Toggle button to display the last value used. Each time the Toggle button is clicked the *last value set* will be recalled. This allows the user to toggle between values with a single click.

Real Time Adjustment mode is only available when repetitive scan mode is active. Some Dashboard parameters are not available for Real Time Adjustment, such as text and information only fields.

<<< PREV <<<

8.9 Multi-Dimensional Sequences

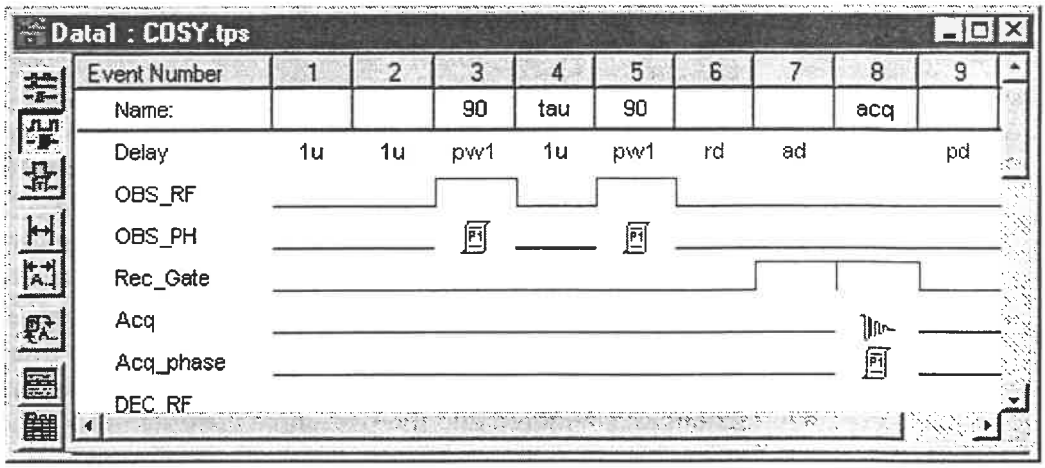
>>> NEXT >>>

Sequence Creation

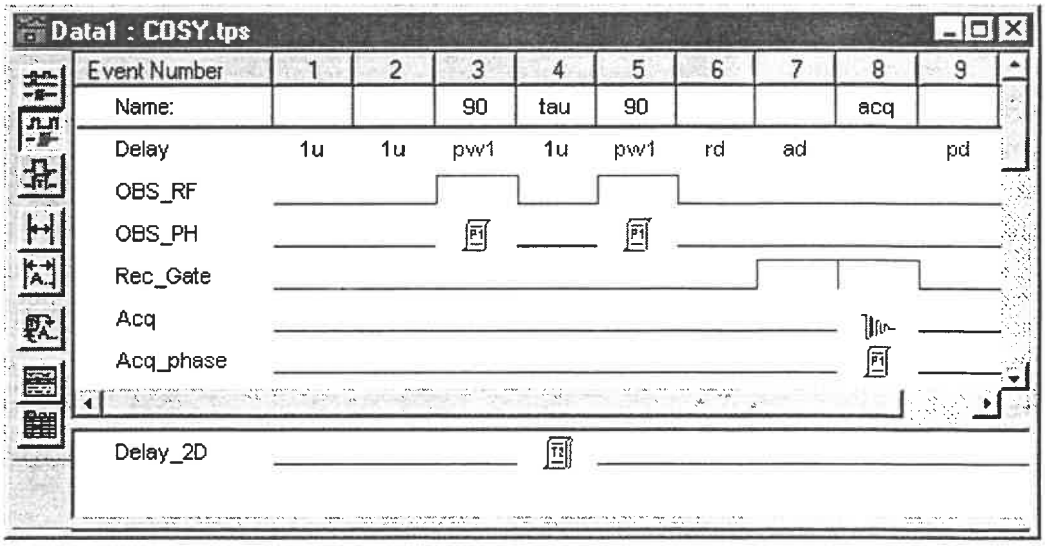
Multi-dimensional acquisitions of up to four dimensions are easily facilitated with NTNMR. Tables can be specified from 1 to 4 dimensions and each dimension in the sequence is displayed in a new section. The example below shows the addition of a 2D-Delay table to a sequence.

A Simple Example

The following starting point for a COSY sequence was created using the general techniques discussed above. Event number 4 (named "tau") has been assigned a value of 1u.



A 2D table was added for the Delay line in Event 4. When a multi-dimensional table is added, a new section is created for that dimension at the bottom of the sequence. Lines are added to the new multi-dimensional section of the sequence only as needed and they are named in the format *linename_dimension*. The example below shows the line "Delay_2D", indicating that this new line is associated with the "Delay" line in the main sequence window (i.e., the first dimension). All 2D tables that are created appear in the 2D section of the sequence. New lines are added as needed.



Multi-dimensional tables are edited in the same manner as their 1D counterparts; right-click on a table or click the Edit Tables button to activate the Edit Tables window.

Multi-Dimensional Table Concepts

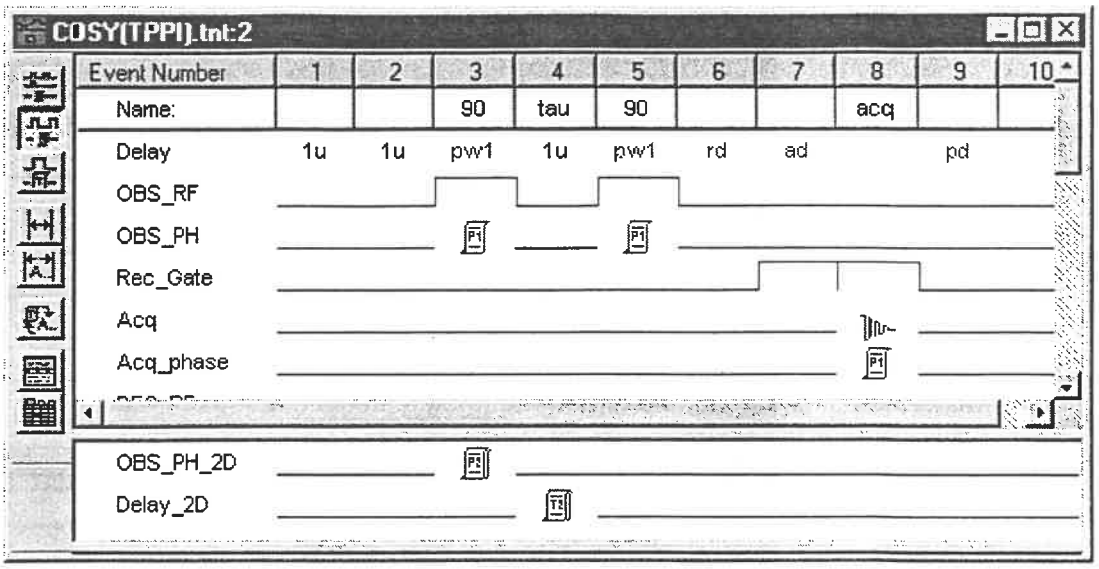
Multi-dimensional tables in NTNMR can function in one of two ways. First, and simplest, the table can be incremented with the dimension counter and the corresponding value used for the Event. This is the case that is illustrated in the sequence above. The 2D delay table that appears in the "Delay_2D" line in Event 4 of the example will simply insert a new value for the "Delay" in Event 4. Each time the 2D counter is incremented (i.e. for each 2D point). In this COSY example, this corresponds to the 2D Dwell time. As discussed in the section above, the Delay tables could be explicitly written out in the form: 2u, 102u, 202u, 302u, … . In this case, the 1D Delay time (1u in the above example) is ignored and the first entry in the 2D table is used for the first 2D point.

The second application of Multi-dimensional tables is where the highest dimension table modifies the next lowest dimension table. This means that a 2D table *can* modify the value set in the corresponding 1D event, whether it is a table or a single value. Similarly, a 3D table can modify a 2D Event and a 4D table can modify a 3D Event.

It is important that the user understand when a multi-dimensional table will *modify* the corresponding (dimension - 1) table and when it will simply control the Event in the sequence.

All tables that are set to the **Auto** mode, such as Delay and Loop tables, will modify the corresponding 1D Event. Consider the basic COSY example shown above. If the Delay_2D table in Event 4 was set to be auto-incremented (**Auto** mode) based on the Dashboard Dwell_2D parameter, the time for Event 4 during acquisition of the first 2D point would be 1u (the 1D Event time). Each 2D point after that will be the accumulation of the Event time for the previous 2D point and the Dashboard parameter Dwell_2D. So, for the second 2D point, the time for Event 4 would be (1u + Dwell_2D). For the third 2D point, the time would be (1u + Dwell_2D + Dwell_2D) and so on. The same logic is applied to Loop tables that are auto-incremented.

Phase tables *always* modify their corresponding (dimension - 1) Events. The extension of the basic COSY example above to a phase sensitive COSY will illustrate this point. First consider the TPPI case.



In the sequence shown above, the basic COSY experiment has been modified to add a 2D-phase table. This table, which appears in the OBS_PH_2D line, modifies the 1D phase table that is in the OBS_PH line of the sequence. The tables have the following entries:

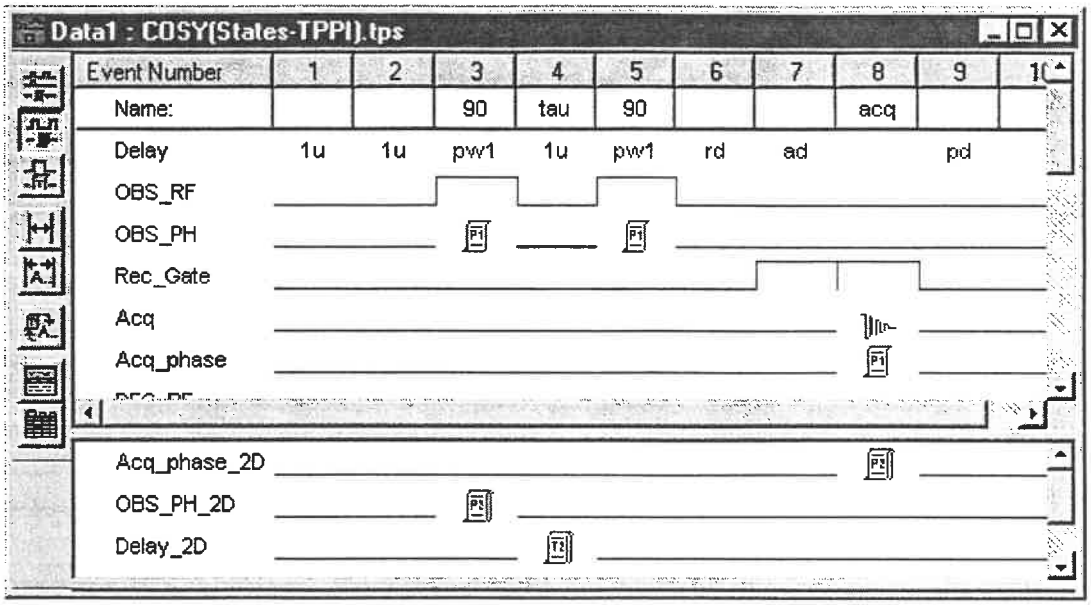
- 1D phase table: 0 2 2 0 1 3 3 1
- 2D phase table: 0 1 2 3

The 2D table is incremented with respect to the 2D scan counter (i.e. with each 2D point) and the entry that is valid for the current 2D point is added to *all entries* in the 1D table. Always keep in mind that 2D tables (also 3D and 4D) are cycled in exactly the same way as 1D tables, except that they are cycled with the second dimension counter (third or fourth for 3D and 4D tables), instead of the first. The following table illustrates what the phase cycling would be for the above example for the first 5 2D points.

2D Point	phase cycle
1	0 2 2 0 1 3 3 1
2	1 3 3 1 2 0 0 2
3	2 0 0 2 3 1 1 3
4	3 1 1 3 0 2 2 0
5	0 2 2 0 1 3 3 1

This achieves the required 90 incrementation on the "preparation" pulse with respect to the 2D point being acquired; that is required for TPPI.

The following, slightly more complicated example, illustrates the implementation of a phase sensitive COSY experiment via the mixed States-TPPI method.



This sequence adds another 2D-phase table which appears in the "Acq_phase_2D" line. This table modifies the "Acq.phase" table. The following phase tables are used in the example above:

Transmitter Phase Tables

- OBS_PH "preparation" pulse (Event 3): 0 2 2 0 1 3 3 1
- OBS_PH_2D (2D Event 3): 0 1 2 3

Acquisition Phase Tables

- Acq_phase (Event 8): 0 2 2 0 1 3 3 1
- Acq_phase_2D (2D Event 8): 0 0 2 2

Additionally, the Delay_2D table (2D, Event 4) is set to **auto-increment** using the Dashboard parameter **Dwell_2D** with the **Increment Scheme** set to "Every 2 Passes". (See the section on tables for details on these table settings)

The following tables show the Phase Cycling and 2D delay with respect to the 2D point number:

2D Point	2D Delay (Event 4)	Transmitter Phase Cycle	Acq. Phase Cycle
1	1u	0 2 2 0 1 3 3 1	0 2 2 0 1 3 3 1
2	1u	1 3 3 1 2 0 0 2	0 2 2 0 1 3 3 1
3	1u + Dwell_2D	2 0 0 2 3 1 1 3	2 0 0 2 3 1 1 3
4	1u + Dwell_2D	3 1 1 3 0 2 2 0	2 0 0 2 3 1 1 3
5	1u + (Dwell_2D * 2)	0 2 2 0 1 3 3 1	0 2 2 0 1 3 3 1
6	1u + (Dwell_2D * 2)	1 3 3 1 2 0 0 2	0 2 2 0 1 3 3 1
7	1u + (Dwell_2D * 3)	2 0 0 2 3 1 1 3	2 0 0 2 3 1 1 3
8	1u + (Dwell_2D * 3)	3 1 1 3 0 2 2 0	2 0 0 2 3 1 1 3

<<< PREV <<<
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>>> NEXT >>>

Pulse Sequence Configuration File

> *This section is provided for the advanced user and is not necessary for understanding pulse sequences in NTNMR. You may also wish to consult the hardware manual for more information.*

The 'config.con' file is a text file used by NTNMR to format the Pulse Sequence Window. This file must be located in the 'System' folder in the NTNMR folder. This file contains the interface information necessary to assign output lines from the Tecmag pulse programmer for spectrometer control functions. In general, this file should not be edited by the user. However, there may be cases, such as the construction of a home built spectrometer based on a Tecmag Pulse Programmer, where it may be necessary to edit the 'config.con' file.

```
;file name = config.con
;
;Definition of LP lines
;
;     -- File Format --
;
; 1 = <Name>
; 2 = <Module Prefix>
; 3 = <Start Address>
; 4 = <Number of Bits>
; 5 = <Minimum delay>
; 6 = <Maximum Delay>
; 7 = <Delay Unit>
; 8 = <Icon type>
; 9 = <Visible?>
; 10 = < Private Data>
; Any text after ";" on each line is ignored.
; Fields are delimited by either spaces or tabs.

; <1>       <2> <3><4><5><6><7> <8> <9> <10>
OBS_RF      ES1 20  1  1  0  0  TX   1   0; OBS_RF gate (p1_SPF1)
OBS_PH      ES1 19  2  1  0  0  PH   1   0; obs. Phase= LP19,LP18
Acq         IO3 1   2  0  0  0  ACQ  1   0;
Acq_phase   IO3 3   2  0  0  0  PH   1   0 ;
DEC_RF      ES1 21  1  1  0  0  TX   1   0 ; Dec_RF gate
DEC_PH      ES1 15  2  1  0  0  PH   1   0 ; decouple phase
BB_MOD      ES1 22  1  1  0  0  TX   1   0 ;
RCP4        EM1  3  1  1  0  0  TX   1   0
;ATN2       EM1  8  2  1  0  0  TX   1   0 ; I3_ATN3
;SPOIL      EM1  1  1  1  0  0  TX   1   0
Rec_Gate    ES1 12  1  1  0  0  TX   1   0;
Gx_Shape    GM1 31 16  0  0  0  SH   1   0;
Gx_Amp      GM1 15 16  0  0  0  GR   1   0;
Gy_Shape    GM2 31 16  0  0  0  SH   1   0;
Gy_Amp      GM2 15 16  0  0  0  GR   1   0;
Gz_Shape    GM3 31 16  0  0  0  SH   1   0;
Gz_Amp      GM3 15 16  0  0  0  GR   1   0;
SH_RF_A     GM5 31 16  0  0  0  SH   1   0;
RFA_Amp     GM5 15 16  0  0  0  GR   1   0;
SH_RF_B     GM6 31 16  0  0  0  SH   1   0;
RFB_Amp     GM6 15 16  0  0  0  GR   1   0;
```

The semi-colon character is used to comment a line. Everything after the ";" on any line is ignored. Individual lines can be commented out. (As in the "ATN2" and "SPOIL" lines in the example above)

NTNMR creates the sequence window with the lines in the order that they appear in the 'config.con' file. This is only the default order and lines can be repositioned in the sequence window.

The fields in the file are labeled as <1>, <2>, ... <8> for informational purposes only. The fields are described below in reference to the labels in the above example.

<1> Line Name. This is the exact text that will appear in the pulse sequence window when NTNMR is run.

<2> Module Prefix. This tells the software what type of module this line in the pulse sequence is controlling. There are several module types: EM (*event module*), ES (*event module slave*), GM (*gradient module*), etc. Each module has a number assigned to it, EM1, IO3, GM4, etc. Consult the hardware documentation for more information about the various module types and their function.

<3> Start Address. This is an integer number that defines the starting address for the pulse programmer lines to use for the current line in the pulse sequence.

<4> Number of Bits. This is an integer number that defines the number of pulse programmer lines to use starting from the Start Address. For example, in the 'config.con' example above, the line Gx_Shape with a starting address of "31" and a number of bits value of 16. This means that there are 16 bits assigned to the control of the GM1 module. The 16 bits are 31, 30, 29, ...16.

<5>, <6>, <7> These fields are currently unused.

<8> Icon Library. This field contains a two-letter code that assigns the type of icon to display in the NTNMR graphical sequence display. The various icon type and their function are discussed in the next section.

<9> Visible. This flag determines whether or not the defined line will be visible in the graphical pulse sequence editor in NTNMR. 1 = visible, 0 = invisible.

<10> Private Data. This field is used for various line-specific data assignments. For example, this field may be used to indicate the resolution of the transmitter phase shifter, the resolution of the transmitter attenuator, etc.

In the Pulse Sequence Window, the **Delay**, **ACQ**, **ACQ Phase** and **Loop** row labels are added to the timing diagram automatically by the software. They are not part of the 'config.con' file.

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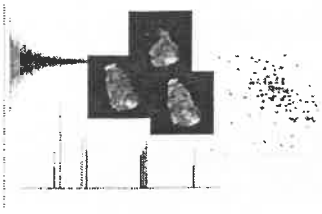
Icon Libraries

Each icon library used in the 'config.con' file is outlined in the table below. For specific examples of the icons that appear in the pulse sequence window, see the section above entitled "Defining and Editing Pulse Sequences."

Library	Icons	Information
TX	Gate on, Gate off	Used for controlling rf transmitter channels, attenuators and external devices.
PH	Fixed phases (+x, +y, -x, -y) and 1 - 4D tables	Used for controlling rf phase shifts and for signal averager phase cycling.
ACQ	Acquisition	Indicates the start of data acquisition by the signal averager.
SH	Shape	Allows the creation of waveform (i.e. shape) tables for gradients or for RF pulse shaping.
GR	Gradient	Gradient amplitude control.
PS	Shape	Phase modulation.
RM	Shape	Transmitter amplitude modulation.
AT	Shape	Transmitter attenuator.
ET	Gate on, Gate off	Activate the external trigger.
LD	Shape, gate	Used to assign a group of lines to be used for clocking out a table of values one value at a time.



9 - Automation

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Introduction

NTNMR provides the ability to automate many of its processes. This allows sophisticated acquisition and processing routines to be created that can be executed from a single click. Applications include complex data processing, automatic execution of a suite of experiments, calibration experiments or even creating a specialized virtual replacement for the NTNMR interface.

The term "Scripting" has been adopted to refer to automating processes in NTNMR because the capabilities far surpass what are typically referred to as "Macros." Conceptually, however, "scripts" in NTNMR can be thought of as "macros."

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OLE Automation

OLE (Object Linking and Embedding) is a method created by Microsoft to allow one application to be controlled by another. NTNMR supports OLE Automation (but *not* Linking and Embedding at this time). This method allows the "Objects" in NTNMR to be "exposed" so that another application can control it. Microsoft Word and Microsoft Excel are other applications that are "OLE compliant."

Both the Document object and the Application object are exposed in NTNMR. Most commands are accessed through the Document. However, some very important functionality is accessed through the application (this will be discussed in detail below).

It is useful to familiarize yourself with the Microsoft terminology used when referring to OLE. The *OLE Server* is the application that exposes its objects to other applications - any of those objects can be used in a Visual Basic application. The *OLE Client* is the application that controls the *OLE Server*. The client can be a 'stand alone' application written in Visual Basic (or another OLE Compliant programming language).

Further Information about OLE automation is available from a variety of books and Internet web pages. Any further discussion of OLE technology is beyond

the scope of the manual, and furthermore, is not necessary for writing"scripts" to control NTNMR.

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9.3 Visual Basic & VBScript

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General Information

Visual Basic 5.0 and VBScript have been adopted by Tecmag as the "official supported" scripting languages. Many other languages such as WinBatch, Visual C++, Java and Python have the ability issue OLE commands and can be used to control NTNMR. The discussion in this manual refers specifically to Visual Basic 5.0 and VBScript; although most of these concepts should generally apply to any other language that may be used to control NTNMR.

Visual Basic or VBScript?

As a general rule, the more complicated the NMRScript, the more likely it is that one would want to use Visual Basic, instead of VBScript. It is important to note that Visual Basic is a programming language, with its own development environment, while VBScript is very much a scripting language.

Compatibility and Support Note

While it is possible to use other programming languages to control NTNMR, Tecmag is unable to guarantee performance and compatibility with other languages. Furthermore, the degree to which Tecmag may be able to support "scripting" languages other than Visual Basic 5.0 may be limited.

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9.4 Automation Commands - Abbreviated List

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The following tables contain shorthand listings of all commands that are currently scriptable in NTNMR. Readers may wish to refer to the Commands Chapter of the manual for specific details. Those commands that are specified as Automation Only, are not available through the NTNMR graphical user interface. Refer to the next section for specific examples of each command.

Scriptable Command: Name(s) of command as used in Visual Basic

AO: Command is available only through automation, i.e. Automation Only

Parameters: Arguments to be supplied with command

Type: Type of data to be supplied or returned

Dashboard: If the command uses parameters from the dashboard, they are specified

NTNMR.Document Object Commands				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
Processing Commands	-	-	-	-
BaselineCorrection, BC	no	-	-	-
BaselineTilt, BT	no	-	-	-
ZeroFill, ZF	no	[optional] points	long	-
EchoZeroFill, EZF	no	[optional] points	long	-
ExponentialMultiplication, EM	no	[optional] lb	double	LB 1D
GaussianMultiplication, GM	no	[optional] gb	double	GB 1D
DoubleExponentialMult, DM	no	[optional] db	double	DM 1D
SinBell, SB	no	[optional] shift, width, skew	double, double, double	SB Shift 1D, SB Width 1D, SB Skew 1D
SinBellSquared, SBS	no	[optional] shift, width, skew	double, double, double	SB Shift 1D, SB Width 1D, SB Skew 1D
Trapezoid, TZ	no	[optional] tz1, tz2, tz3, tz4	long, long, long, long	TZ 1 1D, TZ 2 1D, TZ 3 1D, TZ 4 1D
TrafWindow, TW	no	[optional] tw	double	Traf 1D
BlackmanHarris, BH	no	[optional] shift, width	double, double	SB Shift 1D, SB Width 1D
EchoExponentialMult, EEM	no	[optional] lb	double	LB 1D
FourierTransform, FT	no	-	-	-
InverseFT, IFT	no	-	-	-
RealFT, RFT	no	-	-	-
EchoFT, EFT	no	-	-	-
nDFT	no	[optional] file	file path	-
SetNDPhase	no	dim, ph0, ph0	short, short, short	-
SetNDEchoCenter	no	Dim, Center	short, short	-
SetNDApodization	no	Dim, par1, par2, par3, par4	short, short, short, short, short	-

NTNMR.Document Object Commands Continued				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
SetNDTranspose	no	Dim, Type, Data	short, short, short	-
SetNDParameters	no	Dim, BC, ZeroFill, FT, Reverse, Phase, Apodization	short, bool, short, short, bool, short, short	-
PhaseCorrection, PC	no	[optional] ph0, ph1	-	-
AutoPhase, AP	no	-	-	-
AutoIntegrate, AI	no	-	-	-
ReadFirstHalf	no	-	-	-
ReadSecondHalf	no	-	-	-
LeftShift	no	[optional] points, [optional] zero out	long, BOOL	-
RightShift	no	[optional] points, [optional] zero out	long, BOOL	-
Transpose	no			-
SeparateRecords	no	into or joining, files	BOOL, file path	-
ReverseSpectrumRows	yes	-	-	-
ReverseSpectrumColumns	yes	-	-	-
NDTranspose	yes	nX, nY, nZ, nA	long	-
NDComplexTranspose	yes	nX, nY, nZ, nA	long	-
-	-	-	-	-
File I/O:	-	-	-	-
Save	no	-	-	-
SaveAs	no	file path	string	-
OpenFile	no	file path	string	-
LoadSequence	no	file path	string	-
SaveSequence	no	-	-	
SaveSequenceAs	no	file path	string	-
GetSequenceName	yes	file path	string	-
GetActiveDocPath	yes	-	string	-
-	-	-	-	-

NTNMR.Document Object Commands Continued				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
Acquisition Commands	-	-	-	-
ZeroAndGo, ZG	no	-	-	-
Go	no	-	-	-
CheckAcquisition	yes	-	-	-
Stop	no	-	-	-
Abort	no	-	-	-
reset	no	-	-	-
-	-	-	-	-
Miscellaneous	-	-	-	-
SetNMRParameter	yes	name, value	char, variable	-
GetNMRParameter	yes	name	char, returns variable	-
GetComment	yes		string	-
SetComment	yes	string	string	-
-	-	-	-	-
Data	-	-	-	-
GetData	yes	-	variant (array)	-
SetData	yes	array	variant (array)	-
GetDataPoint	yes	-	variant (array)	-
SetDataPoint	yes	point, array	long, array	-
Get1Drecord	yes	record	long	-
GetDataSize	yes	-	long	-
GetNDSize	yes	dimension	long	-
ReSetDimensionInfo	yes	n1D, n2D, n3D, n4D	long	-
-	-	-	-	-
Display	-	-	-	-
FitToWindow	no	-	-	-
AutoDisplayWhileProcessing	yes	-	boolean	-
UpdateDisplay	yes	-	-	-

NTNMR.Document Object Commands Continued				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
SetNDRecordPointer	no	dimension, record	long	-
SetRecordPointer	no	n2D, n3D, n4D	long	-
GetNDRecordPointer	yes	dimension	long	-
SetSelection	yes	nStart, nEnd	long	-
SetCursorPosition	yes	nPoint	long	-
GetCursorPosition	yes	-	-	-
Get1DSelection	yes	startPt, endPt	string	-
Get1DSelectionEnd	yes	endPt	long	-
-	-	-	-	-
-	-	-	-	-
Zoom	no	nStart, nEnd	long	-
Set2Dcursor	yes	nAxis, nPoint	long	-
Get2Dcursor	yes	nAxis	long	-
Open2DView	no	Init, Mode, Disp, Aspect	bool, short, short, short	-
-	-	-	-	-
Sequence	-	-	-	-
SetTable	yes	table name, entries	string	-
GetTable	yes	table name	string	-
GetTableList	yes	-	string	-
-	-	-	-	-
Option Modes	-	-	-	-
Baseline Fix	-	-	-	-
AutoBaslineFix	no	function type, num of points, apply to all	string, long, boolean	-
DoBaselineFix	no	function type, num of points, array list, units, apply to all	string, long, string (,), units, boolean	-
Peak Pick	-	-	-	-
PickOnePeak	no	position, units	double, string	-

NTNMR.Document Object Commands Continued				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
AutoPeakPick	no	-	-	-
ShowPeakPick	no	-	-	-
ClearPeakPick	no	-	-	-
GetPeakPickList	yes	units	-	-
GetPeakPickAmplitudes	yes		-	-
Line Fits	-	-	-	-
AddOneLineFit	no	left, right, units	double, double, string	-
Integration	-	-	-	-
AutoIntegrate, AI	no	position, units	double, string	-
ShowIntegrals	no	-	-	-
LoadIntegrals	no	file path	-	-
Integrate	no	left, right, parameters	double, double, string	-
ClearIntegrals	no		-	-

NTNMR.Application Object Commands				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
Dashboard Commands	-	-	-	-
GetParameterPageList	yes	-	string	-
GetParameterListInPage	yes	page name	string	-
SetParameterListInPage	yes	page, parameter list	string	-
AddParametersToPage	yes	page, parameter list	string	-
RemoveParameterPage	yes	page	string	-
RemoveAllPages	yes	-	-	-
LoadParameterSetupFromFile	no	path name	string	-
SaveParameterSetupToFile	no	path name	string	-
SetActiveParameterPage	no	page	string	-
LoadParametersFromFile	no	path name	string	-
SaveParametersToFile	no	path name	string	-
-	-	-	-	-
Printing	-	-	-	-
AddActiveDocToPrintPreview	yes	table name, entries	string	-
GetTable	yes	table name	string	-
GetTableList	yes	-	string	-
-	-	-	-	-
Misc. Commands	-	-	-	-
GetActiveDocPath	yes	-	string	-
Quit	no	-	-	-
ShowWindow	no	-	-	-
HideWindow	no	-	-	-
GetDocumentList	no	-	string	-
Shims	-	-	-	-
SetOneShim	no	shim, value	string, long	-
ActivateShims	no	list of shims	string (,)	-
StartShims	no	-	-	-
CheckShimProgress	yes	false = complete	-	-
GetActualShimPrecision	no	-	double	-
SetAutoShimParameters	no	delay, precision, type	string, float, integer	-
Sample	-	-	-	-

NTNMR.Application Object Commands Continued				
Scriptable Command	**AO**	**Parameters**	**Type**	**Dashboard**
LiftSample	no	-	-	-
SpinSample	no	-	-	-
SetSpinRate	no	-	-	-
GetSpinRate	no	-	long	-

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Automation Commands - Syntax & Examples

Abort

Usage:

objectname.Abort

Object:

Document

Description:

Stops the current data acquisition immediately, without completing the current phase cycle.

ActivateShims

Usage:

objectname.ActivateShims "shim_name1, shim_name2, ..."

Object:

Application

Description:

Activates the shims listed "shim_name1, shim_name2, ..." for use in an auto shim operation.

AddActiveToPrintPreview

Usage:

objectname.AddActiveToPrintPreview

Object:

Application

Description:

Adds the active data display to the documents print preview window. Use in conjunction with LoadPrintPreviewTemplate to automate creation of custom plots.

AddOneLineFit

Usage:

objectname.AddOneLineFit *start, stop, unit*

Object:

Document

Description:

Adds a line fit simulation beginning at the left position specified in *start* and ending at the right position specified in *stop* with the units specified in *unit*. Valid units are "points", "hz", or "ppm".

AddParametersToPage

Usage:

objectname.AddParametersToPage "page_name", " param_1, param_2, param_3"

Object:

Application

Description:

Adds the named parameters (*param_1, etc.*) to the named page (*page_name*). Parameters must be valid dashboard parameters and must be comma delimited.

AutoBaselineFix

Usage:

objectname.AutoBaselineFix *"function", num_points, apply_to_all*

Object:

Document

Description:

Performs an auto baseline fix on frequency domain data with the following parameters: *function* = "spline" or "polynomial"; *num_points* = indicates the number of points to include in the calculation; *apply_to_all* = true applies to all records in an nD, false applies only to the active record.

AutoDisplayWhileProcessing

Usage:

objectname.AutoDisplayWhileProcessing *true/false*

Object:

Document

Description:

Allows the data display to be disabled during automatic data processing.

AutoIntegrate
AI

Usage:

objectname. AutoIntegrate
objectname. AI

Object:

Document

Description:

Automatically integrates the spectrum based on peak finding variables set in the Integrate Option mode. See the chapter on Options for more information.

AutoPeakPick

Usage:

objectname.AutoPeakPick

Object:

Document

Description:

Automatically peak picks the active spectrum.

AutoPhase

Usage:

objectname.AutoPhase

Object:

Document

Description:

Performs an auto phase of the type indicated in the 1D preferences (analytical or iterative).

BaselineCorrection
BC

Usage:

objectname.BaselineCorrection
objectname.BC

Object:

Document

Description:

Removes the dc level of the signal by calculating the mean over the last 12% of the data (Commonly applied before Fourier Transform is performed. Note that the NTNMR Fourier Transform *does not* apply any DC correction).

BaselineTilt
BT

Usage:

objectname.BaselineTilt
objectname.BT

Object:

Document

Description:

Corrects for slope and offset of the baseline. (Commonly used before Auto Integrate.)

BlackmanHarris
BH

Usage:

objectname. BlackmanHarris *shift*, *width*
objectname.BH *shift*, *width*

Object:

Document

Description:

Blackman Harris weighting using the phase shift *shift* and the function width *width*. The *shift* and *width* parameters are optional. If they are omitted, the SB Shift and SB Width in the dashboard will be used. Note: The *width* parameter specifies the **full** width of the function meaning that the function will cross zero at (Points 1D * 2).

CheckAcquisition

Usage:

objectname.CheckAcquisition

Object:

Document

Description:

Used to get the current acquisition status of NTNMR. The command is required in scripts that involve data acquisition. The CheckAcquisition command is used inside of a Do loop; the loop is not exited until CheckAcquisition returns a value of False.

Example:

```
Do While Not Data.CheckAcquisition
DoEvents
Loop
```

CheckShimProgress

Usage:

objectname.CheckShimProgress

Object:

Application

Description:

Used to get the current acquisition status of an auto shim operation. The command should be used after starting an auto shim and before the next command. The CheckShimProgress command is used inside of a Do loop; the loop is not exited until CheckShimProgress returns a value of False.

Example:

```
Do While Not Data.CheckShimProgress
DoEvents
Loop
```

ClearIntegrals

Usage:

objectname.ClearIntegrals

Object:

Document

Description:
Clears all integrals.

ClearPeakPick

Usage:
objectname.ClearPeakPick

Object:
Document

Description:
Clears all peak picks.

DoBaselineFix

Usage:
objectname.DoBaselineFix *function, num_points, "point1, point2, ...", unit, apply_to_all*

Object:
Document

Description:
Performs a baseline fix of type *function* ("spline" or "polynomial") with the number of points specified in *num_points*. The spectral positions of the points are specified in a comma delimited list as "*point1, point2, ...*". The units for the list of points are specified as *unit* with valids units being "points", "hz", and "ppm". If *apply_to_all* is true, the baseline fix will be applied to all records. If the data is nD, if *apply_to_all* is false, the baseline fix will be applied to the active record only.

Example:

```
Data.DoBaselineFix "spline", 8, "100, 266, 511, 756, 1200, 1578, 2001, 2020", "points", false
```

DoubleExponentialMult
DM

Usage:
objectname. DoubleExponentialMult *value*

objectname. DM value

Object:

Document

Description:

Performs a Gaussian/exponential weighting using *value*. The *value* parameter is optional; if omitted, DM 1D from Dashboard will be used.

EchoExponentialMult
EEM

Usage:

objectname. EchoExponentialMult *value*
objectname. EEM *value*

Object:

Document

Description:

Performs an echo exponential multiplication on a 1D data set with a function defined by: f(t) = exp - [t * ^{1} * (*value*)]. The *value* parameter is optional; if omitted, LB 1D from Dashboard will be used. The center of the echo, which does not have to be half the number of points, is specified by the Dashboard parameter "Echo Center."

EchoFT
EFT

Usage:

objectname. EchoFT
objectname. EFT

Object:

Document

Description:

Performs a one dimensional fast Fourier Transform on a 1D data set, assuming that echo maximum is at the point specified by the Dashboard Parameter "Echo Center."

EchoZeroFill
EZF

Usage:

objectname. EchoZeroFill
objectname. EZF

Object:

Document

Description:

Doubles the number of data points (Points 1D) in memory and fills with zeros, taking into account that the data is in echo format by zero filling around the point specified by the Dashboard parameter "Echo Center." This command is valid only for 1D data sets.

ExponentialMultiplication
EM

Usage:

objectname. ExponentialMultiplication *value*
objectname. EM *value*

Object:

Document

Description:

Performs an exponential multiplication on the 1D data set with a function defined by: f(t) = exp - [t * ^{1} * (*value*)]. The *value* parameter is options; if omitted, LB 1D from Dashboard is used.

FitToWindow
FTW

Usage:

objectname.FitToWindow
objectname.FTW

Object:

Document

Description:

Performs a one-time auto scale on the data display. If a zoom region is active, the data in the zoom will be auto scaled.

FourierTransform
FT

Usage:

objectname.FourierTransform
objectname.FT

Object:

Document

Description:

Performs a one-dimensional fast Fourier transform on a 1D data set.

GuassianMultiplication
GM

Usage:

objectname.GaussianMultiplication
objectname.GM

Object:

Document

Description:

Performs a Gaussian multiplication on a 1D data set with a function defined by: f(t) = exp - [(t * ¹ * (*value*)) / (1.6651)] exp 2. The *value* parameter is optional; if omitted, GM 1D from Dashboard is used.

Get1DRecord

Usage:

objectname.Get1DRecord *record_number*

Object:

Document

Description:

Returns a variant that contains a 1D array of the data contained in the specified record in the format R, I, R, I, R, ...

Example:

```
MyVariable = Data.Get1DRecord (5)
```

Get1DSelection

Usage:

objectname.Get1DSelection

Object:

Document

Description:

Returns a string that contains the start and stop points of the currently highlighted 1D selection in the data display in the form (*start, stop*). If there is no currently highlighted region, Get1DSelection returns the first and last points in the spectrum.

Example:

```
MyVariable = Data.Get1DSelection
```

Get1DSelectionEnd

Usage:

objectname.Get1DSelection

Object:

Document

Description:

Returns the end point of the currently highlighted 1D selection in the data display.

Example:

```
MyVariable = Data.Get1DSelectionEnd
```

Get2DCursor

Usage:

objectname.Get2DCursor *axis*

Object:

Document

Description:

Returns a string that contains the point value for the current 2D cursor position for the specified axis. The axis is specified as an integer, 1or 2, where 1 is the horizontal axis and 2 is the vertical

Example:

```
MyVariable = Data.Get2Dcursor (2)
```

GetActiveDocPath

Usage:

objectname.GetActiveDocPath

Object:

Application, Document

Description:

Application: Returns the full path the currently active data file. It is recommended that this command be used through the application whenever possible; since no previous link needs to be in place when accessing the application.

Document: Returns the full path to the currently active data file. Note: Remember that a link to a data file must have been previously created before this command can be used. Once a link has been established to any Data file, this command can be used to recognize the front most Data file in NTNMR.

Application Example:

```
CreateObject ("NTNMR.Application")
Set App = GetObject(, "NTNMR.Application")
MyVariable = App.GetActiveDocPath
```

Document Example:

```
MyVariable = Data.GetActiveDocPath
```

GetActualShimPrecision

Usage:

objectname.GetActualShimPrecision

Object:

Application

Description:

Returns the actual shim precision. Use this command to retrieve the actual shim precision to assess the quality of an auto shim operation.

Example:

```
MyVariable = Data. GetActualShimPrecision
```

GetComment

Usage:

objectname.GetComment

Object:
Document

Description:
Returns the current contents of the data file comment field.

GetCursorPosition

Usage:
objectname.GetCursorPosition

Object:
Document

Description:
Returns the point value of the current 1D cursor position.

Example:

```
MyVariable = Data.GetCursorPosition
```

GetData

Usage:
objectname.GetData

Object:
Document

Description:
Returns a variant that contains a 1D array of the current data set in the format R, I, R, I, R, ...

Example:

```
MyVariable = Data.GetData
```

GetDataPoint

Usage:
objectname.GetDataPoint *point_number*

Object:
Document

Description:

Returns a variant that contains a 2-member array in the format R, I of the specified data point.

Example:

```
MyVariable = Data. GetDataPoint (64)
```

GetDataSize

Usage:

objectname.GetDataSize

Object:

Document

Description:

Returns an integer that specifies the total number of points in the current data set (real + img.).

Example:

```
MyVariable = Data.GetDataSize
```

GetDocumentList

Usage:

objectname.GetDocumentList

Object:

Application

Description:

Returns a list of the currently open documents.

GetLockLevel

Usage:

objectname.GetLockLevel

Object:

Application

Description:

Returns at the current lock level.

GetNDRecordPointer

Usage:

objectname.GetNDRecordPointer *dimension*

Object:

Document

Description:

Returns an integer that specifies the active record for the dimension specified by the *dimension* parameter.

Example:

```
MyVariable = Data.GetNDRecordPointer (2)
```

GetNDSize

Usage:

objectname.GetNDSize *dimension*

Object:

Document

Description:

Returns an integer that specifies the number of real points in the specified dimension.

Example:

```
MyVariable = Data.GetNDSize (2)
```

GetNMRParameter

Usage:

objectname. GetNMRParameter "*parameter_name*"

Object:

Document

Description:

Returns the variable associated with the Dashboard Item *parameter_name*. This command is commonly used to assign a Dashboard parameter value to a Visual Basic variable. The Dashboard parameter must be entered **exactly** as it appears in the

Dashboard (case sensitive). Sequence variable values can also be retrieved.

Example:

```
MyVariable = Data.GetNMRParameter ("Points 1D")
```

GetParameterPageList

Usage:

objectname.GetParameterPageList

Object:

Application

Description:

Returns a comma de-limited list of the current pages (i.e. "tabs") in the dashboard.

Example:

```
MyVariable = App.GetParameterPageList
```

GetParameterListInPage

Usage:

objectname.GetParameterListInPage *page_name*

Object:

Application

Description:

Returns a comma de-limited list of the current parameters in the dashboard page specified by *page_name* in the format *"page_name = param1, param2, ..."*.

Example:

```
MyVariable = App.GetParameterListInPage ("Acquisition")
```

GetPeakPickAmplitudes

Usage:

objectname.GetPeakPickAmplitudes

Object:
Document

Description:
Returns a comma de-limited list of the current amplitudes for the current peak picks in the spectrum.

GetPeakPickList

Usage:
objectname.GetPeakPickList *units*

Object:
Document

Description:
Returns a comma de-limited list of the current peak picks in the spectrum in units of *units* where *units* is "points", "hz", or "ppm".

GetSequenceName

Usage:
objectname.GetSequenceName

Object:
Document

Description:
Returns the full path to the sequence that is associated with the active data file.

Example:

```
MyVariable = Data.GetSequenceName
```

GetSpinRate

Usage:
objectname.GetSpinRate

Object:
Application

Description:

Returns the current spin rate.

GetTable

Usage:

objectname.GetTable *table_name*

Object:

Document

Description:

Returns the **name** and **contents** of the specified sequence table as a string in the format "*table_name = value1 value2 value3 ...*".

Example:

```
MyVariable = Data.GetTable
```

GetTableList

Usage:

objectname.GetTableList

Object:

Document

Description:

Returns a space de-limited list of all table names in the sequence.

Example:

```
MyVariable = Data.GetTableList
```

Go

Usage:

objectname.Go

Object:

Document

Description:

Starts a new acquisition using the sequence and parameters from the current window without zeroing the acquisition memory.

Example:

```
Data.Go
```

HideWindow

Usage:

objectname.HideWindow

Object:

Application

Description:

Minimizes AND hides NTNMR. NTNMR will not be visible in the Windows Task Bar after the Hide-Window command has been executed.

Example:

```
App.HideWindow
```

Integrate

Usage:

objectname.Integrate *left_point, right_point, parameters*

Object:

Application

Description:

Integrates the region of the spectrum as specified by *left_point* and *right_point*. The *parameters* string contains *units, offset, slope, curvature, multiplier* where: *units* = "points", "hz", or "ppm"; *offset* = the offset value; *slope* = the slope value; *curvature* = the curvature value; *multiplier* = the multiplier value. Consult the section of the manual on integration for information on the *offset, slope, curvature* and *multiplier* values.

Example:

```
Data.Integrate 1202, 1407, "points, 1, 1.2, 0.75, 2"
```

InverseFT

Usage:

objectname. InverseFT

Object:
Document

Description:
Performs a one-dimensional inverse Fourier transform on a 1D data set.

Example:

```
Data.InverseFT
```

LeftShift

Usage:
objectname.LeftShift *points, true/false*

Object:
Document

Description:

Left Shift the complex data by *points;* number of points with zeroing (*true*) or by circularly shifting the points to the end of the data (*false*). The *points* and *true/false* parameters are optional. If *points* is omitted, "Shift # pts" in the Dashboard will be used. If *true/false* is omitted, the shifted points will be zeroed. See the 1D Preferences for the option to circularly shift data points.

Example:
left shift 5 complex data points...

```
Data.LeftShift 5
```

Circularly left shift 5 complex data points...

```
Data.LeftShift 5, false
```

LiftSample

Usage:
objectname.LiftSample *true/false*

Object:
Application

Description:

Activates the sample eject air when true, deactivates when false.

Example:
lift and hold the sample

```
Data.LiftSample true
```

LoadIntegrals

Usage:
objectname.LoadIntegrals *file_path*

Object:
Document

Description:

Loads the saved integral template specified in *filepath*.

Example:

```
Data.LoadIntegrals "C:\ntnmr\setup\int1.int"
```

LoadParameterSetupFromFile

Usage:
objectname.LoadParameterSetupFromFile *path_name*

Object:

Application

Description:

Loads the dashboard parameter setup file specified by *path_name* and updates the dashboard. This command is a setup command *only*. It does not load parameter values. Use LoadParametersFromFile to load experiment parameters.

Example:

```
App.LoadParameterSetupFromFile "C:\ntnmr\setup\parameters.txt"
```

LoadParametersFromFile

Usage:

objectname.LoadParametersFromFile *path_name*

Object:

Application

Description:

Loads the experiment parameter setup file specified by *path_name* and updates the dashboard. Only the parameters that are currently active in the dashboard will be displayed

Example:

```
App.LoadParameterSetupFromFile "C:\ntnmr\setup\parameters.txt"
```

LoadPrintPreviewTemplate

Usage:

objectname.LoadPrintPreviewTemplate *path_name*

Object:

Application

Description:

Loads the print template file specified by *path_name*.

Example:

```
App. LoadPrintPreviewTemplate "C:\ntnmr\setup\stdplot.prt"
```

LoadSequence

Usage:

objectname.LoadSequence *path_name*

Object:

Document

Description:

Loads the sequence specified by *path_name* and associates it and its variables with the active data file.

Example:

```
Data.LoadSequence ("C:\ntnmr\sequences\cosy.tps")
```

nDFT

Usage:

objectname.nDFT

Object:

Document

Description:

Executes the pre-defined set of processing commands currently set in the nDFT dialog. That can include baseline correction, zero filling, apodization, transformation and phasing. The command can be configured to process 1 to 3 dimensions with a single click. [SHIFT]-select the NDFT command or [shift]-click the NDFT toolbar button.

Example:

```
Data.nDFT
```

NDTranspose

Usage:

objectname.NDTranspose *nX, nY, nZ, nA*

Object:

Document

Description:

Performs a hypercomplex transpose on the data, transposing the dimensions as specified by the *nX, nY, nZ,* and *nA* parameters.

Example:

consider the data set:

record 1	R11	I11	R12	I12

record 2	R21	I21	R22	I22
record 3	R31	I31	R32	I32
record 4	R41	I41	R42	I42

which is stored by NTNMR as R11, I11, R12, I12, R21, I21, R22, I22, ...

The command...

```
Data.NDTranspose 2, 1, 3, 4
```

would result in the following matrix

record 1	R11	R21	R31	R41
record 2	I11	I21	I31	I41
record 3	R12	R22	R32	R42
record 4	I12	I22	I32	I42

NDComplexTranspose

Usage:

objectname.NDComplexTranspose *nX, nY, nZ, nA*

Object:

Document

Description:

Performs a complex transpose on the data, transposing the dimensions as specified by the *nX, nY, nZ,* and *nA* parameters. NDComplexTranspose moves the data in complex pairs.

Example:

Consider the data set:

record 1	R11	I11	R12	I12
record 2	R21	I21	R22	I22

that is stored by NTNMR as R11, I11, R12, I12, R21, I21, R22, I22, ...

The command...

```
Data.NDComplexTranspose 2, 1, 3, 4
```

would result in the following matrix

record 1	R11	I11	R21	I21
record 2	R12	I12	R22	I22

OpenFile

Usage:

objectname.OpenFile *file_path*

Object:

Document, Application

Description:

Opens the file specified in *file_path.*

Example:

```
Data.OpenFile "C:\ntnmr\data\c13.tnt"
```

OpenTwoDView

Usage:

objectname.OpenTwoDView *Init, Mode, Display, Aspect*

Object:

Document

Description:

Opens the 2D display mode of NTNMR with the data display set according to the parameters *init*, *mode*, *display* and *aspect.*
Init = True/False

True = use Mode, Disp, and Aspect information
False = use current NTNMR settings

Mode = 0, 1, 2, 3
0 = Display real data
1 = Display imaginary data
2 = Display magnitude data

3 = Display phase map

Disp = 0, 1, 2, 3
0 = contour
1 = gradient
2 = stack plot
3 = multi-image display

Aspect = 0, 1, 2
0 = force square
1 = by data
2 = none

Example:

```
Data.OpenTwoDView 2, 1, 0
```

PhaseCorrection
PC

Usage:
objectname.PhaseCorrection *ph0, ph1*
objectname.PC *ph0, ph1*

Object:
Document

Description:
Applies the specified zero (*ph0*) and first (*ph1*) order phase corrections to 1D data.

Example:

```
Data.PhaseCorrection 90, -180
```

PickOnePeak

Usage:
objectname.PickOnePeak *position, unit*

Object:
Document

Description:

Places a peak pick at the spectrum location specified in *position* with the units of the position value specified in *unit*. Valid units are "points", "hz" and "ppm".

Example:

```
Data.PickOnePeak 121.5, "ppm"
```

PrintFromPreview

Usage:

objectname.PrintFromPreview

Object:

Application

Description:

Sends the contents of the print preview window to the currently selected printer.

Example:

```
App.PrintFromPreview
```

Quit

Usage:

objectname.Quit

Object:

Application

Description:

Quits NTNMR. This command is the same as selecting Exit from the File menu.

Example:

```
App.Quit
```

ReadFirstHalf

Usage:

objectname.ReadFirstHalf

Object:

Document

Description:

Extracts the first half of a data record. The Points 1D parameter on the dashboard is halved.

Example:

```
Data.ReadFirstHalf
```

ReadSecondHalf

Usage:

objectname.ReadSecondHalf

Object:

Document

Description:

Extracts the second half of a data record. The Points 1D parameter on the dashboard is halved.

Example:

```
Data.ReadSecondHalf
```

RealFT
RFT

Usage:

objectname.RealFT
objectname.RFT

Object:

Document

Description:

Calculates the one-sided Fourier transform where the imaginary part is set to zero. After the transform of n complex points, to get

n/2 complex points back, use the ReadFirstHalf (or ReadSecondHalf) command. The transform is one-sided, 0 -> +SW, with the first point at zero frequency, so the axis will have to be re-defined.

Example:

```
Data.RFT
Data.ReadFirstHalf
```

RemoveAllPages

Usage:

objectname.RemoveAllPages

Object:

Application

Description:

Removes all parameter pages (i.e. "tabs") from the dashboard. Note: NTNMR will automatically regenerate the Sequences tab as needed.

Example:

```
App.RemoveAllPages
```

RemoveParameterPage

Usage:

objectname.RemoveParameterPage *page_name*

Object:

Application

Description:

Removes the parameter page specified parameter page from the dashboard.

Example:

```
App.RemoveParameterPage "Acquisition"
```

Reset

Usage:

objectname.Reset

Object:
Document

Description:
Executes the reset hardware command.

ResetDimensionInfo

Usage:
objectname.ResetDimensionInfo *num_points_X, num_points_Y, num_points_Z, num_points_A*

Object:
Document

Description:
Re-defines the dimension information for a data set by specifying the number of points for each dimension. The number of points for the first ("X") dimension is specified as complex, all other dimensions are specified as total points. The total number of points in a data set CANNOT be changed using this command, only the dimension breaks are changed. An error will result if the total number of points specified by the ResetDimensionInfo command does not match the total number of points in the data set.

Example:
Consider a data set that contains 32 records with each record having 512 points.

```
Data.ResetDimensionInfo 128, 128, 1, 1
```

The resulting data would contain 128 records with each record having 128 points.

ReverseSpectrumColumns

Usage:
objectname.ReverseSpectrumColumns

Object:
Document

Description:

Performs a reverse spectrum on the indirect dimension (displayed vertically in NTNMR) of a 2D data set.

Example:

```
Data.ReverseSpectrumColumns
```

ReverseSpectrumRows

Usage:

objectname.ReverseSpectrumRows

Object:

Document

Description:

Performs a reverse spectrum on the direct dimension (displayed horizontally in NTNMR) of a 2D data set.

Example:

```
Data.ReverseSpectrumRows
```

RightShift

Usage:

objectname.RightShift *points, true/false*

Object:

Document

Description:

Right Shift the complex data by *points* number of points with zeroing (*true*) or by circularly shifting the points to the end of the data (*false*). The *points* and *true/false* parameters are optional. If *points* is omitted, ìShift # ptsî in the Dashboard will be used. If *true/false* is omitted, the shifted points will be zeroed. See the 1D Preferences for the option to circularly shift data points.

Example:

Right shift 5 complex data points

```
Data.RightShift 5, true
```

Circularly right shift 5 complex data points

```
Data.RightShift 5, false
```

Save

Usage:

objectname.Save

Object:

Document

Description:

Saves the current data under the same filename replacing the original data file.

Example:

```
Data.Save
```

SaveAs

Usage:

objectname.SaveAs *file_path*

Object:

Document

Description:

Saves the current data under the filename specified in *file_path*.

Example:

```
Data.SaveAs "C:\mydatafolder\sample1\72397.tnt"
```

SaveIntegrals

Usage:

objectname.SaveIntegrals *file_path*

Object:

Document

Description:

Saves the current integrals under the filename specified in *file_path*.

Example:

```
Data.SaveIntegrals "C:\ntnmr\setup\int1.int"
```

SaveParameterSetupToFile

Usage:

objectname.SaveParameterSetupToFile *file_path*

Object:

Application

Description:

Saves the current dashboard setup to the filename specified in *file_path*. This command DOES NOT SAVE parameter values, only the current dashboard setup.

Example:

```
App.SaveParameterSetupToFile "C:\ntnmr\setup\mysetup.txt"
```

SaveParametersToFile

Usage:

objectname.SaveParametersToFile *file_path*

Object:

Application

Description:

Saves the current parameters from the dashboard to the specified file.

Example:

```
App.SaveParametersToFile "C:\ntnmr\setup\c13.txt"
```

SavePeakPickList

Usage:

objectname.SavePeakPickList *file_path*

Object:
Document

Description:
Saves the current peak pick information in a text file as indicated by *file_path.*

Example:

```
Data.SavePeakPickList "C:\mydata\sample1\sample1_peaks.txt"
```

SaveSequence

Usage:
objectname.SaveSequence

Object:
Document

Description:
Saves the current Sequence under the same filename replacing the original sequence file.

Example:

```
Data.SaveSequence
```

SaveSequenceAs

Usage:
objectname.SaveSequenceAs *file_path*

Object:
Document

Description:
Saves the current Sequence under the filename specified in *file_path.*

Example:

```
Data.SaveSequenceAs "C:\mydatafolder\sample1\cosy.tps"
```

SetLockGain

Usage:

objectname.SetLockGain *value*

Object:

Document

Description:

Sets the lock gain to the value specified in *value*.

Example:

```
Data.SetLockGain 1000
```

Set2DCursor

Usage:

objectname.Set2DCursor *axis, point_number*

Object:

Document

Description:

Sets the 2D cursor for the axis specifed by *axis* to the point value specified by *point_number*. 1 = hoizontal axis, 2 = vertical axis.

Example:

```
Data.Set2DCursor 2, 112
```

SetActiveParameterPage

Usage:

objectname.SetActiveParameterPage *page_name*

Object:

Application

Description:

Forces NTNMR to display the Dashboard page specified by the parameter *page_name*.

Example:

```
App.SetActiveParameterPage "Acquisition"
```

SetComment

Usage:

objectname.SetCursorPoitions *comment*

Object:

Document

Description:

Sets the data file comment to the text specified in *comment*.

Examples:

```
Data.SetComment "C13, July 7, 1998"
```

```
Dim myComment as String
myComment = "C13 Exp." & vbcrlf & "July 7, 1998"
Data.SetComment myComment
```

SetCursorPosition

Usage:

objectname.SetCursorPoitions *point_value*

Object:

Document

Description:

Sets the 1D cursor to the data point specified by the parameter *point_value*.

Example:

```
Data.SetCursorPosition 2012
```

SetData

Usage:

objectname.SetData *array*

Object:

Document

Description:

Sets the data in the active object (data file) to the values contained in the parameter *array*, which is a 1D array of the format R, I, R, I, R... Note that if the data specified in the parameter *array* is larger than the current data buffer, NTNMR will return an error. If the data size specified in the parameter *array* is smaller than the current data buffer, only the portion by *array* will be replaced.

Example:

```
Data.SetData myArray
```

SetDataPoint

Usage:

objectname.SetDataPoint *point_number, array*

Object:

Document

Description:

Sets the data at the point specified by *point_number* in the active object (data file) to the values contained in the parameter *array*, which is a 1D array of the format R, I.

Example:

```
Data.SetDataPoint 5, my2PointArray
```

SetLockField

Usage:

objectname.SetLockField *value*

Object:

Application

Description:

Applicable to DSPect systems only. Sets the lock field on the SCM to the value specified in *value*.

Example:

```
Data. SetLockField 1325
```

SetLockGain

Usage:

objectname.SetLockGain *value*

Object:

Application

Description:

Sets the lock gain to the value specified in *value*.

Example:

```
Data. SetLockGain 500
```

SetLockPhase

Usage:

objectname.SetLockPhase *value*

Object:

Application

Description:

Sets the lock phase to the value specified in *value*.

Example:

```
Data. SetLockPhase 100
```

SetLockPower

Usage:

objectname.SetLockPower *value*

Object:

Application

Description:

Sets the lock power to the value specified in *value*.

Example:

```
Data. SetLockPower 100
```

SetLockState

Usage:

objectname.SetLockState *true/false*

Object:

Application

Description:

Turns the lock on (true) and off (false).

Example:

```
Data. SetLockState false
```

SetNDApodization

Usage:

objectname.SetNDApodization *dimension, par1_value, par2_value[optional] , par3_value [optional] , par4_value [optional]*

Object:

Document

Description:

Sets the apodization values to be used with the apodization function specified by the SetNDParameters command for the specified dimension. This is an initialization command that is used in conjunction with SetNDParameters and NDFT. The values specified by SetNDApodization are applied *only* if SetNDParameters is called with the *apodization* parameter set to 1 through 9 followed by the NDFT command. Parameters indicated as [optional] are required only if the apodization function to be called require them. See SetNDParameters for more information and examples.

Dimension = 1, 2, 3, 4

1 = first dimension
2 = second dimension
3 = third dimension
4 = fourth dimension

par1_value = *value*
value = apodization parameter

par2_value = *value*
value = apodization parameter

par3_value = *value*
value = apodization parameter

par4_value = *value*
value = apodization parameter

SetNDEchoCenter

Usage:

objectname.SetNDEchoCenter *Dimension, center_value*

Object:

Document

Description:

Sets the echo center to be used by the EchoFT and Echo-mode apodization functions for the specified dimension. This is an initialization command that is used in conjunction with SetNDParameters and NDFT. The value specified by SetNDEchoCenter are applied *only* if SetNDParameters is called with the *FT* parameter set to 4, indicating an Echo FT, followed by the NDFT command. See SetNDParameters for more information and examples.

Dimension = 1, 2, 3, 4
1 = firsrt dimension
2 = second dimension
3 = third dimension
4 = fourth dimension

cnter_value = *value*
value = point number of the echo center

SetNDParameters

Usage:

objectname.SetNDParameters *Dimension, BC, ZeroFill, FT, Reverse, Phase, apodization*

Object:

Document

Description:

Initializes the parameters to be used with the NDFT command. This command is used in conjunction with the SetNDPhase, SetNDEchoCenter, SetNDApodization and NDFT commands. The following parameters are used:

Dimension = 1, 2, 3, 4
- 1 = first dimension
- 2 = second dimension
- 3 = third dimension
- 4 = fourth dimension

BC = true/false
- true = apply baseline correction
- false = no baseline correction

ZeroFill = 0, 1, 2...
- *value* = number of zero fills

FT = 0, 1, 2, 3, 4
- 0 = none
- 1 = FFT
- 2 = Inverse FFT
- 3 = Real FFT
- 4 = Echo FFT

Reverse = true/false
- true = apply spectrum reverse
- false = no spectrum reverse

Phase = 0, 1, 2
- 0 = none
- 1 = use values specified by SetNDPhase or set in the NDFT dialog in NTNMR.

2 = use "system" phase parameters

Apodization = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9
0 = none
1 = EM
2 = Gaussian
3 = double exponential
4 = sine bell
5 = sine bell squared
6 = Blackman Harris
7 = trapezoid
8 = traf
9 = echo exponential multiplication

Example:

The following example initializes the NDFT template to apply a baseline correction and courier transform to a two dimensional data set using a standard complex transpose.

```
Data.SetNDTranspose 2, 0, 1
Data.SetNDParameters 1, true, 0, 1, false, 0, 0
Data.SetNDParameters 2, true, 0, 1, false, 0, 0
Data.NDFT
```

SetNDPhase

Usage:

objectname.SetNDPhase *Dimension, ph0_value, ph1_value*

Object:

Document

Description:

Sets the zero and first order phase constants to be applied for the specified dimension. This is an initialization command that is used in conjunction with SetNDParameters and NDFT. The values specified by SetNDPhase are applied *only* if SetNDParameters is called with the *phase* parameter set to 1 followed by the NDFT command. See SetNDParameters for more information and examples.

Dimension = 1, 2, 3, 4
1 = first dimension
2 = second dimension

3 = third dimension
4 = fourth dimension

ph0_value = *value*
value = zero order phase correction

ph1_value = *value*
value = first order phase correction

SetNDRecordPointer

Usage:

objectname.SetNDRecordPointer *dimension, record_number*

Object:

Document

Description:

Sets the NTNMR data display to data specified by the *dimension* and *record_number* parameters.

Example:

```
Data.SetNDRecordPointer 3, 12
```

SetNDTranspose

Usage:

objectname.SetNDTranspose *Dimension, Type, Data*

Object:

Document

Description:

Sets the transpose type and final data for the specified dimension. This is an initialization command that is used in conjunction with NDFT. The specified transpose is applied *only* by the NDFT command. See SetNDParameters for more information and examples.

Dimension = 1, 2, 3, 4
1 = first dimension
2 = second dimension

3 = third dimension
4 = fourth dimension

Type = 0, 1
0 = complex
1 = hypercomplex

Data = 0
0 = keep all data

SetNMRParameter

Usage:

objectname.SetNMRParameter *"parameter_name", value*

Object:

Document

Description:

Sets the Dashboard Item specified in *parameter_name* to the value set in *value.*

Example:

```
Data.SetNMRParameter "Points 1D", 1024
```

SetOneShim

Usage:

objectname.SetOneShim *"shim_name", value*

Object:

Application

Description:

Sets the specified in *shim_name* to the value set in *value.*

Example:

```
Data.SetNMRParameter "x", 1000
```

SetParameterListInPage

Usage:

objectname.SetParameterListInPage *"page_name", "par1, par2, par3"*

Object:

Application

Description:

Sets the list of parameters to be displayed in the dashboard page specified by *page_name*. The dashboard page must exist and the comma de-limited list of dashboard items must be valid. Parameters can, however, be from any page.

Example:

```
App.SetParameterListInPage "Acquisition", "Nucleus, Obs. Freq., LB1D"
```

SetRecordPointer

Usage:

objectname.SetRecordPointer *2D_record_number*

Object:

Document

Description:

Sets the NTNMR display to the 2D record number specified by the parameter *2D_record_number*.

Example:

```
Data.SetRecordPointer 30
```

SetSelection

Usage:

objectname.SetSelection *point_start, point_end*

Object:

Document

Description:

Highlights the region of data in the 1D display area as specified by the parameters *point_start* and *point_end*. This command is

equivalent to a click-drag-release operation in the 1D display area.

Example:

```
Data.SetSelection 100, 200
```

SetSpinRate

Usage:

objectname.SetSpinRate *value*

Object:

Application

Description:

Sets the spin rate to *value*.

Example:

```
Data.SetSpinRate 12
```

SetTable

Usage:

objectname.SetTable *"table_name", "value1 value2 value3 ..."*

Object:

Document

Description:

Sets the contents of the table specified by *table_name* to the values specified by "*value1 value2 value3 ...*". Note: tables entries should be [space] de-limited.

Example:

```
Data.TableName "ph0", "1 2 3 0"
```

ShowIntegrals

Usage:

objectname.ShowIntegrals *true/false*

Object:

Document

Description:
Shows (true) and hides (false) current integrals.

Example:

```
App.ShowIntegrals false
```

ShowLockBar

Usage:
objectname.ShowLockBar *true/false*

Object:
Application

Description:
Shows (true) and hides (false) the lock level display in NTNMR.

Example:

```
App.ShowLockBar false
```

ShowPeakPick

Usage:
objectname.ShowPeakPick *true/false*

Object:
Document

Description:
Shows (true) and hides (false) the current peak picks.

Example:

```
App.ShowPeakPick true
```

ShowWindow

Usage:
objectname.ShowWindow

Object:

Application

Description:

Activates the main NTNMR application window after it has been minimized by clicking on the minimize button in the applications title bar or by executing the Hide Window command.

Example:

```
App.ShowWindow
```

SinBell

Usage:

objectname.SinBell (*shift, width, skew*)
objectname.SB (*shift, width, skew*)

Object:

Document

Description:

Performs a Sine Bell apodization on 1D data using the parameters *shift, width* and *skew*. The *shift, width* and *skew* parameters are optional. If they are omitted, SB Shift, SB Width and SB Skew in the dashboard will be used. Note: The *width* parameter specifies the full width of the function meaning that the function will cross zero at (Points 1D * 2).

Example:

```
Data.SinBell 90, 8192, 1
```

SinBellSquared
SBS

Usage:

objectname.SinBellSquared *shift, width, skew*
objectname.SBS *shift, width, skew*

Object:

Document

Description:

Performs a Sine Bell Squared apodization on 1D data using the parameters *shift, widt,* and *skew*. The *shift, width* and *skew*

parameters are optional. If they are omitted, SB Shift, SB Width and SB Skew in the dashboard will be used. Note: The *width* parameter specifies the full width of the function meaning that the function will cross zero at (Points 1D * 2).

Example:

```
Data.SinBellSquared 90, 8192, 1
```

SpinSample

Usage:

objectname.SpinSample *true/false*

Object:

Application

Description:

Activates (true) and deactivates (false) the sample spinner.

StartShims

Usage:

objectname.StartShims

Object:

Application

Description:

Initiates an auto shim. Use in conjunction with ActivateShims and CheckShimProgress.

Example:

```
App.ActivateShims "x, y, z"

App.StartShims

Do While Not App.CheckShimProgess
DoEvents
Loop
```

Stop

Usage:

objectname.Stop

Object:
Document

Description:
Stops the current data acquisition after completion of the current phase cycle.

Example:

```
Data.Stop
```

TrafWindow
TW

Usage:
objectname.TrafWindow *value*
objectname.TW *value*

Object:
Document

Description:
Performs Traficante Ziessow weighting (J. Mag. Res., 66, 182-186 (1986)) using the parameter *value*. The *value* parameter is optional. If omitted, the Dashboard parameter Traf 1D will be used.

Example:

```
Data.TrafWindow 5
```

Transpose

Usage:
objectname.Transpose

Object:
Document

Description:
Performs a complex transpose on the X and Y dimensions of a 2D data set.

Example:

```
Data.Transpose
```

Trapezoid
TZ

Usage:

objectname.Trapezoid *value1, value2, value3, value4*
objectname.TZ *value1, value2, value3, value4*

Object:

Document

Description:

Performs weighting using the 4 data points *value1, value2, value3 and value 4* as the trapezoid shape de-limiters. The parameters *value1 - 4* are optional. If omitted, the Dashboard parameters TZ 1 1D, TZ 2 1D, TZ 3 1D and TZ 4 1D will be used.

Example:

TZ

```
Data.TW 2, 5, 512, 1024
```

UpdateDisplay

Usage:

objectname.UpdateDisplay

Object:

Document

Description:

Forces a redraw of the 1D NTNMR data display area. This command can be used when AutoDisplayWhileProcessing has been set to false to force redraws at specific times.

Example:

```
Data.UpdateDisplay
```

ZeroFill
ZF

Usage:

objectname.ZeroFill *value*

objectname.ZF *value*

Object:
Document

Description:
Zero fills the data to the number of points specified by *value*. The *value* parameter is optional. If omitted, the data size will be doubled.

Example:

```
Data.ZeroFill 8192
```

ZeroGo
ZG

Usage:
objectname.ZeroGo
objectname.ZG

Object:
Document

Description:
Zeros the signal averager memory and starts an acquisition. Use in conjunction with the CheckAcquisition command.

Example:

```
Data.ZG
 Do While Not Data.CheckAcquisition
Loop
```

Zoom

Usage:
objectname.Zoom *point_start, point_end*

Object:
Document

Description:
Executes a zoom command on the 1D data display using the parameters *point_start* and *point_end*.

Example:

```
Data.Zoom 100, 790
```

<<< PREV <<<
9.6
>>> NEXT >>>

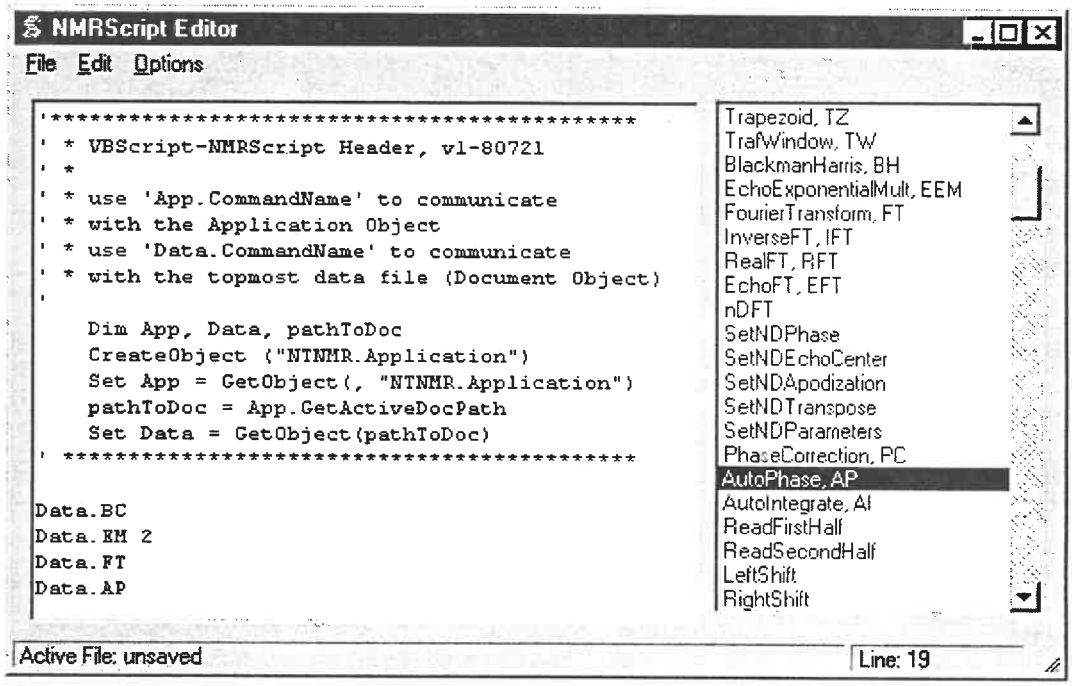
Writing NMRScripts in VBScript

The VBScript language is a subset of Microsoft's Visual Basic programming language. Through the use of the "Windows Scripting Host" or "WSH," VBScript can be used as a system level scripting language. Since VBScript has very limited user interface tools, VBScripts written to control NTNMR are more like macros than Visual Basic programs.

While VBScripts can be written using any text editor, the NMRScriptEditor provided with NTNMR is an excellent tool. The NMRScriptEditor provides several advantages over a standard text editor:

- Built in NTNMR language reference with syntax examples
- Pre-written NTNMR communication header
- Execute a script from the editor without the need to first save to disk

The NMRScriptEditor (shown below) can be launched by selecting it from the Scripts menu in NTNMR or by navigating to the script sub-directory of the NTNMR directory and double-clicking.



When the NMRScriptEditor is launched, a new script file is automatically created with the NTNMR "communication" header inserted. The communication header is required to set up an OLE link with NTNMR. The default header establishes communication with the top most document in

NTNMR. Using the default header will allow any script that is written to automatically act on the top most data file open in NTNMR.

Once the NMRScriptEditor is opened, commands can be added by typing below the header or by double-clicking a command in the right hand NTNMR command reference pane. Note also that selecting and pausing over a command will pop up a tool tip with a syntax example for that command.

Users may wish to install the VBScript language reference from the NTNMR CD or connect to http://www.microsoft.com/scripting for the VBScript language reference.

<<< PREV <<<

9.7 VBScript Examples

>>> NEXT >>>

Example 1: Auto Process 1D

```
'communication header
'*********************************************
   Dim App, Data, pathToDoc
   CreateObject ("NTNMR.Application")
   Set App = GetObject(, "NTNMR.Application")
   pathToDoc = App.GetActiveDocPath
   Set Data = GetObject(pathToDoc)
'*********************************************

'script
  Data.BC
  Data.EM 1
  Data.FT
  Data.AP
Data.FitToWindow
```

Example 2: Chirp Generator

```
'communication header
'*******************************************
   Dim App, Data, pathToDoc
   CreateObject ("NTNMR.Application")
   Set App = GetObject(, "NTNMR.Application")
   pathToDoc = App.GetActiveDocPath
   Set Data = GetObject(pathToDoc)
'*******************************************

'script
dim phase(2048)
titlestring = "NTNMR Chirp Generator"
DeltaT = (inputbox( "Time per point (microsec)", titlestring, "5"))
DeltaT = DeltaT * 1.0e-6
NPts = (inputbox( "Number of points (2-2047)",titlestring,"1024"))
SW = (inputbox( "Sweep Width (Hz)",titlestring,"5000"))

' Check for valid entries
if NPts > 2047 then
  msgbox "Too Many Points !!!",vbCritical
  wscript.quit
end if

' OK... proceed

phase(i)=0
for i = 1 to NPts
  freq = (i-NPts/2)*SW/NPts
  inc = 2 * 3.14159 * freq * DeltaT
  phase(i) = (phase(i-1) + inc) '
  'wscript.echo  phase(i)
  phasetemp = (phase(i) * 360./(2 * 3.14159)) mod 360
  'tempstring = tempstring & " " & (phase(i)) & chr(13) & chr(10)
  tempstring = tempstring & " " & (phasetemp) & chr(13) & chr(10)
next

'msgbox tempstring

tablename = inputbox( "Sequence Table Name",titlestring,"phase0")

Data.SetTable tablename, tempstring
```

<<< PREV <<<
9.8
>>> NEXT >>>

Visual Basic Terminology[1]

While it is beyond the scope of this manual to describe the details of programming in Visual Basic, the following discussion of terminology will facilitate the material presented here.

Control

A control is a tool you use to create objects on a Visual Basic form. You select controls from the toolbox and use the mouse to draw objects on a form. You use most controls to create user interface elements, such as command buttons, image boxes and list boxes.

Object

An object is a type of user interface element you create on a Visual Basic form by using a toolbox control. (In fact, in Visual Basic, the form itself is also an object.) You can move, resize and customize objects by using property settings. Objects also have what is known as inherent functionality-they know how to operate and can respond to certain situations on their own. (A list box "knows" how to scroll, for example.) You can customize Visual Basic objects by using event procedures that are fine-tuned for different conditions in a program.

Property

A property is a value or characteristic held by a Visual Basic object, such as Caption or ForeColor. Properties can be set at design time by using the Properties window or at runtime by using statements in the program code. In code, the format for setting a property is:

- Object.Property = Value

Where

- *Object* is the name of the object you're customizing.
- *Property* is the characteristic you want to change.
- *Value* is the new property setting.

For example,

- Command1.Caption = "Hello"

Could be used in the program code to set the Caption property of the Command1 object to "Hello."

Event Procedure

An event procedure is a block of code that runs when a program object is manipulated. For example, clicking the first command button in a program executes the Command1_Click event procedure. Event procedures typically evaluate and set properties and use other program statements to perform the work of the program.

Program Statement

A program statement is a keyword in the code that does the work of the program. Visual Basic program statements create storage space for data, open files, perform calculations and do several other important tasks.

Method

A method is a special keyword that performs an action or a service for a particular program object. In code, the format for using a method is

- Object.Method Value

Where

- *Object* is the name of the object you want to change.
- *Method* is the command that will change the object.
- *Value* is an optional argument to be used by the method.

For example, this statement uses the AddItem method to put the word *Check* in the List1 list box:

- List1.AddItem "Check"

Variable

A variable is a special container that holds data temporarily in a program. You create variables to store calculation results, create filenames, process input and so on. Variables can store numbers, names and property values.

<<< PREV <<<
9.9
>>> NEXT >>>

Writing NMRScripts in Visual Basic 5.0

Introduction

Visual Basic is a programming language, complete with its own development environment and compiler, that is capable of creating stand alone application executables. Having said that, it is quite easy to learn, has several tools that ease the programming burden and is a very powerful as a scripting language. The syntax is straightforward and the 'Visual' tools for creating windows, buttons, text boxes, etc. are excellent. There are many excellent books on Visual Basic 5.0 to complement the documentation that accompanies the Visual Basic Professional and Learning Editions. A recommended book for learning Visual Basic is "Visual Basic 5 from the Ground Up" by Gary Cornell (Osborne/McGraw-Hill, 1997).

Visual Basic Editions

There are several Editions of Visual Basic available. All will provide the necessary tools for creating NTNMR Scripts. The Professional Edition contains the most complete set of tools and is recommended for advanced users. The Learning Edition (included with each system from Tecmag) is suitable for most applications. The Control Creation Edition is available from Microsoft at no charge, but does not have the ability to create 'stand alone' executables. This means that all scripts created with the Control Creation Edition have to be run from within the Visual Basic Environment. This is generally not convenient unless the script is currently under development. More typically, completed scripts would be saved as *.exe files so that they can be run independently. Nevertheless, the Control Creation Edition is useful for installation on machines that do not have a higher level edition of Visual Basic installed. The development environment is identical for all Editions of Visual Basic and the Project files that are created are compatible making it possible to create and edit scripts in any edition.

General Concepts

Adding NTNMR to the "References" list

Each new Visual Basic Project must have the NTNMR reference activated. This allows the NTNMR object library to be available inside of the Visual Basic script. If the NTNMR reference is not added to the Visual Basic Project, the results will be a compilation error in Visual Basic.

> *You will know that NTNMR reference has been added to your project when you try to call an NTNMR method using the object.method syntax. Immediately after you type a valid objectname followed by a period, the Visual Basic Intellisense feature will pop-up a list of available methods for the NTNMR object type.*

Select **Project|References...** to open the References dialog box. Inactive references are list alphabetically. Activate the NTNMR references by clicking to place a check mark next to the listing for NTNMR. After you set a reference to an object library by selecting the check box next to its name, you can find a specific object and its methods and properties in the Object Browser in Visual Basic.

> *A "Project Template" can be created that has NTNMR in the reference list, commonly used code, code modules loaded, etc. Create a project, add the appropriate references, code, code modules, etc. and save the project into the VB/Templates directory with the name "NTNMR Script.vbp" (you will also need to save the form). The next time you select New Project from the File menu, your template will appear.*

"Linking" to an "Object"

Most automation commands are sent to an NTNMR data file, also referred to as an NTNMR document. OLE Automation requires that the script be linked to an object, which in most cases is an NTNMR data file.

This important concept is slightly different than other scripting languages that may be familiar to you. The result is that in most cases, the script sends commands to an NTNMR *data file*, i.e. "document" and *not* the NTNMR application itself.

In order to create a link to a document, the document (data file) must exist. This does not simply mean that there is a data file open in NTNMR. The data file that you wish to link to must have been saved to disk.

There are three methods for creating a link to an NTNMR Document.

1. Linking to a specific document path

The following lines of code are used in a Visual Basic project to create a link so that a file can be manipulated:

Dim *objectname* as NTNMR.Document

Set *objectname* = GetObject ("path_to_data")

objectname is used here to represent any variable name that you wish to use in the Visual Basic project to refer to the data file. In all of the examples in this chapte, the variable "Data" is used.

path_to_data is used to represent the complete path to the data file. The complete path *must* be specified.

A specific example is shown below:

```
Dim Data as NTNMR.Document
Set Data = GetObject ("C:\ntnmr\data\test1.tnt")
```

> *The Dim objectname as NTNMR.Document statement is usually placed in the declarations section of the Visual Basic project. For simple applications, this is not mandatory, but it is good practice, nonetheless.*

2. Linking to a general document path

This method uses the NTNMR application to first get the path to the top most document. This allows one to create more generalized scripts that are not specific to a particular path name. This is the method that is recommended for scripts that are used to process data.

```
Dim data_objectname as NTNMR.Document
Dim app_objectname as NTNMR.Application
CreateObject ("NTNMR.Application")
Set app_objectname = GetObject(, "NTNMR.Application")
objectpath = App.GetActiveDocPath
Set data_objectname = GetObject (objectpath)
```

The advantage of this method is that the specific path to the data file does not have to be known, allowing generalized scripts to be written that will detect the to most data file.

3. Using the provided GetActiveDoc code module

A code module is supplied to make the task of creating a link to an NTNMR data file even easier. This code module uses the application interface to coerce the current document path and then creates the object using the user supplied *objectname*.

Add the code module called "get_active_doc_path" by selecting Add Module from the Project menu in Visual Basic, clicking on the Exisiting tab and navigating to the modules directory in the NTNMR/Scripts folder. (**Note the location of the supplied code modules may vary depending on the installation. The code modules can be found on the NTNMR CD.)*

Once this code module is loaded, the much simpler syntax below can be used to create a link to the top most document in NTNMR.

```
Dim data_objectname as NTNMR.Document
Dim App as NTNMR.Application
GetActiveDoc data_objectname
```

Note that in this case the object name defined in the Dim statement for the application object *must* be 'App,' as shown above. The code module also provides error checking so that if the document link cannot be created, your project will not crash.

Working on an "Object"

Once a link to an object (i.e. data file) has been created, applying NTNMR commands to the data file is straight forward. The general syntax is as follows:

```
objectname.ntnmr_command
```

Note that this general syntax is illustrated in the preceding section where each scriptable command is discussed in detail.

A specific example is shown below:

```
Data.FourierTransform
```

Many commands also require or have optional parameters that are specified following the command name. Several examples follow:

```
Data.ExponentialMultiplication 5
Data.SaveAs ("C:\ntnmr\data\mydata1.tnt")
Data.SetTable "ph0", "0 1 2 3"
```

Very Important Note for Visual Basic Users

The syntax for using multi-parameter commands in Visual Basic requires some attention to detail. Take the examples below:

1. Data.SetSelection 200, 2500 'okay

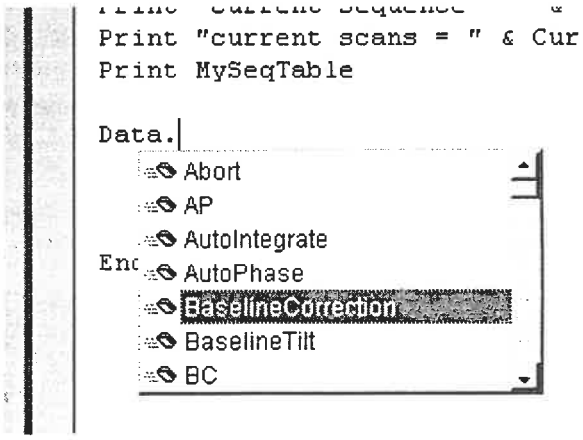
2. Data.SetSelection (200, 2500) 'this example will fail!

At first glance, example 2 might appear to be correct. In fact, that is the form in which all commands are presented in this manual and in the IntelliSense help in Visual Basic. Visual Basic, however, will immediately return a syntax error when the line in example 2 is entered, while it will not object to the code in example 1. Virtually all commands in NTNMR return a 'boolean' (i.e. true/false) which can be used for error checking and when the parentheses are included as in example 2, the expression must be set equal to a variable. The following syntax would not generate a compile error:

3. myVariable = Data.SetSelection (200, 2500) 'okay

In fact, if the above example is written without the parentheses, Visual Basic would return an error! Finally, commands that have only one parameter will compile correctly with or without parentheses when set equal to a variable or when written as in example 1 above.

If a link to a document was created and the NTNMR References have been activated in the current project, Microsoft's IntelliSense feature will be available for NTNMR commands. This is a feature that automatically give visual queues regarding programming syntax. IntelliSense will also recognize the Object type and pop-up a list of available properties and methods for that object. This is true for all Visual Basic Objects, including the NTNMR Object. The graphic below shows the IntelliSense pop-up for the NTNMR Object type.



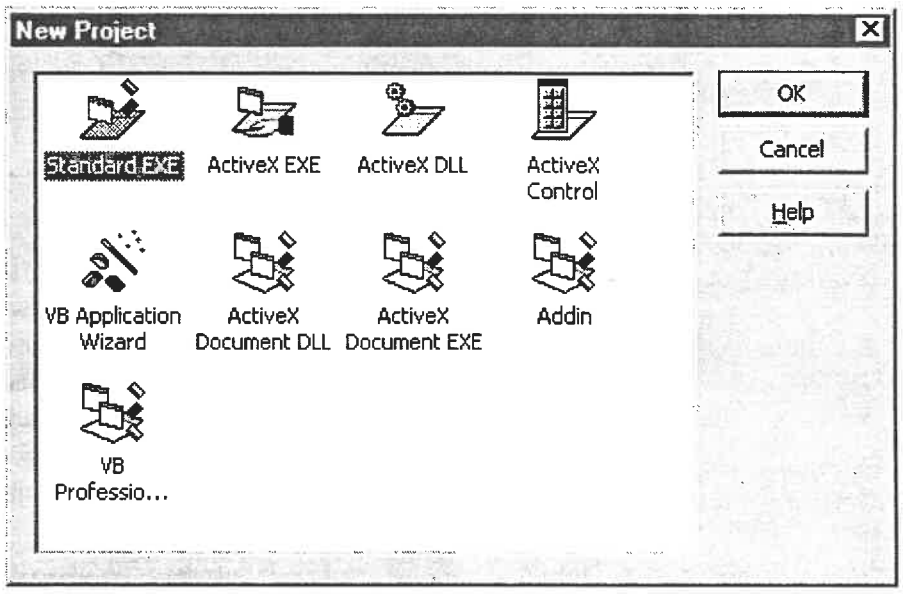
A Step by Step Example

> *If Visual Basic and/or NTNMR have not been installed, install each program using their respective installation programs.*

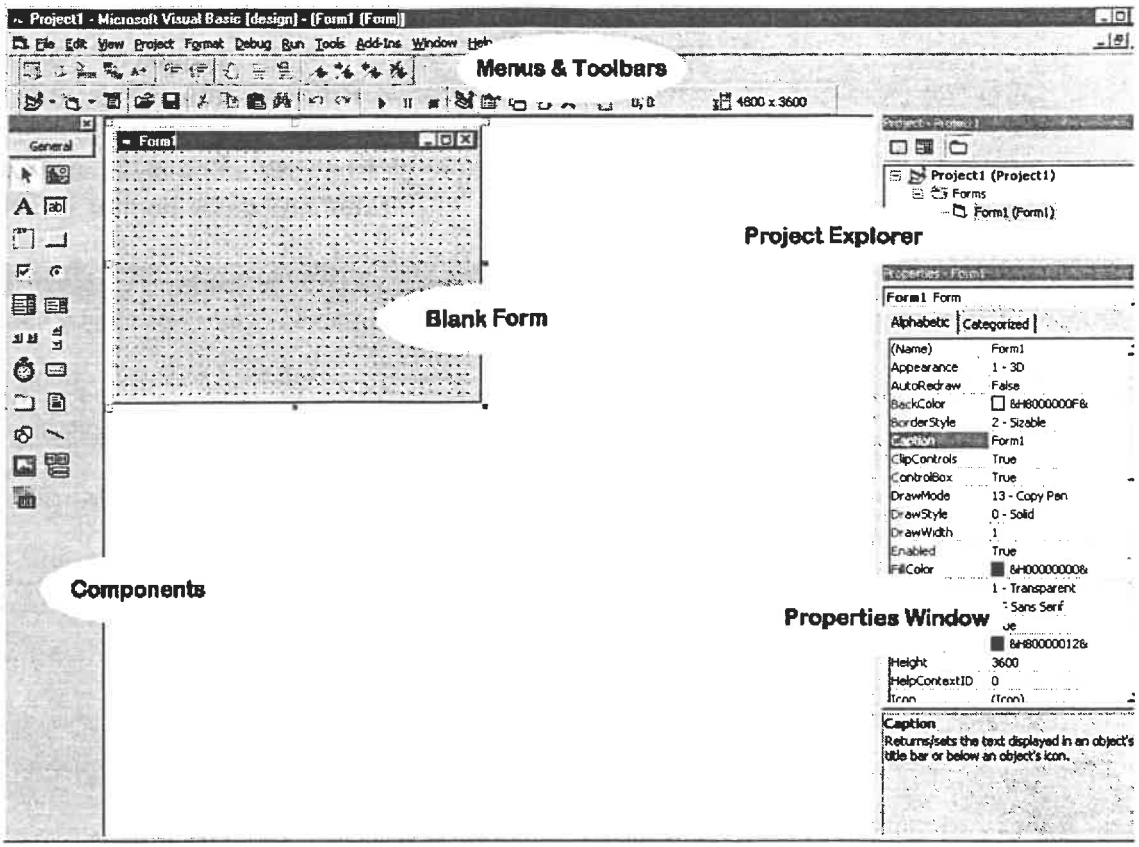
The following step-by-step procedure outlines the creation of a simply script to perform a Baseline Correction, Exponential Multiplication and a Fourier Transform on a 1D data set.

1. Open an NTNMR data file that has previously been saved.

2. Select **File|New Project...** in Visual Basic. The New Project Dialog (shown below) will show several choices depending on the edition of Visual Basic that is used. Choose "Standard EXE" and click "OK."



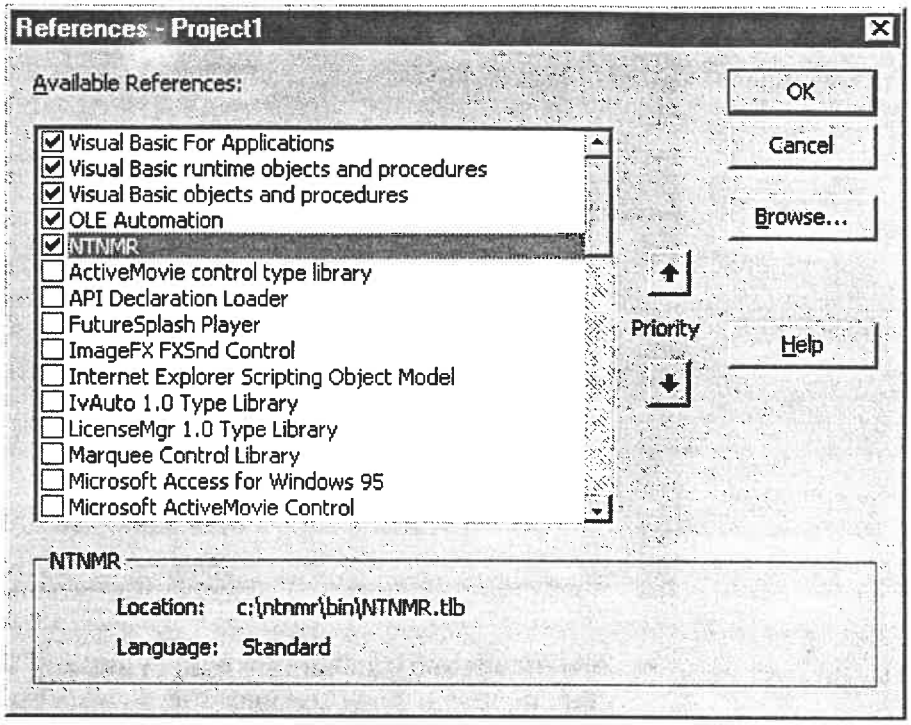
3. A blank project window will appear with a blank Form window visible. The figure below indicates several of the key components of the Visual Basic window.



- The Menus and Toolbars are used to like any Windows style application. Only the menu items and tools that are necessary for basic script writing are discussed here.
- The Project Explorer allows navigation throughout the entire Visual Basic Project. Some advanced script may have several Forms listed in this window. There are also buttons in the upper left of the Project Explorer for toggle between the Form and Code windows.
- The Blank Form window is where buttons, text boxes, etc. are added that will be displayed when the script is run. This is the 'Visual' part of the application.
- The Properties Window will display the details about each of the buttons, text boxes, etc. that are placed on the Blank Form.
- The Components toolbar is a selection of icons representing controls that can be added to the Form window. Click once on a control to select it, and the double-click on the Form to add the selected control. New controls can be added to the toolbar.

4. Select **Project|Reference** and this will open the References dialog shown below. Scroll through the list and select **NTNMR**. You must activate the

NTNMR type library for the current Visual Basic Project; this allows Visual Basic to be "aware" of the NTNMR "document". *This must be done for each new script that you create in Visual Basic.* (Note: It may be necessary to manually locate the NTNMR reference file the first time Visual Basic is run. Do this by clicking on the **Browse...** button and navigating to the NTNMR folder. Locate the "bin" folder and select the file "NTNMR.tlb")



5. Position the mouse pointer over the **Command Button** component on the Components Toolbar. Notice that when the mouse pointer is paused over an item on the Component Toolbar, a tool tip displays the component name.

6. Double-click on the **Command Button** component on the Components Toolbar. This will add a command button to the blank Form in the Visual Basic window. The button can be moved and re-sized on the Form.

7. Double-click in any blank spot on the **Form** window in the Visual Basic window. This will activate the **Code** window. (**Note: the **Code** window can be activated by clicking on the code button in the project explorer window.*)

The **Code** window has several features that are immediately important.

- The **Main Code** window: this is where the Visual Basic code (i.e. the "script") is written.
- The **Event** combo box (at the top right of the code window): this is a pop-up list of all the Events that the working Form can respond to.

- The **Controls** combo box (at the top left of the code window): this is a pop-up list of all of the Controls that are on the working Form.

8. From the **Controls** combo box select "Command1." This activates the portion of the code window that is associated with the command button that was created in step 6. (Note: The name of the button as assigned by Visual Basic can be changed. Also, the name that is used when referring to a control in Visual Basic does not have to be the same as the text name that is used to identify the control in the Form window.)

9. The following lines of code are automatically inserted into the Code Window by Visual Basic:

```
Private Sub Command1_Click()
End Sub
```

This is indicating that all codes inserted in between these two lines will be executed when the button named "Command1" is clicked.

Note that the Control "Command1" that was added to the form can respond to many events. The **Events** pop-up menu allows you to jump to the section of the code window where you would insert code for the selected Event.

10. The first step to writing the code is to insert the lines that create the link between Visual Basic and the NTNMR Data file (i.e. "Document"). This is done using the following two lines:

```
Dim Data As NTNMR.Document
Set Data = GetObject("path_to_data")
```

The Dim statement in Visual Basic is used to define a variable. The first line assigns the variable "Data" to the NTNMR document type.

The second line uses the GetObject command to assign a path name to the data file that the script should work on.

Insert these lines as shown in the example below. Be sure to type the **complete path name** to the data that you opened in NTNMR in step 1.

```
Private Sub Command1_Click()
Dim Data As NTNMR.Document
```

```
Set Data = GetObject("c:\ntnmr\data\sds-c13.tnt")
End Sub
```

11. Next add some data processing lines to the script. The following general syntax in used:

    data_file_variable_name.ntnmr_command

    Add the two lines as shown in the example below to perform a DC Baseline Correction and a Fourier Transform to the data

```
Private Sub Command1_Click()
Dim Data As NTNMR.Document
Set Data = GetObject("c:\ntnmr\data\sds-c13.tnt")
Data.BC
Data.FT
End Sub
```

    Notice that when the defined variable name for the data file is typed ("Data" in this case) followed by a period, Visual Basic pops up a list of available commands that can be applied. The arrow keys on the keyboard can be used to navigate this list. *If you do not see the pop-up list of command,s go back to step 4 and verify that the NTNMR references file has a check next to it.*

12. Select **Run|Start** in Visual Basic (or press the F5 key on the keyboard) to run the script.

13. The Form that was created with a single button named "Commnad1" should appear. Click the "Command1" button.

14. Switch views to display the NTNMR window to check to see that the data was processed.

<<< PREV <<<
9.10
>>> NEXT >>>

Example NMRScripts - Visual Basic 5.0

The scripts below are included as project files in the folder called "example scripts" in the script folder. In cases where specific path names are not needed ready to run, executable versions of the examples are also included. Note that in the examples below the Visual Basic comment character (') has been used to show comment lines.

Example 1: 1D Processing Script

Description:
This script applies simple processing to a data file. This script is mainly for demonstrating scripting syntax and is of little practical use as a script. All of the processing done in this script can be handled in a nDFT processing template.

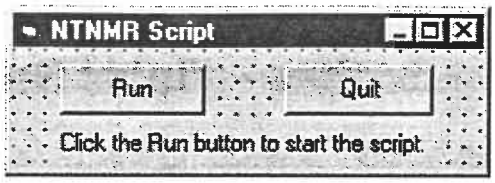
Comments:
A form was created using two buttons and a label. The default button names used by Visual Basic were used - Command1 and Command2. The Command1 button was given the caption "Quit" and the Command2 button was given the caption "Run" by editing the Caption field in the Properties window for both. Similarly, the text label, named Label1, was given the default text string as shown in the form below.

The code is divided into three sections. The top section (Select (General) in the Controls combo box, and (Declarations) from the Events Combo box) declares the variable Data as an NTNMR object of the type Document.

The second section (Control = Command1, Event = Click) is very brief. The single line of code "End" is called when the Command1 button ("Quit" button) is clicked. This quits the script.

The third section of the script is where the data processing actually occurs in response to the "Run" (Command2) button being clicked. Notice also that the Label1 control is utilized to provide feedback to the user on the progress of the script. Just before the processing is started Label1 is set to the text "Working..." Label1 is reset again before the Auto Phase command is called. Finally, when the script is completed, Label1 is set to inform the user that processing is completed. This script also updates the text on the title bar of the window in the line "Form1.Caption ... "

Form:



Script:

```
'define the variable Data as an NTNMR document
Dim Data As NTNMR.Document
----------
Private Sub Command1_Click()
'quit the script when clicking on Quit button
End
End Sub
----------
Private Sub Command2_Click()
'execute the commands below when clicking on Run button
'define the data set to be used
Set Data = GetObject("C:/ntnmr/data/c13.tnt")
'set the title bar of the script window
Form1.Caption = "1d process"
'display some text in the script window
Label1.Caption = "Working..."
'processing...
Data.BC
Data.SBS 90, 9000, 1
Data.FT
Label1.Caption = "Working... Auto Phase"
Data.AP
'prompt the user to quit the script
Label1.Caption = "Script completed. Click Quit to end."
End Sub
```

Example 2: Single Click Acquisition and Processing

Description:

This script demonstrates using Visual Basic to acquire and process a data set.

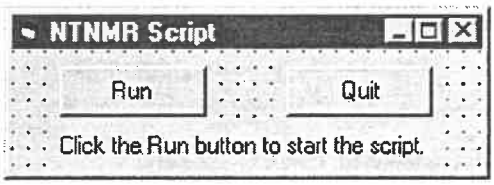
Comments:
A form was created using two buttons and a label. The default button names used by Visual Basic were used - Command1 and Command2. The Command1 button was given the caption "Quit" and the Command2 button was given the caption "Run" by editing the Caption field in the Properties window for both. Similarly, the text label, named Label1, was given the default text string as shown in the form below.

The code is divided into three sections. The top section (Select (General) in the Controls combo box, and (Declarations) from the Events Combo box) declares the variable Data as an NTNMR object of the type Document.

The second section (Control = Command1, Event = Click) is very brief. The single line of code "End" is called when the Command1 button ("Quit" button) is clicked. This quits the script.

The third section of the script is where the data processing actually occurs in response to the "Run" (Command2) button being clicked. Notice also that the Label1 control is utilized to provide feedback to the user on the progress of the script. Just before the processing is started, Label1 is set to the text "Working..." Label1 is reset again before the Auto Phase command is called. Finally, when the script is completed, Label1 is set to inform the user that processing is completed. This script also updates the text on the title bar of the window in the line "Form1.Caption ... "

Form:



Script:

```
'define the variable Data as an NTNMR document
Dim Data As NTNMR.Document
-------------------------------------------------------------------------------------------------------------
----
Private Sub Command1_Click()
'quit the script when clicking on Quit button'
```

```
End
End Sub
-------------------------------------------------------------------------------------------------------------
----
Private Sub Command2_Click()
'execute the commands below when clicking on Run button
'define the data set to be used
Set Data = GetObject("C:/ntnmr/data/c13.tnt")
'set the title bar of the script window
Form1.Caption = "1d Experiment"
'display text in the script window
Label1.Caption = "Acquisition"
'start the acquisition loop
Data.ZG
Data.CheckAcquisition
Do While Not Data.CheckAcquisition
Loop
'change text in the script window
Label1.Caption = "Processing"
'processing...
Data.BC
Data.SBS 90, 9000, 1
Data.FT
Label1.Caption = "Processing... Auto Phase"
Data.AP
'prompt the user to quit the script
Label1.Caption = "Script completed. Click Quit to end."
End Sub
```

Example 3: A 'Batch' Script Example

Description:
Often times you may want to create a script that will simply execute a series of processing steps and then quit, without user interaction. Scripts that run in 'batch' mode, functions essentially the same as user defined commands. Note that in Visual Basic, a Form *must* be created, since the code that is written is associated with its form (and not the other way around!). Even though in batch mode, no user interaction is required, the form is still of some use. The example

shown below uses a label on the form to display text messages updating the user on the progress of the processing. For simple scripts, this may not be useful since the execution is likely to be very fast. For longer, more complicated scripts, however, it is a good practice to inform the user of the progress. This script also uses the provided code module 'get_active_doc_path' to create the link to the active document. Using code modules is a very important concept and can save a good deal of time in script writing.

Comments:
A Form was created and re-sized that contains on a label (called 'label1') in the example. The label is used to inform the user of the progress of the script.

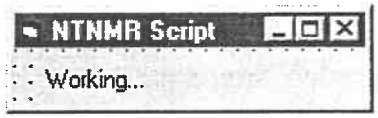
The code is divided into two sections. The top section (Select (General) in the Controls combo box, and (Declarations) from the Events Combo box) declares the variable Data as an NTNMR object of the type Document.

The second section of this script, written in the Form_Initialize event, introduces two new concepts, one specific to NTNMR and one specific to Visual Basic. First, the code module 'get_active_doc_path' is used to create the link to the top most data file. This is a very convenient method of creating a link to a data file. The code module provides what is essentially a new command that can be used in the project: GetActiveDoc *objectname*. The code module must be added to your project before the script below will run!

The second new concept that is introduced is the use of the With ... End With syntax. Earlier, the general syntax of *objectname.ntnmr_command* was introduced. This script shows the shortcut syntax of:

```
With objectname
        .ntnmr_command
        .ntnmr_command
        .ntnmr_command
End With
```

Form:



Script:

```
'define the variable Data as an NTNMR document
Dim Data As NTNMR.Document
```

```
Dim App As NTNMR.Application
--------------------------------------------------------------------------------------------------------------------
--------
Private Sub Form_Initialize()
GetActiveDoc Data
With Data
.BC
.EM
.FT
.AP
End With
'exit the script
End
End Sub
```

EXAMPLE 4: USING "FILE OPEN" DIALOGS

Description:
This example add a directory and a file list dialog boxes so that the path to the data does not have to be hard coded into the script, as in examples 1 and 2. The dialogs used here are the standard (and somewhat clumsy!) Visual Basic dialogs. A Drive list component is also available. This example integrates the drive and file list boxes into the main form. These boxes could, however, be used in a separate form that would only be opened when the user clicked a pre-defined button. Another option illustrated later (see examples 6 & 7) is the more elegant Microsoft Common Dialog control. This control allows the more common File Open dialogs that are used throughout the NTNMR (and the Windows operating system) to be used.

Comments:
A Form was created and several components were added:

- Directory List Box -- *appears at left*
- File List Box -- *appears at right*
- Label3 -- for information only, caption "Select a directory:"
- Label4 -- for information only, caption "Select a file:"
- Label1 -- for information only, caption "Selected file:"
- Command1 --when clicked data processing is executed, caption "Process 1"
- Command2 -- when clicked data processing is executed, caption "Process 2"
- Command3 -- when clicked the script is terminated

The following sections of code were added:

In the General/ Declarations section the variable Data is defined as an NTNMR Document and three other variables are defined using the Dim statement. These other variables are defined in the General section so that they will be available to all of the Sub procedures.

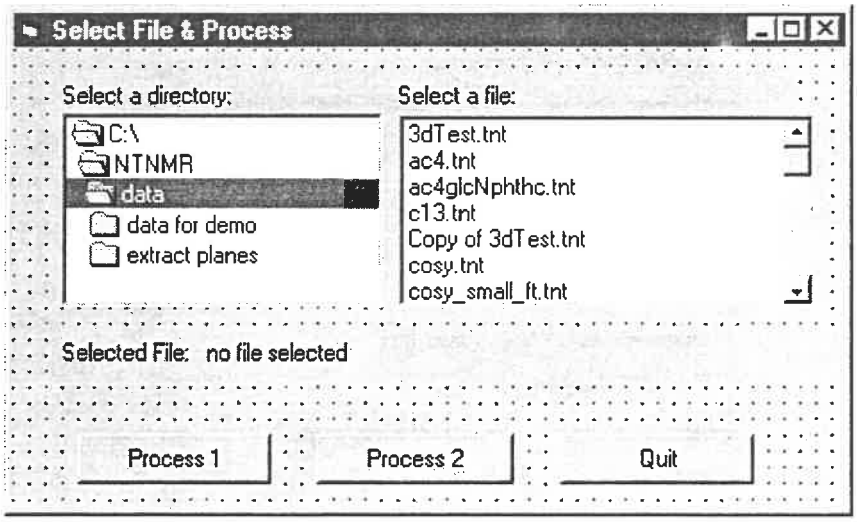
Both the Command1_Click procedures are similar. They both check to see that a data file has been selected using the Directory and File boxes. This is accomplished through an If-Then statement. Note that this code also adds a message dialog if no data file has been selected. The MsgBox line illustrates the syntax for this.

The Command3_Click procedure quits the script.

The Dir1_Change() procedure sets the variable DirPath to the path to the selected folder when changed in the directory box. The path for the file selection box is also set here, "File1.Path = DirPath"

The File1_Click() procedure contains the code to get the complete path to the selected data file in the file selection box. First, the variable DirPath is assigned to the path given by the Directory box (Dir1.Path). The path to the currently selected directory is always available. Next, the variable DataFileName is assigned to the data file selected in the file selection box (File1.filename). The variable PathToData is then created from the DirPath and the DataFileName variables. Finally, the Caption for Label2 is updated to display the complete path to the selected data file.

Form:



Script:

```
'define the variable Data as an NTNMR document
Dim Data As NTNMR.Document
Dim DataFileName, PathToData, DirPath
---------------------------------------------------------------------------------------------------------------
----
Private Sub Command1_Click()
'process 1
If PathToData = "" Then
MsgBox "No data file selected!", vbExclamation, "Error"
Else
Set Data = GetObject(PathToData)
With Data
.BC
.ExponentialMultiplication 5
.FourierTransform
.PhaseCorrection
End With
End If
End Sub
---------------------------------------------------------------------------------------------------------------
----
Private Sub Command2_Click()
'process 2
If PathToData = "" Then
MsgBox "No data file selected!", vbExclamation, "Error"
Else
Set Data = GetObject(PathToData)
With Data
.BC
.ExponentialMultiplication 10
.FourierTransform
.AP
End With
End If
```

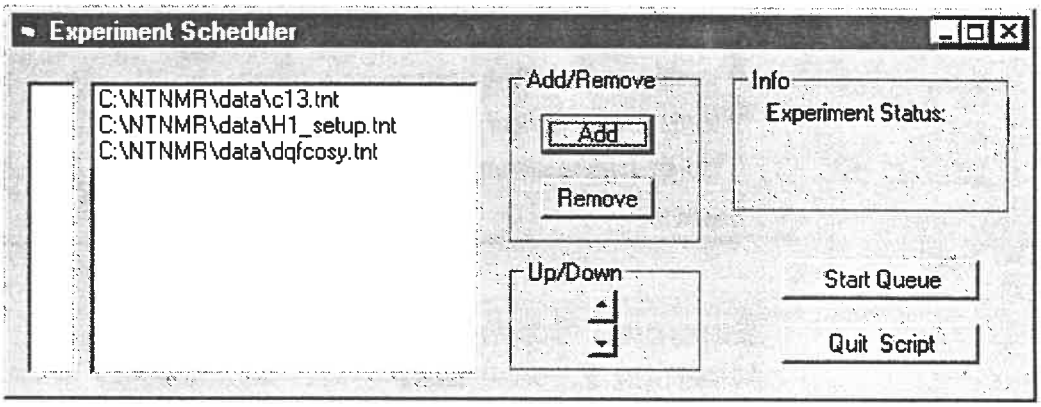
```
End Sub
-------------------------------------------------------------------------------------------------------------
----
Private Sub Command3_Click()
End
End Sub
-------------------------------------------------------------------------------------------------------------
----
Private Sub File1_Click()
DirPath = Dir1.Path
DataFileName = File1.filename
PathToData = DirPath & "\" & DataFileName
Label2.Caption = PathToData
End Sub
```

Examples 5 & 6: Experiment Scheduler & Kinetics Experiment

These two examples are somewhat complicated and intended for the advanced user. They are made available in an *.exe form so that they can be used immediately. The complete project files are also included in the standard distribution of NTNMR. Since these examples are fairly long, the code is not shown here. The Forms are shown for reference and a brief description of the script is given. The complete code can be examined by opening the project file in Visual Basic.

Experiment Scheduler Description:
This example illustrates using Visual Basic to queue several experiments in a row, consecutively. The script allows the user to choose several pre-defined experiments (saved as data files), and queue them to be run. Use the Add button to add a new experiment to the list. The code for the Add button shows an example of using the more elegant Microsoft Common Dialog for file/open operations.

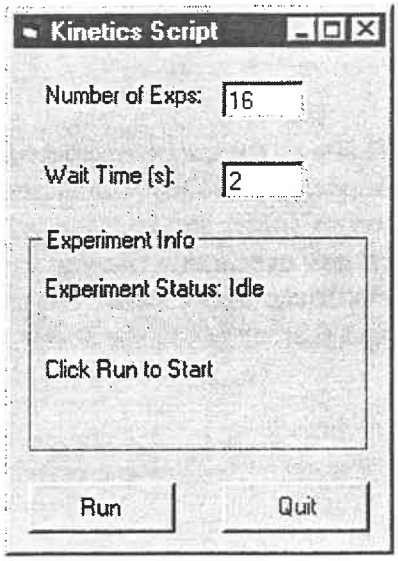
Experiment Scheduler Form:



Kinetics Experiment Description:

The Kinetics experiment works with the open and top most data file to acquire 'Number of Exps:' experiments with the time in between experiments specified by the parameter 'Wait Time' in seconds. The individual data files are saved to a disk in the format *data_file_name.experiment_number*.tnt. Note the use of the timer function for creating the wait time in between experiments.

Kinetics Experiment Form:


Kinetics Script
Number of Exps:
16
Wait Time (s):
2
Experiment Info
Experiment Status: Idle
Click Run to Start
Run
Quit

<<< PREV <<<
9.11
>>> NEXT >>>

The Script Menu

The Script menu in NTNMR allows the user to execute a script saved as an executable (*.exe) without leaving the NTNMR interface. All scripts saved as executables (*.exe) in the 'scripts' folder inside of the NTNMR folder will appear in the menu. Note that any executable file that is saved in the script folder will appear in the Script Menu in NTNMR. The user can also select 'Run Script' to locate and run scripts that are not in the Script Menu.

<<< PREV <<<

9.12

Frequently Asked Questions

Why can't I use a script to process the data that I just acquired?

This is probably because the window that was used to acquire the data was first created by selecting **File|New**. Visual Basic needs a file path to create a link to a document. If the data window was created from the File menu by selecting New, then there is no path since the data has never been written to disk. The solution to this problem is to acquire the data in a window that has previously been saved. When a zero-go command is executed, the data window will be renamed in NTNMR. However, Visual Basic will still be able to create a link to the file.

Can I use a language other than Visual Basic 5.0 to write "scripts?"

Yes - however, Visual Basic 5.0 is the only automation language that is officially supported by Tecmag. This means that languages such as Java, C++, WinBatch, Python, etc. can be used, but Tecmag cannot guarantee functionality and the support, if any. The support Tecmag can offer for languages other than VB will be limited.

References

1. Learn Visual Basic Now, Online (CD) Course Provided with the *Visual Basic Learning Edition*, 1997, Microsoft.

NTNMR File Format (80114)

Quick Start:

The following is the essential information to extract the data from a *.tnt data file.
See the following pages for details about the file format.

Bytes to skip to get to the data: 1056

Data format:
RIRIRIRI, blocks in linear order according to how they were collected

Example:
To read a 1D data file with 2048 points specifiy an offset of 1056 bytes, a data length of 2048, and a format of R, I, R R...

2D data is stored in a serial fashion. To read a 2D file the data length would be specified as (#records * Points 1D).

Data Format Outline
(see below for TECMAG and TECMAG2 data structures)

Item	Size (bytes)	Offset	Comment
"TNT1.000" version ID	8	0	
'TMAG' tag	4	8	
BOOLean value	4	12	
length of Tecmag struct	4	16	usually 1024
TECMAG structure	1024	18	
'DATA' tag	4	1044	
BOOLean	4	1048	
length of data	4	1052	
actual data (floating point - 4 byte in real/imag pairs)	data_offset = 2 * 4 * npts[0] * npts[1] * npts[2] * npts[3]	1056	
'TMG2' tag	4	1056 + data_offset	
BOOLean	4	1056 + data_offset + 4	
length of TECMAG2 struct	4	1056 + data_offset + 8	usually 2048
TECMAG2 structure	2048	1056 + data_offset + 12	
'PSEQ' tag	4	1056 + data_offset + 2060	
BOOLean	4	1056 + data_offset + 2064	
Sequence	variable		
Optional Sections:	Not necessarily in any order		
Peaks:			
'PEAK' tag	4		
BOOLean	4		
number of peaks	4		
sizeof of peak info	8 (long + BOOL)	(long peak_point, BOOL manually_chosen)	
peak info * number of peaks	8 * number of peaks		
Integrals:			
'INTG' tag	4		
BOOLean	4		
number of integrals	4		
size of integral info	28 (4 float + 3 long)	(float slope, float curvature, float fudge_factor, float multiplier, long start_point, long end_point, long bounds_rect.bottom	
integral info * number of integrals	28 * number of integrals		
Comments:			
'COMM' tag	4		
BOOLean	4		
length of string	4		
comment string	length of string		

TECMAG Structure

Number of points and scans in all dimensions:

Type	ID	Size (bytes)	Desc
long	npts[4];	16	points requested 1D, 2D, 3D, 4D
long	actual_npts[4];	16	points completed in each dimension (actual_npts[0] is not really used)
long	acq_points;	4	acq_points will be number of points to acquir during one acquisition icon in the sequence (which may be smaller than npts[0])
long	npts_start[4];	16	scan or pt on which to start the acquisition
long	scans;	4	scans 1D requested
long	actual_scans;	4	scans 1D completed
long	dummy_scans;	4	number of scans to do prior to collecting actual data
long	repeat_times;	4	Number of times to repeat scan
long	sadimension;	4	signal average dimension
char	space1[4];	4	

		76	

Field and frequencies:

double	magnet_field;	8	magnet field
double	ob_freq[4];	32	observe frequency
double	base_freq[4];	32	base frequency
double	offset_freq[4];	32	offset from base
double	ref_freq;	8	reference frequency for axis calculation (used to be freqOffset)
double	NMR_frequency;	8	absolute NMR frequency
char	space2[44];	44	

		164	

Spectral width, dwell and filter:

double	sw[4];	32	spectral width in Hz
double	dwell[4];	32	dwell time in seconds
double	filter;	8	filter
double	experiment_time;	8	time for whole experiment
double	acq_time;	8	acquisition time - time for acquisition
double	last_delay;	8	last delay in seconds
short	spectrum_direction;	2	1 or -1
short	hardware_sideband;	2	
short	Taps;	2	number of taps on receiver filter
short	Type;	2	type of filter
BOOL	bDigRec;	4	toggle for digital receiver
long	nDigitalCenter;	4	number of shift points for digital receiver

char	space3[16];	16	

		128	
Hardware settings:			
short	transmitter_gain;	2	transmitter gain
short	receiver_gain;	2	receiver gain
char	space4[16];	16	

		20	
Spinning speed information:			
unsigned short	set_spin_rate;	2	set spin rate
unsigned short	actual_spin_rate;	2	actual spin rate read from the meter
		----	
		4	
Lock information:			
short	lock_field;	2	lock field value (might be Bruker specific)
short	lock_power;	2	lock transmitter power
short	lock_gain;	2	lock receiver gain
short	lock_phase;	2	lock phase
double	lock_freq_mhz;	8	lock frequency in MHz
double	lock_ppm;	8	lock ppm
double	H2O_freq_ref;	8	H1 freq of H2O
char	space5[16];	16	

		48	
VT information:			
double	set_temperature;	8	non-integer VT
double	actual_temperature;	8	non-integer VT

		16	
Shim information:			
double	shim_units;	8	shim units (used to be SU)
short	shims[36];	72	shim values
double	shim_FWHM;	8	full width at half maximum

		88	
Hardware specific information:			
short	HH_dcpl_attn;	2	decoupler attenuation (0..63 or 100..163); receiver gain is above
short	DF_DN;	2	decoupler
short	F1_tran_mode[7];	14	F1 Pulse transmitter switches
short	dec_BW;	2	decoupler BW

		20	

char	grd_orientation[4];	4	gradient orientation
char	space6[296];	296	space for the middle text below and variables above
		----	
		300	
Text variables:	// 96 below		
char	date[32];	32	experiment date
char	nucleus[16];	16	nucleus
char	nucleus_2D[16];	16	2D nucleus
char	nucleus_3D[16];	16	3D nucleus
char	nucleus_4D[16];	16	4D nucleus
char	sequence[32];	32	sequence name
char	lock_solvent[16];	16	Lock solvent
char	lock_nucleus[16];	16	Lock nucleus

		160	
	TECMAG Structure total =>	1024	

TECMAG2 Structure

Display Menu flags:

Type	ID	Size	Desc
BOOL	real_flag;	4	display real data
BOOL	imag_flag;	4	display imaginary data
BOOL	magn_flag;	4	display magnitude data
BOOL	axis_visible;	4	display axis
BOOL	auto_scale;	4	auto scale mode on or off
BOOL	line_display;	4	TRUE for lines, FALSE for points
BOOL	show_shim_units;	4	display shim units on the data area or not
		----	
		28	

Option Menu flags:

BOOL	integral_display;	4	integrals turned on? - but not swap area
BOOL	fit_display;	4	fits turned on? - but not swap area
BOOL	show_pivot;	4	show pivot point on screen; only used during interactive phasing
BOOL	label_peaks;	4	show labels on the peaks?
BOOL	keep_manual_peaks;	4	keep manual peaks when re-applying peak pick settings?
BOOL	label_peaks_in_units;	4	peak label type
BOOL	integral_dc_average;	4	use dc average for integral calculation
BOOL	integral_show_multiplier;	4	show multiplier on integrals that are scaled
BOOL	Boolean_space[9];	36	

		68	

Processing flags:

BOOL	all_ffts_done[4];	16	
BOOL	all_phase_done[4];	16	

		32	

Vertical display multipliers:

double	amp;	8	amplitude scale factor
double	ampbits;	8	resolution of display
double	ampCtl;	8	amplitude control value
long	offset;	4	vertical offset

		28	

grid_and_axis	axis_set;	256	see Grid and Axis Structure below

short	display_units[4];	8	display units for swap area
long	ref_point[4];	16	for use in frequency offset calcs
double	ref_value[4];	32	for use in frequency offset calcs
long	z_start;	4	beginning of data display (range: 0 to 2 * npts[0] - 2)

long	z_end;	4	end of data display (range: 0 to 2 * npts[0] - 1
long	z_select_start;	4	beginning of zoom highlight
long	z_select_end;	4	end of zoom highlight
long	last_zoom_start;	4	last z_select_start - not used yet (4/10/97)
long	last_zoom_end;	4	last z_select_end - not used yet (4/10/97)
long	index_2D;	4	in 1D window, which 2D record we see
long	index_3D;	4	in 1D window, which 3D record we see
long	index_4D;	4	in 1D window, which 4D record we see

		92	

long	apodization_done[4];	16	masked value showing which processing has been done to the data; see constants.h for values
double	linebrd[4];	32	line broadening value
double	gaussbrd[4];	32	gaussian broadening value
double	dmbrd[4];	32	double exponential broadening value
double	sine_bell_shift[4];	32	sine bell shift value
double	sine_bell_width[4];	32	sine bell width value
double	sine_bell_skew[4];	32	sine bell skew value
long	Trapz_point_1[4];	16	first trapezoid point for trapezoidal apodizati
long	Trapz_point_2[4];	16	second trapezoid point for trapezoidal apodization
long	Trapz_point_3[4];	16	third trapezoid point for trapezoidal apodization
long	Trapz_point_4[4];	16	fourth trapezoid point for trapezoidal apo
double	trafbrd[4];	32	Traficante-Ziessow broadening value
long	echo_center[4];	4	echo center for all dimensions

		320	

long	data_shift_points;	4	number of points to use in left/right shift operations
short	fft_flag[4];	8	fourier transform done? false if time domain, true if frequency domain
double	unused[8];	64	
long	pivot_point[4];	16	for interactive phasing
double	cumm_0_phase[4];	32	cummulative zero order phase applied
double	cumm_1_phase[4];	32	cummulative first order phase applied
double	manual_0_phase,	8	used for interactive phasing
double	manual_1_phase;	8	used for interactive phasing
double	phase_0_value,	8	last zero order phase value applied (not necessarily equivalent to cummulative zero order phase)
double	phase_1_value;	8	last first order phase value applied (not necessarily equivalent to cummulative first order phase)
double	session_phase_0,	8	used during interactive phasing
double	session_phase_1;	8	used during interactive phasing
		----	

long	max_index;	4	index of max data value
long	min_index;	4	index of min data value
float	peak_threshold,	4	threshold above which peaks are chosen
float	peak_noise;	4	minimum value between two points that are above the peak threshold to distinguish two peaks from two points on the same peak
short	integral_dc_points;	2	number of points to use in integral calculation when dc average is used
short	integral_label_type;	2	how to label integrals, see constants.h
float	integral_scale_factor;	4	scale factor to be used in integral draw
long	auto_integrate_shoulder;	4	number of points to determine where integral is cut off
double	auto_integrate_noise;	8	when average of shoulder points is under this value, cut off integral
double	auto_integrate_threshold;	8	threshold above which a peak is chosen in auto integrate
long	s_n_peak;	4	peak to be used for signal to noise calculation
long	s_n_noise_start;	4	start of noise region for signal to noise calculation
long	s_n_noise_end;	4	end of noise region for signal to noise calcula
float	s_n_calculated;	4	calculated signal to noise value

		60	

long	Spline_point[14];	56	points to be used for spline baseline fix calculation
short	Spline_point_avr;	2	for baseline fix
long	Poly_point[8];	32	points for polynomial baseline fix calculation
short	Poly_point_avr;	2	for baseline fix
short	Poly_order;	2	what order polynomial to use

		94	

Blank Space:

char	space[610];	610

Text variables:

char	line_simulation_name[32];	32
char	integral_template_name[32];	32
char	baseline_template_name[32];	32
char	layout_name[32];	32
char	relax_information_name[32];	32
char	username[32];	32
char	user_string_1[16];	16
char	user_string_2[16];	16
char	user_string_3[16];	16
char	user_string_4[16];	16

256

TECMAG2 Structure Total => 2048

Grid and Axis Structure

Type	ID	Size(bytes)	Desc
double	majorTickInc[TOTAL_UNIT_TYPES];	8 * 12 = 96	Increment between major ticks
short	minorIntNum[TOTAL_UNIT_TYPES];	2 * 12 = 24	Number of intervals between major ticks (minor ticks is one less than this)
short	labelPrecision[TOTAL_UNIT_TYPES];	2 * 12 = 24	Number of digits after the decimal point
double	gaussPerCentimeter;	8	Used for calculation of distance axis in frequency domain
short	gridLines;	2	Number of horizontal grid lines to be shown in data area
short	axisUnits;	2	Type of units to show - see constants.h
BOOL	showGrid;	4	Show or hide the grid
BOOL	showGridLabels;	4	Show or hide the labels on the grid lines
BOOL	adjustOnZoom;	4	Adjust the number of ticks and the precision when zoomed in
BOOL	showDistanceUnits;	4	whether to show frequency or distance units when in frequency domain
char	axisName[32];	32	file name of the axis (not used as of 4/10/97)
char	space[52];	52	

		256	

Pulse Sequence:

'PSEQ' tag	4	
BOOLean	4	
SequenceID	8	"1.04 BIN"
Filename Length	4	
File Name	Length	
Number of Rows	4	
Number of Columns	4	
Sequence Rows:	**Number of Rows * (variable length)**	
Number of Columns	4	
Address	4	
BitLength	4	
Icon Library Type	4	
Visible Flag	4	
Private Data	4	
Group	4	
Defalut String Length	4	
Defalut String	Length	
Label String Lerngth	4	
Label String	Length	
Sequence Events	**Number of Columns * (Variable length)**	
Data String Length	4	
Data String	Length	
0D Table Name Length	4	

0D Table Name	Length
0D Table Flag	4
1D Table Name Length	4
1D Table Name	Length
1D Table Flag	4
2D Table Name Length	4
2D Table Name	Length
2D Table Flag	4
3D Table Name Length	4
3D Table Name	Length
3D Table Flag	4
4D Table Name Length	4
4D Table Name	Length
4D Table Flag	4

Sequence Tables: **Number of Tables * variable length**

Table Name Length	4
Table Name	Length
Table Entry Length	4
Table Entry	Length
Increment Operation Length	4
Increment Operation	Length
Increment Value Length	4
Increment Value	Length
Increment Scheme Length	4
Increment Scheme	Length
Repeat Time	4
Type Of Table	4
Dimension	4
StepsPer360Cycle	4
Use As Increment List	4 (BOOL)
Value Type	4 (int)

Sequence Parameter Pages

number of pages 4

Parameters Pages **Number of Pages * variable length**

Page Name Length	4
Page Name	Length
Number on Page	4

Parameter Names **Number on Page * variable length**

Parameter Name Length	4
Parameter Name	Length

Sequence Parameters

Number of Parameters 4

Parameters **Number of Parameters * variable length**

Parameter Name Length	4
Parameter Name	Length
Value String Length	4
Value String	Length
Parameter Type	4
Minimum String Length	4
Minimum String	Length
Maximum Striong Length	4
Maximum String	Length
ReadOnly Flag	4

Sequence comment

'SEQC' tag 4

Length of Comment 4
Comment Length
long Count = m_SeqComment.GetLength();

Tecmag Y2K Compatibility Statement

1. Software Products:

All Tecmag products operate under either Windows NT or the MacOS. Since both of these operating systems are Y2K compliant and Tecmag relies on the respective OS vendors for all date and time functions, there are no known Y2K issues with any version of NTNMR, MacNMR, or MacFID according to the definition below.

2. Hardware Products:

According to the definition below, all Tecmag hardware is Y2K compliant.

Definition of "Year 2000 Compliance"

To the best of our knowledge, we certify that neither the performance nor the functionality of any Tecmag product is affected by dates prior to, during, and after the year 2000.

In particular:

- No value for current date will cause any interruption in operation.
- Date-based functionality will behave consistently for dates prior to, during and after year 2000.
- In all interfaces and data storage, the century in any date is specified either explicitly or by unambiguous algorithms or inferencing rules.
- Year 2000 is recognized as a leap year.