VNMR User Programming VNMR 6.1C Software Pub. No. 01-999165-00, Rev. A1200 VARIAN

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Revision history A0500 – Initial release for VNMR 6.1C A1000 – Revision to shaped gradient pulse sequences in Chapter 3 by Frits Vosman A1200 – Revision to Chapter 1, reserved words in MAGICAL by Rolf Kyburz

Applicability of manual:

UNITY INOVA, MERCURY VxWorks Powered (shortened to MERCURY-VX throughout this manual), MERCURY, UNITYplus, GEMINI 2000, UNITY, and VXR-S NMR spectrometer systems with VNMR 6.1C software installed

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1		nds	
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	dres	ols	
	dsn	Measure signal-to-noise	
	dsnmax	Calculate maximum signal-to-noise	
	getll	Get line frequency and intensity from line list	
	getreg	Get frequency limits of a specified region	
	integ	Find largest integral in specified region	
	mark	Determine intensity of the spectrum at a point	
	nll	Find line frequencies and intensities	
	numreg	Return the number of regions in a spectrum	
	peak	Find tallest peak in specified region	
	select	Select a spectrum or 2D plane without displaying it	
	Input/Output Tools .		
	apa	Plot parameters automatically	
	banner	Display message with large characters	
	clear	Clear a window	
	confirm echo	Confirm message using the mouse Display strings and parameter values in text window	
	flip	Flip between graphics and text window	
	format	Format a real number or convert a string for output	
	input	Receive input from keyboard	
	lookup	Look up and return words and lines from text file	
	nrecords	Determine number of lines in a file	

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autoscale	Resume autoscaling after limits set by scalelimits	42
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abs	Find absolute value of a number	43
acos	Find arc cosine of a number	43
asin	Find arc sine of a number	43
atan	Find arc tangent of a number	43
atan2	Find arc tangent of two numbers	
averaq	Calculate average and standard deviation of input	
COS	Find cosine value of an angle	
exp	Find exponential value of a number	
ln	Find natural logarithm of a number	
sin	Find sine value of an angle	
tan	Find tangent value of an angle	
Creating, Modifying, and Di	splaying Macros	
crcom	Create a user macro without using a text editor	
delcom	Delete a user macro	
hidecommand	Execute macro instead of command with same name	
macrocat	Display a user macro on the text window	
macrocp	Copy a user macro file	
macrodir	List user macros	
macroedit	Edit a user macro with user-selectable editor	
macrold	Load a macro into memory	
macrorm	Remove a user macro	
macrosyscat	Display a system macro on the text window	
macrosyscp	Copy a system macro to become a user macro	
macrosysdir	List system macros	
macrosysrm	Remove a system macro	
macrovi	Edit a user macro with vi text editor	
mstat	Display memory usage statistics	
purge	Remove a macro from memory	
record	Record keyboard entries as a macro	
axis	Provide axis labels and scaling factors	
beepoff	Turn beeper off	
beepon	Turn beeper on	
bootup	Macro executed automatically when VNMR is started	
exec	Execute a VNMR command	
exists	Determine if a parameter, file, or macro exists	
focus	Send keyboard focus to VNMR input window	
gap	Find gap in the current spectrum	
getfile	Get information about directories and files	
graphis	Return the current graphics display status	
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	length	Determine length of a string	17
	listenoff	Disable receipt of messages from send2Vnmr	
	listenon	Enable receipt of messages from send2 vinin	
	login	User macro executed automatically when VNMR activated	
	off	Make a parameter inactive	
	on	Make a parameter active or test its state	
	readlk	Read current lock level	
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SAFETY PRECAUTIONS

The following warning and caution notices illustrate the style used in Varian manuals for safety precaution notices and explain when each type is used:

- **WARNING:** Warnings are used when failure to observe instructions or precautions could result in injury or death to humans or animals, or significant property damage.
- **CAUTION:** Cautions are used when failure to observe instructions could result in serious damage to equipment or loss of data.

Warning Notices

Observe the following precautions during installation, operation, maintenance, and repair of the instrument. Failure to comply with these warnings, or with specific warnings elsewhere in Varian manuals, violates safety standards of design, manufacturing, and intended use of the instrument. Varian assumes no liability for customer failure to comply with these precautions.

WARNING: Persons with implanted or attached medical devices such as pacemakers and prosthetic parts must remain outside the 5-gauss perimeter from the centerline of the magnet.

The superconducting magnet system generates strong magnetic fields that can affect operation of some cardiac pacemakers or harm implanted or attached devices such as prosthetic parts and metal blood vessel clips and clamps.

Pacemaker wearers should consult the user manual provided by the pacemaker manufacturer or contact the pacemaker manufacturer to determine the effect on a specific pacemaker. Pacemaker wearers should also always notify their physician and discuss the health risks of being in proximity to magnetic fields. Wearers of metal prosthetics and implants should contact their physician to determine if a danger exists.

Refer to the manuals supplied with the magnet for the size of a typical 5-gauss stray field. This gauss level should be checked after the magnet is installed.

WARNING: Keep metal objects outside the 10-gauss perimeter from the centerline of the magnet.

The strong magnetic field surrounding the magnet attracts objects containing steel, iron, or other ferromagnetic materials, which includes most ordinary tools, electronic equipment, compressed gas cylinders, steel chairs, and steel carts. Unless restrained, such objects can suddenly fly towards the magnet, causing possible personal injury and extensive damage to the probe, dewar, and superconducting solenoid. The greater the mass of the object, the more the magnet attracts the object.

Only nonferromagnetic materials—plastics, aluminum, wood, nonmagnetic stainless steel, etc.—should be used in the area around the magnet. If an object is stuck to the magnet surface and cannot easily be removed by hand, contact Varian service for assistance.

Warning Notices (continued)

Refer to the manuals supplied with the magnet for the size of a typical 10-gauss stray field. This gauss level should be checked after the magnet is installed.

WARNING: Only qualified maintenance personnel shall remove equipment covers or make internal adjustments.

Dangerous high voltages that can kill or injure exist inside the instrument. Before working inside a cabinet, turn off the main system power switch located on the back of the console, then disconnect the ac power cord.

WARNING: Do not substitute parts or modify the instrument.

Any unauthorized modification could injure personnel or damage equipment and potentially terminate the warranty agreements and/or service contract. Written authorization approved by a Varian, Inc. product manager is required to implement any changes to the hardware of a Varian NMR spectrometer. Maintain safety features by referring system service to a Varian service office.

WARNING: Do not operate in the presence of flammable gases or fumes.

Operation with flammable gases or fumes present creates the risk of injury or death from toxic fumes, explosion, or fire.

WARNING: Leave area immediately in the event of a magnet quench.

If the magnet dewar should quench (sudden appearance of gasses from the top of the dewar), leave the area immediately. Sudden release of helium or nitrogen gases can rapidly displace oxygen in an enclosed space creating a possibility of asphyxiation. Do not return until the oxygen level returns to normal.

WARNING: Avoid liquid helium or nitrogen contact with any part of the body.

In contact with the body, liquid helium and nitrogen can cause an injury similar to a burn. Never place your head over the helium and nitrogen exit tubes on top of the magnet. If liquid helium or nitrogen contacts the body, seek immediate medical attention, especially if the skin is blistered or the eyes are affected.

WARNING: Do not look down the upper barrel.

Unless the probe is removed from the magnet, never look down the upper barrel. You could be injured by the sample tube as it ejects pneumatically from the probe.

WARNING: Do not exceed the boiling or freezing point of a sample during variable temperature experiments.

A sample tube subjected to a change in temperature can build up excessive pressure, which can break the sample tube glass and cause injury by flying glass and toxic materials. To avoid this hazard, establish the freezing and boiling point of a sample before doing a variable temperature experiment.

Warning Notices (continued)

WARNING: Support the magnet and prevent it from tipping over.

The magnet dewar has a high center of gravity and could tip over in an earthquake or after being struck by a large object, injuring personnel and causing sudden, dangerous release of nitrogen and helium gasses from the dewar. Therefore, the magnet must be supported by at least one of two methods: with ropes suspended from the ceiling or with the antivibration legs bolted to the floor. Refer to the *Installation Planning Manual* for details.

WARNING: Do not remove the relief valves on the vent tubes.

The relief valves prevent air from entering the nitrogen and helium vent tubes. Air that enters the magnet contains moisture that can freeze, causing blockage of the vent tubes and possibly extensive damage to the magnet. It could also cause a sudden dangerous release of nitrogen and helium gases from the dewar. Except when transferring nitrogen or helium, be certain that the relief valves are secured on the vent tubes.

WARNING: On magnets with removable quench tubes, keep the tubes in place except during helium servicing.

On Varian 200- and 300-MHz 54-mm magnets only, the dewar includes removable helium vent tubes. If the magnet dewar should quench (sudden appearance of gases from the top of the dewar) and the vent tubes are not in place, the helium gas would be partially vented sideways, possibly injuring the skin and eyes of personnel beside the magnet. During helium servicing, when the tubes must be removed, carefully follow the instructions and safety precautions given in the manual supplied with the magnet.

Caution Notices

Observe the following precautions during installation, operation, maintenance, and repair of the instrument. Failure to comply with these cautions, or with specific cautions elsewhere in Varian manuals, violates safety standards of design, manufacturing, and intended use of the instrument. Varian assumes no liability for customer failure to comply with these precautions.

CAUTION: Keep magnetic media, ATM and credit cards, and watches outside the 5-gauss perimeter from the centerline of the magnet.

The strong magnetic field surrounding a superconducting magnet can erase magnetic media such as floppy disks and tapes. The field can also damage the strip of magnetic media found on credit cards, automatic teller machine (ATM) cards, and similar plastic cards. Many wrist and pocket watches are also susceptible to damage from intense magnetism.

Refer to the manuals supplied with the magnet for the size of a typical 5-gauss stray field. This gauss level should be checked after the magnet is installed.

Caution Notices (continued)

CAUTION: Keep the PCs, (including the LC STAR workstation) beyond the 5gauss perimeter of the magnet.

Avoid equipment damage or data loss by keeping PCs (including the LC workstation PC) well away from the magnet. Generally, keep the PC beyond the 5-gauss perimeter of the magnet. Refer to the *Installation Planning Guide* for magnet field plots.

CAUTION: Check helium and nitrogen gas flowmeters daily.

Record the readings to establish the operating level. The readings will vary somewhat because of changes in barometric pressure from weather fronts. If the readings for either gas should change abruptly, contact qualified maintenance personnel. Failure to correct the cause of abnormal readings could result in extensive equipment damage.

CAUTION: Never operate solids high-power amplifiers with liquids probes.

On systems with solids high-power amplifiers, never operate the amplifiers with a liquids probe. The high power available from these amplifiers will destroy liquids probes. Use the appropriate high-power probe with the high-power amplifier.

CAUTION: Take electrostatic discharge (ESD) precautions to avoid damage to sensitive electronic components.

Wear a grounded antistatic wristband or equivalent before touching any parts inside the doors and covers of the spectrometer system. Also, take ESD precautions when working near the exposed cable connectors on the back of the console.

Radio-Frequency Emission Regulations

The covers on the instrument form a barrier to radio-frequency (rf) energy. Removing any of the covers or modifying the instrument may lead to increased susceptibility to rf interference within the instrument and may increase the rf energy transmitted by the instrument in violation of regulations covering rf emissions. It is the operator's responsibility to maintain the instrument in a condition that does not violate rf emission requirements.

Introduction

Varian's VNMR software provides NMR users with an exceptionally responsive user programming environment that allows customizing the system software and the operator interface. This manual explains how to use these capabilities:

- Chapter 1, "MAGICAL II Programming," describes MAGICAL II (MAGnetics Instrument Control and Analysis Language), a powerful software application that enables full automation of spectrometer operation and data analysis using macros.
- Chapter 2, "Pulse Sequence Programming," covers pulse sequence programming, via menus as well as user-written programs, using Varian's powerful and extensive set of pulse sequence statements.
- Chapter 3, "Pulse Sequence Statement Reference," is an alphabetical reference to each pulse sequence statement in VNMR.
- Chapter 4, "UNIX-Level Programming," is a short overview of UNIX, the operating system used with VNMR.
- Chapter 5, "Parameters and Data," covers manipulating parameters, using data files, modifying parameter displays, and writing user-defined weighting functions
- Chapter 6, "Customizing Graphics Windows," describes how to customize the interactive graphics display windows for the enter, status, and dg programs.

Notational Conventions

The following notational conventions are used throughout all VNMR manuals:

- Typewriter-like characters identify VNMR and UNIX commands, parameters, directories, and file names in the text of the manual. For example: The shutdown command is in the /etc directory.
- Typewriter-like characters also show text displayed on the screen, including the text echoed on the screen as you enter commands. For example: Self test completed successfully.
- Text shown between angled brackets (<...>) in a syntax entry is optional. For example, if the syntax is seqgen s2pul<.c>, entering the ".c" suffix is optional, and typing seqgen s2pul.c or seqgen s2pul is functionally the same.
- Lines of text containing command syntax, examples of statements, source code, and similar material are often too long to fit the width of the page. To show that a line of text had to be broken to fit into the manual, the line is cut at a convenient point (such as at a comma near the right edge of the column), a backslash (\) is inserted at the cut, and the line is continued as the next line of text. This notation will be familiar to C programmers. Note that the backslash is not part of the line and, except for C source code, should not be typed when entering the line.
- Because pressing the Return key is required at the end of almost every command or line of text you type on the keyboard, use of the Return key will be mentioned only in cases where it is *not* used. This convention avoids repeating the instruction "press the Return key" throughout most of this manual.

• Text with a change bar (like this paragraph) identifies material new to VNMR version 6.1C that was not in the previous version of VNMR. Refer to the *VNMR 6.1C Release Notes* for a description of new features to the software.

Other Manuals

This manual should be your basic source of information on MAGICAL programming, pulse sequence programming, manipulating parameters and data, and customizing graphics windows. Other VNMR 6.1 manuals you should have include:

- Getting Started
- Walkup NMR Using GLIDE
- User Guide: Liquids NMR
- User Guide: Solid-State NMR
- User Guide: Imaging
- VNMR Command and Parameter Reference
- VNMR and Solaris Software Installation

All of these manuals are shipped with the VNMR software. These manuals, other Varian hardware and installation manuals, and most Varian accessory manuals are also provided online so that you can view the pages on your workstation and print copies.

Types of Varian Software and Spectrometers

VNMR is the trademark name of Varian's NMR software, which includes acquisition, data processing, menus, macros, and pulse sequences. Occasionally you will also see "Vnmr" mentioned in VNMR manuals as well as in the online help. Vnmr is the name of the main NMR program that runs on UNIX, forming the nucleus of VNMR. Specific applications of VNMR include VNMR for computers using the X Window System (VnmrX), VNMR for IBM workstations (VnmrI), and VNMR for Silicon Graphics computers (VnmrSGI).

In parts of this manual, the type of system (UNITY INOVA, MERCURY, MERCURY-VX, GEMINI 2000, UNITY plus, UNITY, or VXR-S) must be considered in order to use the software properly.

- UNITY INOVA and MERCURY-VX are the current systems sold by Varian.
- UNITYplus, UNITY, and VXR-S are spectrometer lines that preceded the UNITYINOVA.
- *GEMINI 2000* is a separate line of spectrometers that preceded the *MERCURY* and *MERCURY-VX*.

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Chapter 1. MAGICAL II Programming

Sections in this chapter:

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- 1.2 "Programming with MAGICAL," page 29
- 1.3 "Relevant VNMR Commands," page 38
- 1.4 "Using Dialog Boxes from a Macro," page 49
- 1.5 "Customizing the Menu System," page 52
- 1.6 "Customizing the Files Menus," page 58

Many of the actions performed on an NMR spectrometer are performed many times, day after day. To make these actions easier on the user, VNMR software provides for the use of macros and a high-level programming language designed for NMR.

1.1 Working with Macros

A *macro* is a user-defined command that can duplicate a long series of commands and parameter changes you would otherwise have to enter one by one. To plot a spectrum, a scale under the spectrum, and parameters on the page would require a sequence of commands such as

pl pscale hpa page

It would be possible to define a macro, say, plot, that would be the equivalent of these commands. Or, perhaps you routinely plot 2D spectra using certain parameters. In this case, you might define a macro plot_2d as equivalent to the following:

```
wc=160
sc=20
wc2=160
sc2=20
pcon(10,1.4)
page
```

But macros in the VNMR software are much more than this. Macros are written in Varian's special high-level "NMR" language, MAGICAL II[™] (MAGnetics Instrument Control and Analysis Language, version II—usually just called MAGICAL in this chapter). MAGICAL provides an entire series of programming tools, such as if statements and loops, that can be used as part of macros. In addition, MAGICAL provides other NMR-related tools that allow macros to access NMR information like peak heights, integrals, and spectral regions. Using these two sets of tools, "NMR algorithms" are easily implemented with MAGICAL.

Writing a Macro

Consider the following problem: Find the largest peak in a spectrum in which the peaks may be positive or negative (such as an APT spectrum) and adjust the vertical scale of the spectrum so that the tallest peak is 180 mm high. The following macro (or MAGICAL program) that we call vsadj illustrates how the MAGICAL tools can be used to quickly and simply find a solution:

"vsadj --- Adjust scale of spectrum"
peak:\$height,\$frequency "Find largest peak"
if \$height<0 then \$height=- "If negative, make positive"
\$height endif
vs=180*vs/\$height "Adjust the vertical scale"</pre>

As written, the macro vsadj has four lines:

- The material in double-quotation marks (the first line and parts of other lines) are comments. MAGICAL permits comments, and as is good programming practice, this example is filled with comments to explain what is happening.
- The second line of the macro ("peak:\$height,...") illustrates the ability of MAGICAL to extract spectral information. The peak command looks through the spectrum and returns to the user the height and frequency of the tallest peak in the spectrum, which are then stored (in this example) in temporary variables named \$height and \$frequency.
- The third line of the macro ("if \$height<0...") illustrates that MAGICAL is a high-level programming language, with conditional statements (e.g., if... then...), loops, etc. This particular line ensures that the peak height we measure is always a positive value, which is necessary for the calculation in the next line.
- The last line ("vs=180*vs...") illustrates the use of NMR parameters (like vs, which sets the vertical scale) as simple variables in our macro. This line accomplishes the task of calculating a new value of vs that will make the height of the tallest peak equal to 180 mm.

Part of the power of the MAGICAL macro language is its ability to build on itself. For example, we can create first-level macros out of existing commands, second-level macros out of first-level macros and commands, and so on. Suppose we created a macro plot, for example, we might also create a macro setuph, another macro acquireh, and yet another macro processh. Now we might create a "higher-level" macro, H1, which is equivalent to setuph acquireh processh plot. Perhaps we have created two more similar macros, C13 and APT. Now we might create yet another higher-level macro HCAPT, equivalent to H1 C13 APT. At every step of the way, the power of the macro increases, but without increasing the complexity.

Many macros are part of the standard VNMR software. These macros are discussed in the relevant chapters of the manual *Getting Started*—processing macros are discussed along with processing commands, acquisition setup macros along with acquisition setup commands, etc. Refer to the *VNMR Command and Parameter Reference* for a concise description of standard macros. The examples used here are instructive examples and do not necessarily represent standard Varian software.

Executing a Macro

When any program is executed, the command interpreter first checks to see if it is a standard VNMR command. If the program is not a command, the command interpreter then attempts to find a macro with the program name. Unlike a built-in VNMR command, which

is a built-in procedure containing code that normally cannot be changed by users, the code inside a macro is text that is accessible and can be changed by users as needed.

If a VNMR command and a macro have the same name, the VNMR command always takes precedence over a macro. For example, there is a built-in VNMR command named wft. If someone happens to write a macro also named wft, the macro wft will never get executed because the VNMR command wft takes precedence. To get around this restriction, the hidecommand command can rename a command so that a macro with the same name as a command is executed instead of the built-in command. If the user who wrote the wft macro enters hidecommand('wft'), the command is renamed to Wft (first letter made upper case) and the macro wft is now executable directly. The new wft macro can access the hidden wft built-in command by calling it with the name Wft. To go back to executing the command wft first, enter hidecommand('Wft').

Macro files can reside in four separate locations:

- 1. In the user's maclib directory.
- 2. In the directory pointed to by the maclibpath parameter (if maclibpath is defined in the user's global parameter file).
- 3. In the directory pointed to by the sysmaclibpath parameter (if defined).
- 4. In the system maclib directory.

When macros are executed, the four locations are searched in this order. The first location found is the one that is used. For example, rt is a standard VNMR macro in the system maclib. If a user puts a macro named rt in the user's maclib, the user's rt macro takes precedence over the system rt macro.

The which macro can search these locations and display on line 3 the information it finds about which location contains a macro. For example, entering which ('rt') determines the location of the macro rt.

The system macro directory /vnmr/maclib can be changed by the system operator only, but changes to it are available to all users. Each user also has their own private macro directory maclib in the user's vnmrsys directory. These macros take precedence over the system macros if a macro of the same name is in both directories. Thus, users can modify a macro to their own needs without affecting the operation of other users. If the command interpreter does not find the macro, it displays an error message to the user.

Macros are executed in exactly the same way as normal system commands, including the possibility of accepting optional arguments (shown by angled brackets "<...>"): macroname<(argument1<,argument2,...>)>

Arguments passed to commands and macros can be constants (examples are 5.0 and 'apt'), parameters and variables (pw and \$ht), or expressions (2*pw+5.0). Recursive calls to procedures are allowed. Single quotes must be used around constant strings.

Macros can also be executed three other ways:

- When the VNMR program is first run, a system macro bootup is run. This macro in turn runs a user macro named login in the user's local maclib directory if such a macro exists.
- When any parameter x is entered, if that parameter has a certain "protection bit" set (see "Format of a Stored Parameter," page 301), a macro by the name _x (that is, the same name as the parameter with an underline as a prefix) is executed. For example, changing the value of sw executes the macro _sw.
- Whenever parameters are retrieved with the rt, rtp, or rtv commands, a macro named fixpar is executed.

If the macro needs to know what macro invoked it, that information is stored by the string parameter macro available in each experiment.

Transferring Macro Output

Output from many commands and macros, in addition to being displayed on the screen or placed in a file, can also be transferred into any parameter or variable of the same type. To receive the output of a program of this type, the program name (and arguments, if any) are followed by a colon (:) and one or more names of variables and parameters that are to take the output:

macroname<(arg1<,arg2,...>)>:variable1,variable2,...

For example, the command peak (described below in more detail) finds the height and frequency of the tallest peak. Entering the command: peak:r1,r2

results in r1 containing the height of the tallest peak and r2 its frequency. Therefore, entering the command

peak:\$ht,cr

would set \$ht equal to the height of the tallest peak and set the cursor (parameter cr) equal to its frequency, and thus would be the equivalent of a "tallest line" command (similar to but different than the command nl to position the cursor at the nearest line).

It is not necessary to receive all of the information. For example, entering peak:\$peakht

puts the height of the tallest peak into the variable \$peakht, and does not save the information about the peak frequency.

The command that displays a line list, dll, also produces one output—the number of lines. Entering

dll:\$n

reads the number of lines into variable \$n. dll alone is perfectly acceptable although the information about the number of lines is then "lost."

Loading Macros into Memory

Every time a macro is used, it is "parsed" before it is executed. This parsing takes time. If a macro is used many times or if faster execution speed is desirable, the parsed form of the macro, user or system, can be loaded into memory by the macrold command. When that macro is executed, it runs substantially faster. You can even "pre-load" one or more macros automatically when you start VNMR by inserting some macrold commands into your login macro.

Macros are also loaded into memory when you use the macrovi or macroedit commands to edit the macro. The only argument in each is the name of the macro file; for example, enter macrovi('pa') or macroedit('pa') if the macro name is pa. Which command you use depends on the type of macro and the text editor you want:

- For a user macro from the UNIX vi editor, use macrovi.
- For a user macro from an editor you select, use macroedit.
- To edit a system macro, copy the macro to your personal macro directory and edit it there with macrovi or macroedit.

To select the editor for macroedit, set the UNIX variable vnmreditor to its name (vnmreditor is set through the UNIX env command). You must have also a script for

the editor in the bin subdirectory of the VNMR system directory. For example, you can select Emacs by setting vnmreditor=emacs and having a script vnmr_emacs.

Several minor problems need to be considered in loading macros into memory:

- These macros consume a small amount of memory. In memory-critical situations, you might want to remove one or more macros from memory. This is done with the purge<(file)> command, where file is the name of a macro file to be removed from memory. Entering purge with no arguments removes all macros loaded into memory.
- **CAUTION:** The purge command with no arguments should never be called from a macro, because it will remove all macros from memory, including the macro containing purge. Furthermore, purge, where the argument is the name of the macro containing the purge command, should never be called.
 - If a macro is loaded in memory and you try to modify the macro from a separate UNIX window, the copy in memory is *not* changed, so if you execute the macro again, VNMR executes the old copy. To avoid this, use macrovi or macroedit to edit the macro, or if you have already edited the macro from another window, use macrold to replace the macro loaded in memory with the new version.
 - If you wish to create a personal macro with the same name as a system macro already in memory, you must use purge to clear the system macro from memory so the version in your personal maclib directory will subsequently be executed.

If one macro calls another macro inside a loop, you might improve performance by having the calling macro load the called macro before entering the loop, execute the loop, and then remove the called macro from memory with the purge command.

1.2 Programming with MAGICAL

MAGICAL has many features, including tokens, variables, expressions, conditional statements, and loops. To program in MAGICAL, you need to know about the main features described in this section.

Tokens

In a computer language, a token is defined as a character or characters that is taken by the language as a single "thing" or "unit." There are five classes of tokens in MAGICAL: identifiers, reserved words, constants, operators, and separators.

Identifiers

An identifier is the name of a command, macro, parameter, or variable, and is a sequence of letters, digits, and the characters _ \$ #. The underline _ counts as a letter. Upper and lower case letters are different. The first letter of identifiers, except temporary variable identifiers, must be a letter. Temporary variable identifiers start with the dollar-sign (\$) character. Identifiers can be any length (but be reasonable). Examples of identifiers are pcon, _pw, or \$height.

Reserved Words

The identifiers listed in Table 1 are reserved words and may not be used otherwise. Reserved words are recognized in both upper and lower case formats (e.g., do not use either and or AND except as a reserved word).

abort	endif	repeat	then	
abortoff	endwhile	return	until	
aborton	if	size	while	
and	mod	sqrt		
do	not	trunc		
else	or	typeof		

Table 1. Reserved Words in MAGICAL

Constants

Constants can be either floating or string.

- A floating constant consists of an integer part, a decimal point, a fractional part, the letter E (or e) and, optionally, a signed integer exponent. The integer and fraction parts both consist of a sequence of digits. Either the integer part or the fraction part (but not both) may be missing; similarly, either the decimal point, or the E and the exponent may be missing. Some examples are 1.37E–3, 4e5, .2E2, 1.4, 5.
- A string constant is a sequence of characters surrounded by single-quote characters ('...') or by backward single-quote characters ('...'). 'This is a string' and 'This is a string' are examples of string constants.

To include a single-quote character in a string, place a backslash character ($\)$ before the single-quote character, for example:

'This string isn\'t permissible without the backslash' To include a backslash character in the string, place another backslash before the backslash, such as

```
'This string includes the backslash \backslash \backslash '
```

Alternatively, the two styles of single quote characters can be used. If backward single quotes are used to delimit a string, then single quotes can be placed directly within the string, for example:

```
'This isn't a problem'
```

Or the single-quote styles can be exchanged, for example:

```
'This isn't a problem'
```

The single quote style that initiates the string must also terminate the string.

Operators

Table 2 lists the operators available in MAGICAL. Each operator is placed in a group, and groups are shown in order of precedence, with the highest group precedence first. Within each group, operator precedence in expressions is from left to right, except for the logical group, where the respective members are listed in order of precedence.

There are four "built-in" special operators:

- sqrt returns the square root of a real number.
- trunc truncates real numbers.

Group	Operation	Description	Example
special	sqrt()	square root	a = sqrt(b)
	trunc()	truncation	\$3 = trunc(3.6)
	typeof()	return argument type	if typeof('\$1') then
	size()	return argument size	r1 = size('d2')
unary	-	negative	a = -5
multiplicative	*	multiplication	a = 2 * c
	/	division	b = a / 2
	00	remainder	\$1 = 4 % 3
	mod	modulo	$\$3 = 7 \mod 4$
additive	+	addition	a = x + 4
	-	subtraction	b = y - sw
relational	<	less than	if a < b then
	>	greater than	if a > b then
	<=	less than or equal to	if a <= b then
	>=	greater than or equal to	if a >= b then
equality	=	equal to	if a = b then
	<>	not equal to	if a <> b then
logical	not	negation	if not (a=b) then
	and	logical and	if r1 and r2 then
	or	logical inclusive or	if (r1=2) or (r2=4) then
assignment	=	equal	a = 3

Table 2. Order of Operator Precedence (Highest First) in M	MAGICAL
--	---------

- typeof returns an identifier (0 or 1) for the type (real or string) of an argument.
- size returns the number of elements in an arrayed parameter.

The unary, multiplicative, and additive operators apply only to real variables. The + (addition) operator can also be used with string variables to concatenate two strings together. The mathematical operators can not be used with mixed variable types.

If the variable is an array, the mathematical operators try to do simple matrix arithmetic. If two matrices of the same size are equated, added, subtracted, multiplied, divided, or one matrix is taken as a modulus, each element of the first matrix is operated on with the corresponding element of the second. If two matrices of the same size are compared with an and operator, the resulting Boolean is the AND of each individual element. If two matrices of the same size are ORed together, the resulting Boolean is the OR of each individual element. If the two matrices have unequal sizes, an error results.

An arrayed variable *cannot* be operated on (added, multiplied, etc.) by a single-valued constant or variable. For example, if pw is an array of five values, pw=2*pw does *not* double the value of each element of the array.

Separators and Comments

Blanks, tabs, new lines, and comments serve to separate tokens and are otherwise ignored. Characters between double quote marks ("...") are comments, except when the double quotes are in a literal string, such as 'The word "and" is a reserved word '. Comments can appear anywhere— at the beginning, middle, or end of a line—but may not span multiple lines. At the end of a comment place a second double quote; otherwise, the comment is automatically terminated when the end of a line occurs.

Variable Types

As with many programming languages, MAGICAL provides two classes of variables:

- Global variables (also called external) that retain their values on a permanent or semipermanent basis.
- Local variables (also called temporary and automatic) that are created for the time it takes to execute the macro in question, after which the variables no longer exist.

Global and local variables can be of two types: real and string. Global real variables are stored as double-precision (64-bit) floating point numbers. The real(variable) command creates a real variable without a value, where variable is the name of the variable to be created.

Although global real variables have potential limits from 1e308 to 1e-308, when such variables are created, they are given default maximum and minimum values of 1e18 and -1e18; these can subsequently be changed with the setlimit command. For example, setlimit('r1', 1e99, -1e99, 0) sets variable r1 to limits of 1e99 and -1e99. Local real variables have limits slightly less than 1e18 (9.999999843067e17, to be precise) and cannot be changed.

String variables can have any number of characters, including a null string that has no characters. The command string(variable), where variable is the name of the variable to be created, creates a string variable without a value.

Both real and string variables can have either a single value or a series of values (also called an array).

Global and local variables have the following set of attributes associated with them:

name	group	array size
basictype	display group	enumeration
subtype	max./min. values	protection status
active	step size	

The variable's attributes are used by programs when manipulating variables.

Global Variables

The most important global variables used in macros are the VNMR parameters themselves. Thus parameters like vs (vertical scale), nt (number of transients), at (acquisition time), etc., can be used in a MAGICAL macro. Like any variable, they can be used on the left side of an equation (and hence their value changed) or they can be used on the right side of an equation (as part of a calculation, perhaps to set another parameter).

The real-value parameters r1, r2, r3, r4, r5, r6, and r7, and the string parameter n1, n2, and n3 are not NMR variables but can be used by macros. In using these parameters, it is important to remember that they are experiment-based parameters. If you are in expl and a macro changes experiments by using the command jexp3, for example, a new set of such parameters appears. Similarly, recalling parameters or data with the rt or rtp commands overwrites the current values of these parameters, just as it overwrites the values of all other parameters.

Within a single experiment, and assuming that the rt and rtp commands are not used, however, these parameters do act like global parameters in that all macros can read or write information into these parameters, and hence information can be passed from one macro to another in this way. They thus provide a useful place to store information that must be retained for some time or must be accessed by more than one macro—be sure that some other macro does not change the value of this variable in the meantime!

Local Variables

Any number of local variables can be created within a macro. These temporary variables are distinguished by beginning with the dollar-sign (\$) character, such as \$number and \$peakht. The type of variable (real or string) is decided by the first usage—there is no variable declaration, as in many languages. Therefore, setting, \$number=5 and \$select='all' establishes \$number as a real variable and \$select as a string variable.

A special initialization is required in one situation. When the first use of a string variable is as the return argument from a procedure, it must be initialized first by setting it to a null string. For example, a line such as

```
input('Input Your Name: '):$name
```

produces an error. Use instead
\$name=' ' input('Input Your Name: '):\$name.

By definition, local variables are lost upon completion of the macro. Furthermore, they are completely local, which means that each macro, even a macro that is being run by another macro, has its own set of variables. If one macro sets \$number=5 and then runs another macro that sets \$number=10, when the second macro completes operation and the execution of commands returns to the first macro, \$number equals 5, not 10. If the first macro is run again at a later time, \$number starts with an undefined value. It is good practice to use local variables whenever possible.

Local variables can also be created on the command input line. These variables are automatically created but are not deleted, and hence this is not a recommended practice; use r1, r2, etc., instead.

Accessing a variable that does not exist displays the error message: Variable "variable_name" doesn't exist.

Arrays

Both global and local variables, whether real or string, can be arrayed. Array elements are referred to by square brackets ([...]), such as pw[1]. Indices for the array can be fixed numbers (pw[3]), global variables (pw[r1]), or local variables (pw[\$i]). Of course, the index must not exceed the size of the array. You can use the size operator to determine the array size. For example, the statement r1=size('d2') sets r1 to number of elements in variable d2. If the variable has only a single value, size returns a 1; if the variable doesn't exist, it returns a 0.

Some arrays, such as a pulse width array, are user-created by keyboard entry. Other arrays, such as llfrq and llamp, are created by the software (in this case when a line list is performed). In both these cases, a macro can refer to any existing element of the array, pw[4] or llfrq[5], for example.

A MAGICAL macro can also create local variables containing arrayed information by itself. No dimensioning statement is required; the variable just expands as necessary. The only constraint is that the array must be created in order: element 1 is first, element 2

second, and so on. The following example shows how an array might be created and all values initialized to 0:

```
$i=1
repeat
    $newarray[$i]=0
    $i=$i+1
until $1>10
```

Arrays of string variables are identical in every way to arrays of real variables, except that the values are strings. If, for example, a user has entered dm='nny', 'yyy', the following macro plots each spectrum with the proper label:

```
$i=1
repeat
select($i)
pl
write('plotter',0,wc2max-10,'Decoupler mode: %s',dm[$i])
page
$i=$i+1
until $i>size('dm')
```

Accessing an array element that does not exist displays the error message: variable_name["index"] index out of bounds

Using a string as an index, rather than an integer, displays the error message: Index for variable_name['index'] must be numeric

or Index must be numeric

Finally, using an array as an index displays the error message: Index for variable_name must be numeric scalar

or

```
Index must be numeric scalar.
```

Expressions

An *expression* is a combination of variables, constants, and operators. Parentheses can be used to group together a combination of expressions. Multiple nesting of parentheses is allowed. In making expressions, combine only variables and constants of the same type:

- · Real variables and constants only with other real variables and constants.
- String variables and constants only with other string variables and constants.

The type of a local variable (a variable whose name begins with a \$) is determined by the context in which it is first used. The only ambiguity is when a local variable is first used as a return argument of a command such as input, as discussed in the previous section on local variables.

If an illegal combination is attempted, an error message is displayed: Can't assign STRING value "value" to REAL variable \ "variable_name" or Can't assign REAL value (value) to STRING variable \ "variable_name"

Mathematical Expressions

Expressions can be classified as mathematical or Boolean. Mathematical expressions can be used in place of simple numbers or parameters. Expressions can be used in parameter assignments, such as in pw=0.6*pw90, or as input arguments to commands or macros, such as in pa(-5+sc, 50+vp).

When parameters are changed as a result of expressions, the normal checks and limits on the entry of that particular parameter are followed. For example, if nt=7, the statement nt=0.5*nt will end with nt=3, just as directly entering nt=3.5 would have resulted in nt=3. Other examples of this include the round-off of fn entries to powers of two, limitation of various parameters to be positive only, etc.

Boolean Expressions

Boolean expressions have a value of either TRUE or FALSE. Booleans are represented internally as 0.0 for FALSE and 1.0 for TRUE, although in a Boolean expression any number other than zero is interpreted as TRUE. Boolean expressions can only compare quantities of the same type—real numbers with real numbers, or strings with strings. Some examples of Boolean expressions include pw=10, sw>=10000, at/2<0.05, and (pw<5) or (pw>10).

The explicit use of the words "TRUE" and "FALSE" is not allowed. All Boolean expressions are implicit—they are evaluated when used and given a value of TRUE or FALSE for the purpose of some decision.

Input Arguments

Arguments passed to a macro are referenced by \$n, where n is the argument number. An unlimited number of arguments (\$1, \$2, and so on) can be passed. The name of the macro itself may be accessed using the special name \$0. For example, if the macro test1 is running, \$0 is given the value test1. A second special variable \$# contains the number of arguments passed and can be used for routines having a variable number of arguments. Arguments can be either real or string types, as with all parameters.

```
An example of using an input arguments such as $1:
"vsmult(multiplier)"
"Multiply vertical scale (vs) by input argument"
vs=$1*vs
```

Another example, which uses two input arguments:

```
"offset(arg1,arg2)"
"Increment vertical position (vp) and horizontal position (sc)"
vp=$1+vp
sc=$2+sc
```

The typeof operator returns a zero (FALSE) if the variable is real or does not exist, and returns a non-zero (TRUE) if the variable is a string. For example, in the conditional statement if typeof('\$1') then ..., the then part is executed only if \$1 is a string.

Name Replacement

An identifier surrounded by curly braces $(\{...\})$ results in the identifier being replaced by its value before the full expression is evaluated. If the name replacement is on the left side of the equal sign, the new name is assigned a value. If the name replacement is on the right

side of the equal sign, the value of the new name is used. The following are examples of name replacement:

\$a = 'pw'	"variable \$a is set to string 'pw'"
{\$a} = 10.3	"pw is set to 10.3"
pw = 20.5	"pw is set to 20.5"
\$b = {\$a}	"variable \$b is set to 20.5"
{\$a}[2]=5	"pw[2] is set to 5.0"
\$b = {\$a}[2]	"variable \$b is set to 5.0"
<pre>\$cmd='wft'</pre>	"\$cmd is set to the string 'wft'"
{\$cmd}	"execute wft command"

The use of curly braces for command execution is subject to a number of constraints. In general, using the VNMR command exec for the purpose of executing an arbitrary command string is recommended. In this last example, this would be exec(\$cmd).

Conditional Statements

The following forms of conditional statements are allowed:

```
if booleanexpression then ... endif
if booleanexpression then ... else ... endif
```

Any number of statements (including none) can be inserted in place of the ellipses (...). If booleanexpression is TRUE, the then statements are executed; if booleanexpression is FALSE, the else statements (if any) are executed instead. Note that endif is required for both forms and that no other delimiters (such as BEGIN or END) are used, even when multiple statements are inserted. Nesting of if statements (the use of if statement as part of another if statement) is allowed, but be sure each if has a corresponding endif.

The following example uses a simple if ... then conditional statement:

```
"error --- Check for error conditions"
if (pw>100) or (d1>30) or ((tn='H1') and (dhp='y'))
    then write('line3','Problem with acquisition parameters')
endif
```

```
This example adds an else conditional statement:
"checkpw --- Check pulse width against predefined limits"
if pw<1
    then pw=1 write('line3','pw too small')
    else if pw>100
        then pw=100 write('line3','pw too large')
    endif
endif
```

Loops

Two types of loops are available. The while loop has the form: while booleanexpression do ... endwhile

This type of loop repeats the statements between do and endwhile, as long as booleanexpression is TRUE (if booleanexpression is FALSE from the start, the statements are not executed).

The other type of loop is the repeat loop, which has the form:

repeat ... until booleanexpression

This loop repeats statements between repeat and until, until booleanexpression becomes TRUE (if booleanexpression is TRUE at the start, the statements are executed once).

The essential difference between repeat and while loops is that the repeat type always performs the statements at least once, while the while type may never perform the statements. The following macro is an example of using the repeat loop:

```
"maxpk(first,last) -- Find tallest peak in a series of spectra"
$first=$1
repeat
   select($1) peak:$ht
   if $1=$first
      then $maxht=$ht
      else if $ht>$maxht then $maxht=$ht endif
   endif
   $1=$1+1
until $1>$2
```

Both types of loops are often preceded by n=1, then have a statement like n=n+1 inside the loop to increment some looping condition. Beware of endless loops!

Macro Length and Termination

Macros have no restriction on length. Execution of a macro is terminated when the command return is encountered. This is usually inserted into the macro after testing some condition, as shown in the example below:

```
"plotif--Plot a spectrum if tallest peak less than 200 mm" peak:$ht
```

if \$ht>200 then return else pl endif

The syntax return(expression1, expression2, ...) allows the macro to return values to another calling macro, just as do commands. This information is captured by the calling macro using the format :argument1, argument2, ... Here is an example of returning a value to the calling macro:

```
"abs(input):output -- Take absolute value of input"
if $1>0 then return($1) else return(-$1) endif
```

In nested macros, return terminates the currently operating macro, but not the macro that called the current macro.

To terminate the action of the calling macro (and all higher levels of nesting), the abort command is provided. abort can be made to act like return at any particular level by using the abortoff command. Consider the following sequence: abortoff macrol macro2

If macrol contains an abort command and it is executed, abort terminates macrol; however, macro2 still will be executed. If the macro sequence did not contain the abortoff statement, however, execution of an abort command in macrol would have prevented the operation of macro2. The aborton command nullifies the operation of abortoff and restores the normal functioning of abort.

Command and Macro Tracing

The commands debug('c') and debug('C') turn on and off, respectively, VNMR command and macro tracing. When tracing is on, a list of each executed command and

macro is displayed in the Terminal (in CDE) or Command Tool (in OpenWindows) window from which VNMR was started. Nesting of the calls is shown by indentation of the output. A return status of "returned" or "aborted" can help track down which macro or command failed.

If VNMR is started when the user logs in, or if it started from a drop-down menu or the CDE tool, the output goes to a Console window. If no Console window is present, the output goes into a file in the /var/tmp directory. This last option is not recommended.

1.3 Relevant VNMR Commands

Many VNMR commands are particularly well-suited for use with MAGICAL programming. This section lists some of those commands with their syntax (if the command uses arguments) and a short summary taken from the *VNMR Command and Parameter Reference*. Refer to that publication for more information. (Remember that string arguments must be enclosed in single quotes.)

Spectral Analysis Tools

dres	Measure linewidth and digital resolution
Syntax:	<pre>dres<(<frequency<,fractional_height>>)> \ :linewidth,resolution</frequency<,fractional_height></pre>
Description:	Analyzes line defined by current cursor position (cr) for linewidth and digital resolution. frequency overrides cr as the line frequency. fractional_height specifies the height at which linewidth is measured.
dsn	Measure signal-to-noise
Syntax:	dsn<(low_field,high_field)>:signal_to_noise,noise
Description:	Measures signal-to-noise of a spectrum. Noise region can be specified by supplying low_field and high_field frequencies, in Hz.
dsnmax	Calculate maximum signal-to-noise
Syntax:	dsnmax<(noise_region)>
Description:	Finds best signal-to-noise in a region. noise_region, in Hz, can be specified, or the cursor difference (delta) can be used by default.
getll	Get line frequency and intensity from line list
Syntax:	getll(line_number)<:height,frequency>
Description:	Returns the height and frequency of the specified line number.
getreg	Get frequency limits of a specified region
Syntax:	getreg(region_number)<:minimum,maximum>
Description:	Returns the minimum and maximum frequencies, in Hz, of the specified region number.

integ	Find largest integral in specified region
-------	---

Syntax: integ<(highfield,lowfield)><:size,value>

Description: Finds the largest absolute-value integral in the specified region or the total integral if no reset points are present between the specified limits. The default values for highfield and lowfield are parameters sp and sp+wp, respectively.

mark	Determine intensity of the spectrum at a point
Syntax:	<pre>mark<(fl_position)> mark<(left_edge,region_width)> mark<(fl_position,f2_position)> mark<(fl_start,fl_end,f2_start,f2_end)> mark<('trace',<options>)> mark('reset')</options></pre>
Description:	Functions similarly to the MARK button of ds and dconi. 1D or 2D operations can be performed in the cursor or box mode for a total of four separate functions. In the cursor mode, the intensity at a particular point is found. In the box mode, the integral over a region is calculated. For 2D operations, this is a volume integral. In addition, the mark command in the box mode finds the maximum intensity and the coordinate(s) of the maximum intensity.
nll	Find line frequencies and intensities
Syntax:	<pre>nll<('pos'<,noise_mult))><:number_lines></pre>
Description:	Returns the number of lines using the current threshold, but does not display or print the line list.
numreg	Return the number of regions in a spectrum
numreg Syntax:	Return the number of regions in a spectrum
_	Return the number of regions in a spectrum numreg:number_regions
Syntax:	Return the number of regions in a spectrum numreg:number_regions
Syntax: Description:	Return the number of regions in a spectrum numreg:number_regions Finds the number of regions in a previously divided spectrum. Find tallest peak in specified region
Syntax: Description: peak	Return the number of regions in a spectrum numreg:number_regions Finds the number of regions in a previously divided spectrum. Find tallest peak in specified region
Syntax: Description: peak Syntax:	Return the number of regions in a spectrum numreg:number_regions Finds the number of regions in a previously divided spectrum. Find tallest peak in specified region peak<(min_frequency,max_frequency)><:height,freq> Finds the height and frequency of the tallest peak in the selected region. min_frequency and max_frequency are the frequency limits, in Hz, of
Syntax: Description: peak Syntax: Description:	Return the number of regions in a spectrum numreg:number_regions Finds the number of regions in a previously divided spectrum. Find tallest peak in specified region peak<(min_frequency,max_frequency)><:height,freq> Finds the height and frequency of the tallest peak in the selected region. min_frequency and max_frequency are the frequency limits, in Hz, of the region to be searched; default values are the parameters sp and sp+wp. Select a spectrum or 2D plane without displaying it

Input/Output Tools

apa	Plot parameters automatically
Description:	Selects the appropriate command on different devices to plot the parameter list.
banner	Display message with large characters
Syntax:	<pre>banner(message<,color><,font>)</pre>
Description:	Displays the text given by message as large-size characters on the VNMR graphics windows.
clear	Clear a window
Syntax:	<pre>clear<(window_number)></pre>
Description:	Clears window given by window_number on the Sun or GraphOn terminal. With no argument, clears the text screen.
confirm	Confirm message using the mouse
Syntax:	confirm(message):\$response
Description:	Displays dialog box with message and two buttons: Confirm and Cancel. response is 1 if the user clicks the mouse on Confirm; response is 0 if the user clicks the mouse on Cancel.
echo	Display strings and parameter values in text window
Syntax:	echo<(<'-n',>string1,string2,)>
Description:	Functionally similar to the UNIX echo command. Arguments to VNMR echo can be strings or parameter values, such as pw. The $-n'$ option suppresses advancing to the next line.
flip	Flip between graphics and text window
Syntax:	<pre>flip<('graphics' 'text' \ <,'off' 'on' 'autooff' 'autoon'>)></pre>
Description:	Brings the graphics or text window to the top of the screen. It also controls whether parameter changes or commands that write to a window cause a window to appear.
format	Format a real number or convert a string for output
Syntax:	format(real_number,length,precision):string_var format(string,'upper' 'lower' 'isreal'):return_var
Description:	Using first syntax, takes a real number and formats it into a string with the given length and precision. Using second syntax, converts a string variable into a string of characters, all upper case or all lowercase, or tests the first argument to verify that it satisfies the rules for a real number (1 is returned if the first argument is a real number, otherwise a zero is returned).

input	Receive input from keyboard
Syntax:	<pre>input<(<prompt><,delimiter>)>:var1,var2,</prompt></pre>
Description:	Receives characters from the keyboard and stores them into one or more string variables. prompt is a string that is displayed on the command line. The default delimiter is a comma.
lookup	Look up and return words and lines from text file
Syntax:	<pre>lookup(options):return1,return2,,number_returned</pre>
Description:	Searches a text file for a word and returns to the user subsequent words or lines. options is one or more keywords ('file', 'seek', 'skip', 'read', 'readline', 'count', and 'delimiter') and other arguments.
nrecords	Determine number of lines in a file
Syntax:	nrecords(file):\$number_lines
Description:	Returns the number of "records," or lines, in the given file.
psgset	Set up parameters for various pulse sequences
Syntax:	<pre>psgset(file,param1,param2,,paramN)</pre>
Description:	Sets up parameters for various pulse sequences using information in a file from the user or system parlib.
vnmr_confirme	er Display a confirmer window (UNIX)
Syntax:	<pre>vnmr_confirmer message <label value="">\ <"-x"posx> <"-y"posy> <"-fn"name></label></pre>
Description:	Displays a confirmer window consisting of a message (a single-line multicharacter string) and one or more buttons. The default window location and font can be changed by the arguments posx, posy, and name. Each button has a unique label (a short string) and value (a number or string) that are set by arguments label and value. When the user clicks on one of the buttons, vnmr_confirmer returns a value. Because it is a UNIX command, vnmr_confirmer cannot be called directly from VNMR; it must be accessed using the VNMR shell command (e.g., shell ('vnmr_confirmer "This is a test" "Label 1" 1 "Label 2" 2 "Label 3" 3'):\$ret displays the message "This is a test" and makes three buttons available, returning 1, 2, or 3, respectively).
write	Write output to various devices
Syntax:	<pre>write('graphics' 'plotter'<,color pen> \ <,'reverse'>,x,y<,template>)<:height> write('alpha' 'printer' 'line3' 'error',template) write('reset' 'file',file<,template>)</pre>
Description:	

Regression and Curve Fitting

analyze	Generalized curve fitting
Syntax:	<pre>(Curve fitting) analyze('expfit', xarray<, options>) (Regression) analyze('expfit', 'regression'<, options>)</pre>
Description:	Provides an interface to the UNIX curve fitting program expfit, supplying input data in the form of the text file analyze.inp in the current experiment.
autoscale	Resume autoscaling after limits set by scalelimits
Description:	Returns to autoscaling in which the scale limits are determined by the expl command such that all the data in the expl input file is displayed.
expfit	Least-squares fit to exponential or polynomial curve (UNIX)
Syntax:	expfit options <analyze.inp>analyze.list</analyze.inp>
Description:	A UNIX command that takes a least-squares curve fitting to the data supplied in the file analyze.inp.
expl	Display exponential or polynomial curves
Syntax:	<pre>expl<(<options,>line1,line2,)></options,></pre>
Description:	Displays exponential curves resulting from T_1 , T_2 , or kinetic analyses. Also displays polynomial curves from diffusion or other types of analysis.
pexpl	Plot exponential or polynomial curves
Syntax:	<pre>pexpl<(<options><,line1,line2,)></options></pre>
Description:	Plots exponential curves from T_1 , T_2 , or kinetics analysis. Also plots polynomial curves from diffusion or other types of analysis.
poly0	Display mean of the data in the file regression.inp
Description:	Calculates and displays the mean of data in the file regression.inp.
rinput	Input data for a regression analysis
Description:	Formats data for regression analysis and places it into the file regression.inp.
scalelimits	Set limits for scales in regression
Syntax:	<pre>scalelimits(x_start,x_end,y_start,y_end)</pre>
Description:	Causes the command expl to use typed-in scale limits.

Mathematical Functions

abs	Find absolute value of a number
Syntax:	abs(number)<:value>
Description:	Finds absolute value of a number.
acos	Find arc cosine of a number
Syntax:	<pre>acos(number)<:value></pre>
Description:	Finds arc cosine of a number. The optional return value is in radians.
asin	Find arc sine of a number
Syntax:	asin(number)<:value>
Description:	Finds arc sine of a number. The optional return value is in radians.
atan	Find arc tangent of a number
Syntax:	atan(number)<:value>
Description:	Finds arc tangent of a number. The optional return value is in radians.
atan2	Find arc tangent of two numbers
Syntax:	atan2(y,x)<:value>
Description:	Finds arc tangent of y/x . The optional return argument value is in radians.
averag	Calculate average and standard deviation of input
Syntax:	<pre>averag(num1,num2,) \</pre>
Description:	Finds average, standard deviation, and other characteristics of a series of numbers.
cos	Find cosine value of an angle
Syntax:	-
5	Finds cosine of an angle given in radians.
exp	Find exponential value of a number
Syntax:	exp(number)<:value>
Description:	
ln	Find natural logarithm of a number
Syntax:	ln(number)<:value>
Description:	Finds natural logarithm of a number. To convert to base 10, use $log_{10}x = 0.43429 \ *ln(x)$.

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sin		Find sine value of an angle
	Syntax:	<pre>sin(angle)<:value></pre>
	Description:	Finds sine an angle given in radians.

tan	Find tangent value of an angle
Syntax:	tan(angle)<:value>
Description:	Finds tangent of an angle given in radians.

Creating, Modifying, and Displaying Macros

crcom	Create a user macro without using a text editor
Syntax:	<pre>crcom(file,actions)</pre>
Description:	Creates a user macro file in the user's macro directory. The actions string is the contents of the new macro.
delcom	Delete a user macro
Syntax:	delcom(file)
Description:	Deletes a user macro file in the user's macro directory. The actions string is the contents of the new macro.
hidecommand	Execute macro instead of command with same name
Syntax:	hidecommand(command_name)<:\$new_name> hidecommand('?')
Description:	Renames a built-in VNMR command so that a macro with the same name as the built-in command is executed instead of the built-in command. command_name is the name of the command to be renamed. '?' displays a list of renamed built-in commands.
macrocat	Display a user macro on the text window
Syntax:	<pre>macrocat(file1<,file2><,>)</pre>
Description:	Displays one or more user macro files, where file1, file2, are names of macros in the user macro directory.
macrocp	Copy a user macro file
Syntax:	<pre>macrocp(from_file,to_file)</pre>
Description:	Makes a copy of an existing user macro.
macrodir	List user macros
Description:	Lists names of user macros.
macroedit	Edit a user macro with user-selectable editor

Syntax: macroedit(file)

Description: Modifies an existing user macro or creates a new macro. To edit a system macro, copy it to a personal macro directory first.

macrold	Load a macro into memory
Syntax:	<pre>macrold(file)<:dummy></pre>
Description:	Loads a macro, user or system, into memory. If macro already exists in memory, it is overwritten by the new macro. Including a return value suppresses the message on line 3 that the macro is loaded.
macrorm	Remove a user macro
Syntax:	<pre>macrorm(file)</pre>
Description:	Removes a user macro from the user macro directory.
macrosyscat	Display a system macro on the text window
Syntax:	<pre>macrosyscat(file1<,file2><,>)</pre>
Description:	Displays one or more system macro files, where file1, file2, are names of macros in the system macro directory.
macrosyscp	Copy a system macro to become a user macro
Syntax:	<pre>macrosyscp(from_file,to_file)</pre>
Description:	Makes a copy of an existing system macro.
macrosysdir	List system macros
Description:	Lists names of system macros.
macrosysrm	Remove a system macro
Syntax:	macrosysrm(file)
Description:	Removes a system macro from the macro directory.
macrovi	Edit a user macro with vi text editor
Syntax:	macrovi(file)
Description:	Modifies an existing user macro or creates a new macro using the vi text editor. To edit a system macro, copy it to a personal macro directory first.
mstat	Display memory usage statistics
Syntax:	<pre>mstat<(program_id)></pre>
Description:	Displays memory usage statistics on macros loaded into memory.
purge	Remove a macro from memory
Syntax:	<pre>purge<(file)></pre>

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Description: Removes a macro from memory, freeing extra memory space. With no argument, removes all macros loaded into memory by macrold.

record Record keyboard entries as a macro

Syntax: record<(file 'off')>

Description: Records keyboard entries and stores the entries as a macro file in the user's maclib directory.

Miscellaneous Tools

axis	Provide axis labels and scaling factors
Syntax:	<pre>axis('fn' 'fn1' 'fn2')<:\$axis_label, \ \$frequency_scaling,\$factor></pre>
Description:	Returns axis labels, the divisor to convert from Hz to units defined by the axis parameter with any scaling, and a second scaling factor determined by any scalesw type of parameter. The parameter 'fn' 'fn1' 'fn2' describes the Fourier number for the axis.
beepoff	Turn beeper off
Description:	Turns beeper sound off. The default is beeper sound on.
beepon	Turn beeper on
Description:	Turns beeper sound on. The default is beeper sound on.
bootup	Macro executed automatically when VNMR is started
Syntax:	bootup<(foreground)>
Description:	Displays a message, runs a user login macro (if it exists), starts Acqstat and acqi (spectrometer only), and displays the menu system. bootup and login can be customized for each user (login is preferred because bootup is overridden when a new VNMR release is installed). foreground is 0 if VNMR is being run in foreground; non-zero otherwise.
exec	Execute a VNMR command
Syntax:	exec(command_string)
Description:	Takes as an argument a character string constructed from a macro and executes the VNMR command given by command_string.
exists	Determine if a parameter, file, or macro exists
Syntax:	exists(name,type):\$exists
Description:	Checks for the existence of a parameter, file, or macro with the given name. type is 'parameter', 'file', 'maclib', 'ascii', or 'directory'.

focus	Send keyboard focus to VNMR input window
Description:	Sends keyboard focus to the VNMR input window.
gap	Find gap in the current spectrum
Syntax:	gap(gap,height):found,powition,width
Description:	Looks for a gap between lines of the currently displayed spectrum, where gap is the width of the desired gap and height is the starting height. found is 1 is search is successful, or 0 if unsuccessful.
getfile	Get information about directories and files
Syntax:	getfile(directory,file_index):\$file,\$file_extension getfile(directory):\$number_files
Description:	If file_index is specified, the first return argument is the name of the file in the directory with the index file_index, excluding any extension, and the second return argument is the extension. If file_index is not specified, the return argument contains the number of files in the directory (dot files are not included in the count).
graphis	Return the current graphics display status
Syntax:	graphis(command):\$yes_no graphis:\$display_command
Description:	Determines what command currently controls the graphics window. If no argument is supplied, the name of the currently controlling command is returned.
length	Determine length of a string
Syntax:	length(string):\$string_length
Description:	Determines the length in characters of the given string.
listenoff	Disable receipt of messages from send2Vnmr
Description:	Deletes file \$vnmruser/.talk, disallowing UNIX command send2Vnmr to send commands to VNMR.
listenon	Enable receipt of messages from send2Vnmr
Description:	Writes files with VNMR port number that UNIX command send2Vnmr needs to talk to VNMR. The command then to send commands to VNMR is /vnmr/bin/send2Vnmr \$vnmruser/.talk command where command is any character string (commands, macros, or if statements) normally typed into the VNMR input window.
login	User macro executed automatically when VNMR activated
Description:	When VNMR starts, the bootup macro executes, and then, if the login macro exists, bootup executes the login macro. By creating and

Make a parameter inactive
Syntax: off(parameter|'n'<,tree>)

Description: Makes a parameter inactive. tree is 'current', 'global', 'processed', or 'systemglobal'.

Make a parameter active or test its state

off

on

customizing the login macro, a VNMR session can be tailored for an individual user. The login macro does not exist by default.

	•
Syntax:	on(parameter 'y'<,tree>)<:\$active>
Description:	Makes a parameter active or tests the active flag of a parameter. tree is 'current', 'global', 'processed', or 'systemglobal'.
readlk	Read current lock level
Syntax:	readlk<:lock_level>
Description:	Returns the same information as would be displayed on the digital lock display using the manual shimming window. It cannot be used during acquisition or manual shimming, but can be used to develop automatic shimming methods such as shimming via grid searching.
rtv	Retrieve individual parameters
Syntax:	<pre>rtv<(file,par1<,index1<,par2,index2>>)><:val></pre>
Description:	Retrieves one or more parameters from a parameter file to the experiment's current tree. If a return argument is added, rtv instead returns values to macro variables, which avoids creating additional parameters in the current tree. For arrayed parameters, array index arguments can specify which elements to return to the macro. The default is the first element.
shell	Start a UNIX shell
Syntax:	<pre>shell<(command)>:\$file1,\$file2,</pre>
Description:	If no argument is given, brings up a normal UNIX shell. If a UNIX command entered as an argument, shell executes the command. The text lines usually displayed as a result of the UNIX command given in the argument can be returned to \$file1, \$file2, etc.

solppm Return ppm and peak width of solvent resonances

Syntax: solppm:chemical_shift,peak_width

Description: Returns information about the chemical shift in ppm and peak spread of solvent resonances in various solvents for either ¹H or ¹³C, depending on the observe nucleus tn and the solvent parameter solvent. This macro is used "internally" by other macros only.

substr	Select a substring from a string
Syntax:	substr(string,word_number):substring substr(string,index,length):substring
Description:	Picks a substring out of a string. If two arguments are given, substring returns the word_number word in string. If three arguments, it returns a substring from string where index is the number of the character at which to begin and length is the length of the substring.
textis	Return the current text display status
Syntax:	textis(command):\$yes_no textis:\$display_command
Description:	Determines what command currently controls the text window. If no argument is supplied, the name of the currently controlling command is returned.
unit	Define conversion units
Syntax:	<pre>unit<(suffix,label,m<,tree><,'mult' 'div'>, \ b<,tree><,'add' 'sub'>)></pre>
Description:	Defines a linear relationship that can be used to enter parameters with units. The unit is applied as a suffix to the numerical value (e.g., 10k, 100p). suffix identifies the name for the unit (e.g., 'k'). label is the name to be displayed when the axis parameter is set to the value of the suffix (e.g., 'kHz'). m and b are the slope and intercept, respectively, of the linear relationship. A convenient place to put unit commands for all users is in the bootup macro.

Put private unit commands in a user's login macro.

1.4 Using Dialog Boxes from a Macro

A macro can pop up a dialog box for obtaining user input through the dialog command. This command has the following syntax: dialog(definition_file,output_file<,'nowait'>)

The definition_file argument is the name of the definition file (specified as an absolute path) that specifies the layout of the dialog box. The syntax of this file is the same as the .def files for *GLIDE* discussed in the manual *Walkup NMR Using GLIDE*. Normally this file is stored in \$vnmruser/dialoglib or \$vnmrsystem/dialoglib. Note, however, that dialog does not follow the VNMR standard of first looking for a file in \$vnmruser and then in \$vnmrsystem.

The output_file argument is a text output file as specified in the definition file. A good place for the output file is in /tmp. After the user answers the prompts and clicks the OK button, the answers are written to this output file. The macro can then use the command lookup to read the results.

Existing macros can be written to take advantage of the pop up dialog box. Listing 1 is the array macro, rewritten using dialog. Note the following in this macro:

- Lines 1–7 are comments explaining what the macro does.
- Line 8 checks if none (interactive) or all arguments are supplied (non-interactive). If only part of the arguments are supplied, an error message (Lines 9–11) is displayed.
- Line 12 forces \$par to a string type.

Listing 1. The array Macro, Rewritten Using the dialog Command

```
2: " array - macro for easy setup of arrays
 4: " usage: array
                    interactive mode
 5: "array(parameter_name,steps,start,stsize) "
 6: "
           optional fifth argument avoids da "
 7:
 8: if (\$\# > 1) and (\$\# < 4) then
 9: write('error','usage: array<(parameter_name<,steps, \
          start,stepsize>)>')
10: return(1)
11: endif
12: $par = `'
13: exists('/tmp/array','file'):$e
14: if ($e > 0) then
     shell('rm /tmp/array')
15:
16: endif
17: dialog(userdir+'/dialoglib/array','/tmp/array')
18: exists('/tmp/array','file'):$e
19: if (\$e = 0) then
20: return
21: endif
22: lookup(`file','/tmp/array')
23: lookup(`readline'):$par
24: lookup(`readline'):$steps
25: lookup(`readline'):$start
26: lookup('readline'):$delta
27:
28:
29: gain='y'
30: $count=0
31: repeat
32: {$par}[$count+1] = $start + $count*$delta
33:
     $count = $count+1
34: until $count>=$steps
35: if ($# <> 5) then
36:
     da
37: endif
```

Lines 13–16 checks if the output file /tmp/array exists, and if so, deletes it. Next, the dialog command is called (Line 17), which pops up the dialog box, as shown in Figure 1.

The dialog command
waits for the user to click
the OK or Cancel button.

OK executes the SAVE

Ĩ	rai alletei .		
	Size:		
	Start:		
	Step:		
Ir			
	OK)	(Cancel)	(Help)

Figure 1. Dialog Box for array Macro

command; that is, dialog saves the output to the output file, and then CLOSE closes the dialog box.

Cancel closes the dialog box without creating the output file.

• Lines 18–21 check if the output file exists.

If Cancel was clicked, the output file does not exist and return is executed (this is why it was deleted in lines 12–16).

If OK was clicked, the output file can be read by the lookup macro, as is done in lines 22–26.

• The remainder of the macro stores the values into the array.

Listing 2 is the definition file, in this case \$vnmruser/dialoglib/array.

Listing 2. Definition File for dialog Version of array Macro

```
ł
 label: Parameter:
 input:
output:
                $input
cols:
         30
remark: Enter the name of the parameter
}
 label: Size:
 input:
 output: $input
 cols:
           30
 remark: Enter the number of steps in the array
}
ł
  label: Start:
  input:
 output: $input
 cols:
           30
 remark: Enter the first value in the array
}
{
 label: Step:
 input:
 cols:
           30
 output: $input
 remark: Enter the increment for the array
}
{
  button(1): OK
   exec(1): SAVE CLOSE
  remark(1): Done with this window
  button(2): Cancel
   exec(2): CLOSE
   remark(2): Cancel this command
  button(3): Help
   rtoutput(3): man(`array')
   remark: Show help for array
}
```

Note that the dialog command runs until the OK button or Cancel button is clicked. VNMR is therefore busy, because the macro still executes. However, the man command, used with the rtoutput(3) on button(3) is executed before dialog returns. rtoutput provides a back door into VNMR.

1.5 Customizing the Menu System

Fully integrated into the VNMR software package are a series of user-programmable, menus. Accessible to the user at all times are two rows of menu buttons, selected by clicking the left mouse button on the relevant choice or by pressing the corresponding function key on the keyboard. The upper row of buttons, called the Permanent menu, contains functions that must be accessible to the user at all time. The next section describes how to customize the Permanent menu.

The lower row of buttons contains choices for a large number of different menus. These menus can make many operations easier and faster than using the command line. All menu buttons are user-programmable through menu files, which is covered below.

 Table 3 lists the commands and parameters connected with programming menus. The manual *Getting Started* covers menus from the user viewpoint.

Commands	
<pre>clear<(window_number)></pre>	Clear a window
glide	Toggle on and off the GLIDE interface
help	Display the current help file
<pre>menu<(menu_name 'off')></pre>	Change status of menu system
<pre>menuvi(menu_name)</pre>	Edit a menu with vi text editor
newmenu(menu)<\$current_menu>	Select menu without activation
Parameters	
helppath {absolute path}	Path to user's help directory
lastmenu {menu name}	Menu to display if Return clicked
menulibpath {absolute path}	Path to user's menu directory
<pre>mlabel {string}</pre>	Menu label
<pre>mstring {command string}</pre>	Menu string

 Table 3. Menu-Related Commands and Parameters

Customizing the Permanent Menu

The Permanent menu is the upper fixed row of buttons. This menu provides easy user access to the most important functions of the system:



The Permanent menu is fixed in the sense that the labels must be defined when VNMR starts; however, you can customize the labels and functions of the buttons by editing a text file. When VNMR is started, if the variable vnmrmenu is present in the UNIX environment, it is used as the path to the text file defining the menu buttons (you can display this environment by entering the command env from UNIX). For example, if the *GLIDE* option is installed, the vnmrmenu variable displayed by env is set to a file named vnmrmenu in the glide subdirectory.

If the vnmrmenu variable does not exist, the default text file defining the menu is still named vnmrmenu but is instead located in the VNMR system directory.

The definition text file is a list of up to eight button descriptions. Each menu button is defined with three fields:

- The first field is the word Function.
- The second is the action to be performed when that button is pressed. The available actions are the following:

abort	Abort acquisition
cancel	Cancel the current VNMR command
glide	Toggle the GLIDE interface
menu	Select the current menu
mainmenu	Select the main menu
flip	Hide and show the text window
resize	Toggle the graphics window between large and small size
help	Display help file for the current menu
exit	Exit from VNMR
usermacrol to usermacro8	Call user-defined macros usermacro1, usermacro2,usermacro8

• The third field, which starts one character after the second field and extends to the end of the line, is the label displayed for the button.

The default Permanent menu definition, found in the vnmrmenu file, includes the following definitions:

```
Function abort Abort Acq
Function cancel Cancel Cmd
Function menu Menu On
Function mainmenu Main Menu
Function help Help
Function flip Flip
Function resize Resize
```

Using one of the actions usermacrol to usermacro8 sets the name to the macro called. That macro then determines the action of the button. For example, to label the first button as Send Plot and make it the same as calling the page command, use the following definition in the vnmrmenu file:

Function usermacrol Send Plot

Then edit the macro usermacrol to contain the page command.

Customizing Menu Files and Help Files

The standard system menu files are stored in the directory /vnmr/menulib. For example, the file /vnmr/menulib/display_1D contains main choices for the 1D Data Display Menu. Most often a menu is activated by selecting a button on a menu that involves switching to another menu. Alternately, a menu can be activated by pressing on a function key associated with menu-switching button or by entering the menu command with the name of the menu as an argument. An example of using the menu command, would be entering menu('display_1D') to open the 1D Data Display Menu.

Every menu has associated with it a help file, stored in the /vnmr/help system directory with the same name as the menu itself. The help file for the current menu is displayed when the Help button in the upper menu is selected or the help command is entered. For

example, the file /vnmr/menulib/display_1D contains the main choices for the 1D Data Display Menu; the corresponding help file is found in /vnmr/help/display_1D.

Menu Files

Menu files are simple text files that can be examined or modified as desired (assuming appropriate permission). The menuvi command is available for editing a menu file using the UNIX vi editor. For example, entering menuvi('display_lD') opens for editing the text file for the 1D data display menu.

After editing, menu files can reside in several places. When the user selects a button that opens another menu (or if the menu command is entered with the name of a menu as an argument), VNMR looks for the menu file name in the following order:

- 1. In the user's menulib directory.
- 2. In the directory pointed to by the menulibpath parameter (if the menulibpath parameter is defined in the user's global parameter file). This parameter must contain an absolute path, not a relative path.
- 3. In the system menulib directory. If the file name is not found, the command interpreter displays an error message.

This order of search means that each user can have their own private menu directory menulib in their vnmrsys directory. User menus take precedence over the system menus if a menu of the same name exists is in both directories. This allows users to modify each menu to their own needs without affecting the operation of other users. The system menu directory /vnmr/menulib can be changed by the system administrator only; however, changes to it are available to all users.

Menus are themselves a special form of macros. Specifically, menus are macros containing other macros. Invoking a menu macro sets up the menu bar in which each button is itself a macro. This combination of macros allows the entire system to be run using menus without limiting operation to just a "simplified" mode.

Help Files

Custom help files can be created to go with custom menus. The help file for a particular menu has the same name as the menu file. When a user clicks on the Help button or enters the help command, VNMR looks for the help file in the following order:

- 1. In the user's help directory. This directory is a subdirectory of the user's VNMR directory. A typical path is /home/vnmr1/vnmrsys/help.
- 2. In the directory pointed to by the helppath parameter (if the parameter helppath is defined in the user's global parameter file). This parameter must contain an absolute path, not a relative path.
- 3. In the system help directory. This directory is a subdirectory of the system VNMR directory. A typical path might be /vnmr/help.

The same as with menu files, each user can have their own private help files. A file in the user's help directory takes precedence over the system help directory. The system help directory can only be changed by the system administrator; however, changes to the help directory are available to all users.

Manual Files

A VNMR manual directory contains text files with information about VNMR commands, macros, and parameters. When a user enters the man command to look at a manual file (e.g., man('go')), VNMR looks for the manual directory in the following order:

- 1. In the user's manual directory. This directory is a subdirectory of the user's VNMR directory. A typical path is /home/vnmr1/vnmrsys/manual.
- 2. In the directory pointed to by the manualpath parameter (if the parameter is defined in the user's global parameter file). manualpath contains the absolute path to a user's directory of VNMR manual entries. This parameter must contain an absolute path, not a relative path.

To create manualpath, enter the following command:

create('manualpath','string','global')

3. In the system manual directory. This directory is a subdirectory of the system VNMR directory. A typical path is /vnmr/manual.

Each user can have private manual files. A file in the user's manual directory takes precedence over the system manual directory. The system manual directory can only be changed by the system administrator; however, changes to the manual directory are available to all users.

Controlling Menus

To turn on the menu system and display the current menu, enter the menu command with no arguments. menu('off') turns off the menu system. menu(menu_name) turns on the menu system and displays the menu menu_name (e.g., menu('workspace')).

To select a menu without immediate activation, enter newmenu(menu_name). This is most useful when selecting which menu will be active when an interactive command exits. For example, entering newmenu('manipulate_1D') ds causes the menu "manipulate_1D" to be displayed when the Return button in the ds menu is selected. The command newmenu:\$current_menu returns the name of the currently active menu to the string parameter current_menu.

The lastmenu parameter contains the name of the menu that displays when the Return button is selected

Programming Menus

An active menu consists of two arrayed string parameters, mlabel and mstring:

- mlabel[i] contains the label that is displayed on the ith button. The total length of all the displayed labels cannot exceed the width of the screen (80 characters).
- mstring[i] contains the text string that is executed when the ith button is selected.

The mstring text string is essentially identical to a macro, with three exceptions:

- No new lines (that is, carriage returns) should appear in the text string.
- As with all strings, single quotes in the text string must be replaced by reverse single quotes (`...`) or by the escape sequence backslash with single quote (\'...).
- The length for the text string is subject to a maximum. Of course, a menu string can simply contain the name of a macro, which is not subject to any limitation.

Listing 3 shows what a typical menu looks like (this menu is somewhat simplified from the actual system menu). In this menu, the first three lines is a comment with the name of the menu. Like regular macros, comments are indicated by double quotation marks ("...").

Listing	3.	Typical	Menu
---------	----	---------	------

```
mlabel=' '
mstring=' '
mlabel[1]='Plot'
  mstring[1]='pl'
mlabel[2]='Scale'
  mstring[2]='pscale'
if (plotter='HP7550A')or(plotter='HP7570A')
     or(plotter='HP7570A_C')or(plotter='HP7570A_D')
     or(plotter='HP7475A') then
mlabel[3]='HP Params'
  mstring[3]='hpa'
else
  mlabel[3]=' 'mstring[3]=' '
endif
mlabel[4]='Params'
 mstring[4]='ppa'
mlabel[5]='All Params'
  mstring[5]='pap'
mlabel[6]='Peaks'
  mstring[6]='ppf'
mlabel[7]='Page'
  mstring[7]='page menu(`display_1D`)'
mlabel[8]='Return'
  mstring[8]='menu(`display_1D`)'
```

In the first active line of the menu, mlabel and mstring are set to a null string. This removes any trace of the previously active menu. After that, a series of assignments are made for each of up to eight values of mlabel[i] and mstring[i].

The labels are just that, button labels, and hence can contain anything appropriate. The strings, on the other hand, are themselves macros to be executed later, and hence they must contain valid commands, parameters, macros, and other MAGICAL language statements. In Listing 3, strings 1 through 6 contain a single command. If one of these buttons is selected, the command is executed, and the same menu is reactivated. String 7, however, issues a page command and then a second command that changes to the "display_1D" menu. The assumption here is that several of the choices 1 through 6 may be made on a single plot, but that once choice 7 is made, the user is finished with this menu and wants to revert back to the "parent" menu.

Note the reverse quotation marks (`...`) in strings 7 and 8, which are converted to regular quotation marks when the string is executed.

The sample menu in Listing 4 illustrates additional features of menus.

Notice the new features in this menu:

- The clear command appears near the start of the file. Executing clear(2) clears the graphics window. Because this command is in the menu itself and not in any particular string, it is executed each time the menu is activated.
- A number of comments are included in addition to the title—these are perfectly permissible and are encouraged to make the statement action clearer.

Listing 4	. Typical	Menu	with	Additional	Features
-----------	-----------	------	------	------------	----------

```
mlabel='
mstring=' '
clear(2) "clear any spectrum from screen"
mlabel[1]='No WT'
  mstring[1]='sb='n' sbs='n' lb='n' gf='n' gfs='n' awc='n''
mlabel[2]='Resolve'
  mstring[2]='resolv(0.1,0.3,`noft`)'
mlabel[3]='Broaden'
  mstring[3]='lb=sw/(fn/2) "set to digital resolution"'
if (dmg='ph') then
  mlabel[4]='->AV' mstring[4]='av'
else
  mlabel[4]='->PH' mstring[4]='ph'
endif
mlabel[5]='FN: Small'
  mstring[5]='fn=np/4'
mlabel[6]='Normal'
  mstring[6]='fn=`n`'
mlabel[7]='Large'
  mstring[7]='fn=2*np'
mlabel[8]='Return'
  mstring[8]='menu(`process_1D`)'
```

• The label and action of button 4 depend on the value of a particular parameter, dmg. If the spectrum is in the phase-sensitive mode, button 4 displays the label ->AV; clicking on the button switches the spectrum to the absolute-value mode. If the spectrum is in the absolute-value mode, button 4 displays ->PH; clicking on it switches the spectrum to the phase-sensitive mode.

Menus are redisplayed after any choice is made from the menu, and also after any other action, such as entering a parameter. For this reason, menus can respond dynamically to changed conditions by displaying different choices or taking different actions in response to different situations.

Consider the menu in Listing 5 that allows the user to display the experiment library, join different experiments, and create and delete experiments.

Of course, we only want to allow experiments that exist to be joined. It is meaningless to join the current experiment. The macro that sets up the menu evaluates the current situation and prepares the menu accordingly. Note that if you select this menu (by selecting Workspace in the Main menu) and then create an experiment (with the Create New button), the menu changes immediately. Note also in this menu, the creation of menu strings is not by simple assignments but with string concatenation operations. Those interested in exploring the limits of creating complex macros should find this menu an interesting model.

User-Programmable Menus in Interactive Programs

Many of the various interactive programs that are part of VNMR, such as dconi and df, have user-programmable menus. Entering a command to start one of these programs displays a menu from the menulib directory: For example,

- dconi automatically brings up the menu dconi when started.
- df (or dfid) automatically brings up the menu dfid when started.

```
mlabel=' '
mstring=' '
mlabel[1]='Library'
mstring[1]='explib'
$x='' $v=''
jexp:$x
$i=2 $e=1 $firstfree='10'
repeat
  format($e,1,0):$y
  exists(userdir+'/exp'+$y,'file'):$expexists
  if NOT($expexists) and ($firstfree='10')
   then $firstfree=$y endif
 if $expexists AND ($y<>$x) then
   mlabel[$i]='Exp '+$y
   mstring[$i]='jexp'+$y+' menu(`main`)'
   $i=$i+1
 endif
 $e=$e+1
until ($i>7) or ($e>9)
if ($firstfree<>'10') AND ($i<8) then
  mlabel[$i]='Create New'
  mstring[$i]='cexp('+$firstfree+')'
  \dot{s}_{i=\dot{s}_{i+1}}
endif
mlabel[$i]='Delete'
mstring[$i]='input('Enter # of Experiment to Delete: '):$exp
  delexp($exp)'
```

Listing 5. Typical Menu with Dynamic Changes

- ds automatically brings up the menu ds_1 when started.
- inset automatically brings up the menu inset when started.

A user or system administrator wishing to change the opening menu displayed when one of these commands is executed must edit the menulib file listed above for the command. Similarly, all the menus available for each program can be modified. For further information, see "Programming Menus," page 55.

In order not to redraw the display after every menu selection, these menus generally involve special calls to the program in question. For example, entering ds('thresh') activates the display of a horizontal threshold on the ds display. For 1D displays (df, ds), any change in a display parameter (e.g., vs) causes the display to be updated, whereas for 2D displays (dconi) the display must be deliberately reactivated, either by dconi('restart'), which reactivates the display without redrawing it, or by dconi('again'), which redraws the display with any parameter changes in effect.

1.6 Customizing the Files Menus

The Files program in VNMR provides an interface with the UNIX file system. You can use the menus in the program to create, delete, copy, and rename files, or to select a data set or parameter set to load into your experiment. Because the Files program relies on the standard menu and help file mechanism, the special-purpose menus and help files reside in the same libraries as other menus and help files. The manual *Getting Started* covers the

standard Files program menus as seen by the user. In this section, we look at programming these menus.

Starting the Program

To start the Files program, take one of the following actions:

- Enter the files command in the VNMR input window.
- Click on the File button in the Main Menu.

By default, either action selects the menu files_main (also called the Files Main Menu) or the last active files menu. You can also call up a particular menu by entering the command files(file), where file is the file name of the menu. For example, entering files('files_main') calls up the Files Main Menu.

Selecting and Accessing Files

At startup, the program reads the entries in the current directory and displays them on the screen. To select a file, click on each entry you want with the mouse. Each name is highlighted in reverse video to show it has been selected. You then click on the button with the desired function in the menu. To deselect a file name, click on the entry again.

Use the filesinfo command to access the list of selected files. This command expects at least one of the following input arguments:

- filesinfo('number') returns the number of selected files. If no files have been selected, it returns a value of 0.
- filesinfo('name'<, num>) returns the names of the selected files. If you have selected more than one file, all their names are returned, each separated with a space from its neighboring names in the list. An optional second argument lets you return an individual file name. This argument is a number giving the position in the list of the file names to return.
- filesinfo('redisplay') displays again the files in the current directory. Use the filesinfo command with this argument whenever a change occurs in the file system, for example, a file is deleted or created.

Using the Files Program with the Menu System

To better understand how the filesinfo command interacts with MAGICAL programming, consider how the Display button might work. We will use the cat command to display the file.

The first requirement is to limit the number of selected files to 1, because additional steps would be necessary to distinguish between the different files if more than one file is selected (later we will show how to work with more than one file). A first attempt might be as follows:

```
filesinfo('number'):$f
$n=' '
if ($f = 1) then
    filesinfo('name'):$n
    cat($n)
else
    write('error','You must select one element')
    abort
endif
```

This becomes the text of a macro that the menu arranges to have executed when the Display button is pressed. But suppose the user selected a directory or a compiled binary program file. Neither is really suitable for display. Fortunately the exists command has options to determine if a file is a directory or a text file.

The test for a directory is to include the statement exists(\$n, 'directory'): \$e and display an error message if the return argument \$e is nonzero. To test for an ASCII file, include exists(\$n, 'ascii'): \$e and display an error message if \$e is zero. Files that make it through the macro without an error message can be considered suitable for display. So our second version might be the following:

```
filesinfo('number'):$f
$n=' '
if (\$f = 1) then
    filesinfo('name'):$n
    exists($n,'directory'):$e
    if ($e <> 0) then
        write('error','
                          \backslash
        %s is a directory and cannot be displayed', $n)
        abort
    endif
    exists($n,'ascii'):$e
    if (\$e = 0) then
        write('error','%s is not an ASCII file',$n)
        abort
    endif
    cat($n)
else
    write('error','You must select one element')
    abort
endif
```

Now we would like to display the text file in that directory if it turns out that if the user selected a FID or an experiment directory. Programming this extra capability is simple: filesinfo('number'):\$f

```
$n=' '
if (\$f = 1) then
    filesinfo('name'):$n
    exists($n,'directory'):$e
    if ($e <> 0) then
        exists($n+'/text','file'):$e
        if ($e <> 0) then
        cat($n+'/text')
        else
        write('error', \
        '%s is a directory and cannot be displayed',$n)
        abort
    endif
    exists($n,'ascii'):$e
    if (\$e = 0) then
    write('error','%s is not an ASCII file',$n)
        abort
    endif
    cat($n)
else
    write('error','You must select one element')
    abort
endif
```

Notice in each case the macro first establishes that the user selected exactly one file and then obtains that file name. Each successive example shows how one can program more operations using the file name.

Several files can be displayed by selecting individual file names with filesinfo. To avoid obscuring the macro's structure, we shall return to the original function of just displaying the selected files, not checking for directories or non-ASCII files:

```
filesinfo('number'):$f
if ($f < 1) then
    write('error','You must select one element')
    abort
endif
$i=1
repeat
    filesinfo('name',$i):$n
    write('alpha','Contents of %s:',$n)
    cat($n)
    write('alpha','')
    $i=$i+1
until ($i >= $f)
```

To illustrate using the 'redisplay' keyword argument, we show how one might program a Delete button. Again we limit the user to deleting one file at a time.

```
filesinfo('number'):$f
$n=' '
if ($f = 1) then
    filesinfo('name'):$n
    delete($n)
    filesinfo('redisplay')
else
    write('error','You must select one element')
    abort
endif
```

Once the macro deletes the selected file, it displays again the files in the current directory using filesinfo('redisplay').

Chapter 1. MAGICAL II Programming

Chapter 2. Pulse Sequence Programming

Sections in this chapter:

- 2.1 "Programming Pulse Sequences from Menus," this page
- 2.2 "Overview of Pulse Sequence Programming," page 69
- 2.3 "Spectrometer Control," page 79
- 2.4 "Pulse Sequence Statements: Phase and Sequence Control," page 98
- 2.5 "Real-Time AP Tables," page 104
- 2.6 "Accessing Parameters," page 110
- 2.7 "Using Interactive Parameter Adjustment," page 120
- 2.8 "Hardware Looping and Explicit Acquisition," page 125
- 2.9 "Pulse Sequence Synchronization," page 131
- 2.10 "Pulse Shaping," page 131
- 2.11 "Shaped Pulses Using Attenuators," page 138
- 2.12 "Internal Hardware Delays," page 142
- 2.13 "Indirect Detection on Fixed-Frequency Channel," page 146
- 2.14 "Multidimensional NMR," page 148
- 2.15 "Gradient Control for PFG and Imaging," page 150
- 2.16 "Programming the Performa XYZ PFG Module," page 153
- 2.17 "Imaging-Related Statements," page 155
- 2.18 "User-Customized Pulse Sequence Generation," page 157

Programming pulse sequences on VNMR-based spectrometer systems is a process called pulse sequence generation (PSG). To simplify this process, the software includes a menudriven mode for writing new pulse sequences. This mode allows generation of the most common pulse sequences and presents a useful starting point, even for those users who wish to make use of pulse sequence features not accessible from the menus. The chapter starts, therefore, by describing this simplified mode of pulse sequence programming.

2.1 Programming Pulse Sequences from Menus

One way to begin is by making a diagram of the pulse sequence you want to program, then adding to the diagram the names of the parameters that describe the pulses and delays shown. Also, write down the phase cycling to be used. Finally, decide the points in the pulse sequence at which the status needs to change (see the manual *Getting Started* for a discussion of the status concept). With this information, you can quickly program the pulse sequence using the menu system.

For example, Figure 2 displays the diagram for a homonuclear-2D-J pulse sequence (A, B, and C represent the status).

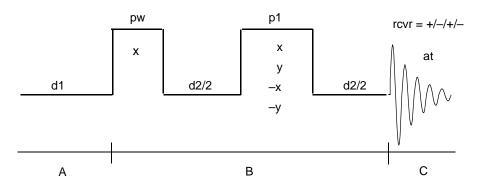


Figure 2. Homonuclear-2D-J Pulse Sequence

Here are the steps to program this sequence:

- 1. In the Permanent menu (the top row of buttons), click on Main Menu.
- 2. Click on More > Write Pulse Sequence > Start.

You are now in the Pulse Sequence Entry Main Menu with the prompt: Enter a Name for the Pulse Sequence:

3. Enter **hom2dj**.

A new prompt appears:

Enter Basic Phase Cycle Length (without additional phase cycling):

4. Because HOM2DJ has a basic phase cycle that is four transients long, enter 4.

This action produces a total phase cycle 16 transients long, 4 for the basic cycle, with the whole cycle repeated 4 times in successively incremented phases.

You are now ready to start programming the sequence. Start with status A. Select a delay d1 with homospoil. Adding homospoil means that a homospoil pulse can occur at the start of this delay, depending on your choice of parameters when the experiment is run.

5. Click on Status > A > Delay > Allow Homospoil > D1

If you are using a *GEMINI 2000* system, no homospoil is possible; however, you can enter homospoil-related statements and parameters without an error occurring.

Next, consider status B. Looking at Figure 2, we see that in status B we want the following elements: (1) a pulse of phase x and length pw, (2) a delay d2/2 (because this experiment has a split evolution time), (3) a pulse of length p1 whose phase cycles 0, 3, 2, 1 during the course of four transients, and (4) another d2/2 delay.

 Click on Status > B > Pulse > X > PW > Delay > D2/2. Then click on Pulse > More > 0321 > P1 > Delay >D2/2.

In status C, we need only one action-to select alternating receiver phase.

- 7. Click on Status > C > Status > Set Rcvr Phase > +-+-.
- 8. The programming is finished. Click on **Finish**.

This closes the pulse sequence file and compiles the pulse sequence. Some messages appear in the text window, and then the output is saved in the user pulse sequence directory.

If you have followed this procedure correctly, a homonuclear-2D-J pulse sequence is now ready to use. You can view it graphically by entering dps in the input window. Notice that you have just used a few keystrokes and the mouse to write a complete computer program in the C language!

Pulse Sequence Programming Menus

By clicking the buttons Main Menu -> More -> Write Pulse Sequence, many pulse sequence entry menus are available on your system to help you program pulse sequences, including the following menus:

Pulse Sequence Entry Main Menu

Start Delay Pulse DecPulse Status Other Finish Show Seq.

Pulse Sequence Entry Delay Menu



Pulse Sequence Entry Phases Menu

SELECT PHASE: Use Previous X Y -X -Y Fixed:0 +-+- More

Pulse Sequence Entry Phases Secondary Menu

3210 0321 0022 2200 Fixed:90 Fixed:180 Return

Pulse Sequence Entry Pulses Menu

PW	P1	2PW	2P1	Other	Return
----	----	-----	-----	--------------	--------

Pulse Sequence Entry Decoupler Pulses Menu

PP 2PP Other Return

Pulse Sequence Entry Status Menu



The only tricky part is that the Pulse Sequence Entry Pulses Menu and Pulse Sequence Entry Decoupler Pulses Menu are not directly accessible from the Main Menu. Instead, any time a pulse is called for, a phase menu appears for you to set phase, and *then* the appropriate pulse menu appears for you to set the pulse width. This occurs because the phase of the pulse must be known to the sequence before the pulse can occur.

In all menus, to make a selection, move the mouse arrow to the desired button on the screen and press the left mouse button. The center and right mouse buttons are inactive.

For information on the VNMR menu system in general, refer to the manual Getting Started.

The following sections describe the choices on the pulse sequence entry menus.

Pulse Sequence Entry Main Menu

The Pulse Sequence Entry Main Menu is typically entered by selecting Write Pulse Sequence in the Secondary Main Menu or by entering menu ('psg_main').

Button	Description
Start	Show prompts "Enter a Name for the Pulse Sequence:" and "Enter Basic Phase Cycle Length (without additional phase cycling):" and uses the information you enter to initialize a pulse sequence file in your pulse sequence directory (use Start button first and only once).
Delay	Display Pulse Sequence Entry Delay Menu (see below) to add a delay at this point of the sequence.
Pulse	Display Pulse Sequence Entry Phases Menu (page 67) to select the phase and add a pulse at this point of the sequence.
DecPulse	Display Pulse Sequence Entry Decoupler Pulses Menu (page 68) to select decoupler phase and add a decoupler pulse at this point of the sequence.
Status	Display the Sequence Entry Status Menu (page 68) to change the decoupler and receiver status at this point of the sequence.
Other	Show prompt "Enter Pulse Sequence Statement:" and use the information you enter.
Finish	Close the pulse sequence file and compile the pulse sequence, placing the output in the user pulse sequence directory.
Show Seq.	Display a listing of the pulse sequence in the text window.

Pulse Sequence Entry Delay Menu

The Pulse Sequence Entry Delay Menu is typically entered by selecting Delay in the Pulse Sequence Entry Main Menu or by entering menu('psg_delay'). After each button action is complete, the Pulse Sequences Entry Main Menu (see above) is displayed.

Button	Description
D1	Add delay d1 at this point in the sequence.
D2	Add delay $d2$ at this point in the sequence (automatically made the evolution time in 2D experiments).
D2/2	Add a delay $d2/2$ at this point in the sequence (for split evolution times in 2D experiments).
D3	Add delay d3 at this point in the sequence.
MIX	Add a delay mix at this point in the sequence.
Other	Show prompt "Input Name of Delay:" and add the name you enter as a delay at this point in the sequence.
Allow Homospoil	Make the delay that follows start with a homospoil pulse of length hst. (You must use this button before selecting buttons 1 through 6 if that delay is to have a homospoil pulse.) Note that homospoil is not possible on the <i>GEMINI 2000</i> .
Return	Display Pulse Sequence Entry Main Menu (page 66) without adding a delay at this point in the sequence.

Pulse Sequence Entry Phases Menu

The Pulse Sequence Entry Phases Menu is typically entered by selecting Pulse or DecPulse in the Pulse Sequence Entry Main Menu, by selecting Set Rcvr Phase in the Pulse Sequence Entry Status Menu, or by entering menu ('psg_phase'). For buttons 1 to 7, the Pulse Sequence Entry Pulses Menu (page 67), the Pulse Sequence Entry Decoupler Pulses Menu (page 68), or the Pulse Sequences Entry Main Menu is displayed (page 66), as appropriate.

Button	Description	
SELECT PHASE: Use Previous		
	Use the phase of the previous pulse for this pulse as well.	
Х	Use a phase of X, which will have additional phase cycling automatically added to it. For example, if the phase cycle length has been set to be 2, the additional phase cycle will be 00112233 (or 0, 0, 90, 90, 180, 180, 270, 270) and an "X" pulse will have the same phase (00112233). This choice will be common if this menu is used to set receiver phase.	
Y	Use a phase of Y (see description of X).	
-X	Use a phase of –X (see description of X).	
-Y	Use a phase of –Y (see description of X).	
Fixed:0	Use a fixed phase of 0° that is not phase cycled.	
+-+-	Use phase alternation for this pulse. Phase cycling will be automatically added; the minimum phase cycle length that should have been selected for this to be meaningful is 2. For example, if the phase cycle length has been set to be 4, the additional phase cycle is 0000111122223333 and selecting this button will give a phase 0202131320203131.	
More	Display Pulse Sequence Entry Phases Secondary Menu (below) for more phase choices.	

Pulse Sequence Entry Phases Secondary Menu

The Pulse Sequence Entry Phases Menu is typically entered by selecting More in the Pulse Sequence Entry Phases Menu or by entering menu('psg_phase2'). For buttons 1 to 6, the Pulse Sequence Entry Pulses Menu (see below), the Pulse Sequence Entry Decoupler Pulses Menu (page 68), or the Pulse Sequences Entry Main Menu is displayed (page 66), as appropriate.

Button	Description
3210	Use a cycling phase 3, 2, 1, 0 (= 270, 180, 90, 0).
0321	Use a cycling phase 0, 3, 2, 1 (= 0, 270, 180, 90).
0022	Use a cycling phase 0, 0, 2, 2 (= 0, 0, 180, 180).
2200	Use a cycling phase 2, 2, 0, 0 (= 180, 180, 0, 0).
Fixed:90	Use a fixed phase of 90° that is not phase cycled.
Fixed:180	Use a fixed phase of 180° that is not phase cycled.
Return	Display Pulse Sequence Entry Phases Menu (page 67).

Pulse Sequence Entry Pulses Menu

The Pulse Sequence Entry Pulses Menu is typically entered by selecting a phase value in the Pulse Sequence Entry Phases Menu or in the Pulse Sequence Entry Phases Secondary Menu, or by entering menu('psg_pulse'). After each button action is complete, the Pulse Sequences Entry Main Menu (page 66) is displayed.

Button	Description
PW	Add a pulse pw at this point in the sequence.
P1	Add a pulse p1 at this point in the sequence
2PW	Add a pulse 2*pw at this point in the sequence.
2P1	Add a pulse 2*p1 at this point in the sequence.
Other	Show prompt "Input Name of Pulse:" and add name you enter as a pulse at this point in the sequence.
Return	Display Pulse Sequence Entry Main Menu (page 66) without adding a pulse at this point in the sequence.

Pulse Sequence Entry Decoupler Pulses Menu

The Pulse Sequence Entry Decoupler Menu is typically entered by selecting DecPulse in the Pulse Sequence Entry Main Menu or by menu('psg_decpulse'). After each button action is complete, the Pulse Sequences Entry Main Menu (page 66) is displayed.

Button	Description
РР	Add a decoupler pulse pp at this point in the sequence.
2PP	Add a decoupler pulse 2*pp at this point in the sequence.
Other	Show prompt "Input Name of Pulse:" and add the name you enter as a decoupler pulse at this point in the sequence.
Return	Display Pulse Sequence Entry Main Menu (page 66) without adding a decoupler pulse at this point in the sequence.

Pulse Sequence Entry Status Menu

The Pulse Sequence Entry Status Menu is typically entered by selecting Status in the Pulse Sequence Entry Main Menu or by entering menu('psg_status'). After each button action is complete, the Pulse Sequences Entry Main Menu (page 66) is displayed.

Button	Description
A	Change status of decoupler to "A" at this point in the sequence. This corresponds to the first letter of parameters dm (decoupler mode) and dmm (decoupler modulation mode). Thus, if $dm = 'yny'$, the decoupler will be turned on (because of the first 'y') during status "A".
В	Select status "B" at this point in the sequence.
С	Select status "C" at this point in the sequence.
D	Select status "D" at this point in the sequence.
RcvrOn	Turn receiver on at this point in the sequence.
RcvrOff	Turn receiver off at this point in the sequence.
Set Rcvr Phase	Display Pulse Sequences Entry Phases Menu (page 67) to set receiver phase different than default 0123 (= 0, 90, 180, 270).
Return	Display Pulse Sequence Entry Main Menu (page 66) without changing status at this point in the sequence.

2.2 Overview of Pulse Sequence Programming

Pulse sequences are written in C, a high-level programming language that allows considerable sophistication in the way pulse sequences are created and executed. New pulse sequences are added to the software by writing and compiling a short C procedure. This process is greatly simplified, however, and need not be thought of as programming if you prefer not to. As shown in the previous section, simple pulse sequences can be written completely using the menu system, without any knowledge of C programming. For example, the hom2dj pulse sequence that we "wrote" in the step-by-step example is a simple text file similar to Listing 6. We will return in a moment to the specifics of what is included in this text file.

Spectrometer Differences

This manual contains information on how to write pulse sequences for UNITY *INOVA*, *MERCURY-VX*, *MERCURY*, UNITY *plus*, *GEMINI 2000*, UNITY, and VXR-S spectrometers. Each class of spectrometer has different capabilities, so not all statements may be executed on all platforms.

For example, because *MERCURY-VX* hardware differs significantly from UNITY *INOVA* hardware, sections in this manual covering waveform generators and imaging are not applicable to the *MERCURY-VX* even though the pulse sequence programming language is the same. Pay careful attention to comments in the text regarding the system applicability of the pulse sequence statement or technique.

Pulse Sequence Generation Directory

Pulse sequence generation (PSG) text files (like hom2dj.c in Listing 6) are stored in a directory named psglib. There are many such psglib directories, including the system /vnmr/psglib directory and a psglib directory that belongs to each user.

Listing 6. Text File for hom2dj.c Pulse Sequence Listing

```
/* VARIAN VNMR MENU GENERATED PULSE SEQUENCE: hom2dj */
#include <standard.h>
pulsesequence()
{
    initval(4.0,v9); divn(ct,v9,v8);
    status(A);
    hsdelay(d1);
    status(B);
    add(zero,v8,v1); pulse(pw,v1);
    delay(d2/2.0);
    mod4(ct,v1); add(v1,v8,v1); pulse(p1,v1);
    delay(d2/2.0);
    status(C);
    mod2(ct,oph); dbl(oph,oph); add(oph,v8,oph);
}
```

The user psglib is stored in the user's private directory system (e.g., for user vnmr1, in /export/home/vnmr1/vnmrsys/psglib). All pulse sequence files stored in these directories are given the extension .c to indicate that the file contains C language source code. For instance, the homonuclear-2D-J sequence that you may have written as an

example was automatically stored in your private pulse sequence directory and thus has a name like /export/home/vnmr1/vnmrsys/psglib/hom2dj.c.

You may find that a pulse sequence you need is already available. Numerous sequences are in the standard Varian-supplied directory /vnmr/psglib and in the user library directory /vnmr/userlib/psglib, or you can program a sequence using the menu system or write a sequence using any of the standard text editors such as vi or textedit. Once a pulse sequence exists, it can subsequently be modified as desired, again using one of a number of text editors.

Compiling the New Pulse Sequence

After a pulse sequence is written, the source code is compiled by one of these methods:

- By clicking on the Finish button in the Pulse Sequence Entry Main Menu (only if the sequence was created using the VNMR menu system).
- By entering seqgen(file<.c>) within VNMR.
- By entering seqgen file<.c> from a UNIX shell.

For example, entering seqgen('hom2dj') compiles the hom2dj.c sequence in VNMR and entering seqgen hom2dj does the same in UNIX. Note that a full path, such as seqgen('/export/home/vnmr1/vnmrsys/psglib/hom2dj.c') or even seqgen('hom2dj.c') is not necessary or possible—the seqgen command knows where to look to find the source code file and knows that it will have a .c extension.

During compilation, the system performs the following steps:

- 1. If the program dps_ps_gen is present in /vnmr/bin, extensions are added to the pulse sequence to allow a graphical display of the sequence by entering the dps command. Statements dps_off, dps_on, dps_skip, and dps_show can be inserted in the pulse sequence to control the dps display.
- 2. The source code is passed through the UNIX program lint to check for variable consistency, correct usage of functions, and other program details.
- 3. The source code is converted into object code.
- 4. If the conversion is successful, the object code is combined with the necessary system psg object libraries (libparam.so and libpsglib.so), in a procedure called link loading, to produce the executable pulse sequence code. This is actually done at run-time. If compilation of the pulse sequence with the dps extensions fails, the pulse sequence is recompiled without the dps extensions.

If the executable pulse sequence code is successfully produced, it is stored in the user seqlib directory (e.g., /export/home/vnmr1/vnmrsys/seqlib). If the user does not have a seqlib directory, it is automatically created.

Like psglib, different seqlib directories exist, including the system directory and each user's directory. The user's vnmrsys directory should have directories psglib and seqlib. Whenever a user attempts to run a pulse sequence, the software looks first in the user's personal directory for a pulse sequence by that name, then in the system directory.

A number of sequences are supplied in /vnmr/seqlib, compiled and ready to use. The source code for each of these sequences is found in /vnmr/psglib. To compile one of these sequences, or to modify a sequence in /vnmr/psglib, copy the sequence into the user's psglib, make any desired modifications, then compile the sequence using seqgen. (seqgen will not compile sequences directly in /vnmr/psglib). All sequences in /vnmr/psglib have an appropriate macro to use them.

Troubleshooting the New Pulse Sequence

During the process of pulse sequence generation (PSG) with the seqgen command, the user-written C procedure is passed through a utility to identify incorrect C syntax or to hint at potential coding problems. If an error occurs, a number of messages usually are displayed. Somewhere among them are these statements: Pulse Sequence did not compile. The following errors can also be found in the file /home/vnmr1/vnmrsys/psglib/errmsg:

As a rule of thumb, focus on the lines in the errmsg text file that begin with the name of the pulse sequence enclosed in double quotes followed by the line number and those that begin with a line number in parentheses. In both cases, a brief description of the problem is also displayed. If the line of code looks correct, often the preceding line of code is the culprit. Note that a large number of error messages can be generated from the same coding error.

```
If a warning occurs, the following message appears:
Pulse Sequence did compile but may not function properly.
The following comments can also be found in the
file /home/vnmr1/vnmrsys/psglib/errmsg:
```

This message means that although the pulse sequence has some inconsistent C code that may produce run-time errors, the pulse sequence did compile. Three warnings to watch for are the following:

```
warning: conversion from long may lose accuracy
warning: parameter_name may be used before set
warning: parameter_name redefinition hides earlier one
```

The first warning may be generated by less than optimum usage of the ix variable: conversion from long may lose accuracy

An example can be found in a few of the earlier pulse sequences implementing TPPI. The following construct, which was taken from an older version of hmqc.c, generates the warning:

```
initval((double) ((int)((ix - 1) / (arraydim / ni) \
+1e-6)), v14);
```

avoids the warning and also provides for roundoff of the floating point expression to give proper TPPI phase increments.

Even the above expression can fail under some circumstances. That construction will not work for 3D and 4D experiments. With the availability of increment counters such as id2, id3, and id4, and the predefined phasel variable, this example can be rewritten as

```
if (phase1 == 3)
    assign(id2,v14);
```

The second warning generally suggests an uninitialized variable: parameter_name may be used before set

This should be corrected; otherwise, unpredictable execution of the pulse sequence is likely. A common cause is the use of a user variable without first using a getval or getstr statement on the variable.

The third warning generally suggests that a variable is defined within the pulse sequence that has the same name as one of the standard PSG variables. parameter_name redefinition hides earlier one

This warning is normally avoided by renaming the variable in the pulse sequence or, if the variable corresponds to a standard PSG variable, by removing the variable definition and initialization from the pulse sequence and just using the standard PSG variable. A list of the standard PSG variable names is given in "Accessing Parameters," page 110.

Finally, if the pulse sequence program is syntactically correct, the following message is displayed:

Done! Pulse sequence now ready to use.

Types of Acquisition Controller Boards

Hardware looping, timing, and other system capabilities are often determined by the type of acquisition controller board used on the system. The following list describes the types of acquisition controller boards used on Varian UNITY *INOVA*, UNITY *plus*, UNITY, and VXR-S systems. *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* controller boards are directly described.

- Data Acquisition Controller boards, Part No. 01-902010-00. Varian started shipping this board in mid-1995 with the introduction of the UNITY INOVA system.
- Pulse Sequence Controller boards, Part No. 00-992560-00. Varian started shipping this board in early 1993 with the introduction of the UNITYplus system.
- Acquisition Controller boards, Part No. 00-969204-00 or 00-990640-00. Varian started shipping 00-969204-00 in late 1988 as a replacement for the Output boards, and then 00-990640-00 replaced 00-969204-00 in mid-1990.
- Output boards, Part No. 00-953520-0#, where # is an integer. These boards were used on systems prior to 1988.

Creating a Parameter Table for Pulse Sequence Object Code

The ability to modify or customize acquisition parameters to fit a given user-created pulse sequence is provided by a small number of commands. These commands make it possible to perform the following operations on an existing parameter table:

- Create new parameters
- Control the display and enterability of parameters
- Control the limits of the parameter
- · Create a parameter table for two-dimensional experiments

The commands that enable the creation and modification of parameters are discussed in Chapter 5 of this manual.

C Framework for Pulse Sequences

Each pulse sequence is built onto a framework written in the C programming language. Look again at the hom2dj sequence in Listing 6. The absolutely essential elements of this framework are these:

```
#include <standard.h>
pulsesequence()
{
}
```

This framework must be included exactly as shown. Between the two curly braces $(\{\})$ are placed pulse sequence statements, each statement ending with a semicolon.

The majority of pulse sequence statements allow the user to control pulses, delays, frequencies, and all functions necessary to generate pulse sequences. Most are in the general form statement(argument1, argument2,...), where statement is the name of the particular pulse sequence statement, and argument1, argument2,... is the information needed by that statement in order to function.

Many of these arguments are listed as real number. Because of the flexibility of C, a realnumber argument can take three different forms: variable (e.g., d1), constant (e.g., 3.4, 20.0e-6), or expression (e.g., 2.0*pw, 1.0-d2).

Times, whether delays or pulses, are determined by the type of acquisition controller board used on the system (listed on page 72):

- On Data Acquisition Controller boards, times can be specified in increments as small as 12.5 ns with a minimum of 100 ns.
- On Acquisition Controller boards and Pulse Sequence Controller boards, times can be specified in increments as small as 25 ns with a minimum of 200 ns.
- On Output boards and the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*, times can be specified in increments as small as 0.1 μs. The smallest possible time interval in all other cases is 0.2 μs, or 0.

Any pulse widths or delays less than the minimum generate a warning message and are then eliminated internally from the sequence. (Note that time constants within a pulse sequence are always expressed in seconds.)

A series of internal, real-time variables named v1, v2, ..., v14 are provided to perform calculations in real-time (by the acquisition computer) while the pulse sequence is executing. Real-time variables are discussed in detail later in this chapter. For now, note that all of the phases, and a small number of the other arguments to the pulse sequence statements discussed here, must be real-time variables. A real-time variable must appear as a simple argument (e.g., v1), and *cannot* be replaced by anything else, including an integer, a real number, a "regular" variable such as d1, or an expression such as v1+v2.

Any variables you choose to use in writing a pulse sequence must be declared. Most variables will be of type double, while integers will be of type int, and strings, such as dmm, are of type char with dimension MAXSTR. Table 4 lists the length of these basic types on the Sun computer. Many variables that refer to parameters used in an experiment are already declared (see "Accessing Parameters," page 110).

Real-time variables are of type codeint (int on *MERCURY-VX* and UNITY*INOVA*, 32 bits), whose size is 16 bits—you will probably not be declaring new variables of this type. A framework including variable declarations of the main types might look like this: #include <standard.h>

```
pulsesequence()
{
   double delta; /* declare delta as double */
   char xpolar[MAXSTR]; /* declare xpolar as char */
...
}
```

Туре	Description	Length (bits)
char	character	8
short	short integer	16
int	integer	32
long	long integer	32
float	floating point	32
double	double-precision floating point	64

Table 4. Variable Types in Pulse Sequences

Implicit Acquisition

The hom2dj.c pulse sequence listing in Listing 6 on page 69 has one notable omission data acquisition. In most pulse sequences, the sequence of events consists of a series of pulses and delays, followed at the very end by the acquisition of an FID; the entire process is then repeated for the desired number of transients, and then again (for arrayed and nD experiments) for subsequent elements of the arrayed or nD experiment.

In all these cases, pulse sequences use *implicit acquisition*, that is, following the pulse sequence as written by the user, an FID is automatically (implicitly) acquired. This acquisition is preceded by a delay that combines the parameter alfa with a delay based on the type of filter and the filter bandwidth. In addition, the phase of all channels of the spectrometer (except the receiver) is set to zero at this time.

Some pulse sequences are not described by this simple model; many solids NMR sequences are in this category, for example. These sequences use explicit acquisition, in which the preacquisition and acquisition steps must be explicitly programmed by the user. This method is described further in "Hardware Looping and Explicit Acquisition," page 125. (Explicit acquisition is not available on the *MERCURY* and *GEMINI 2000*.)

Acquisition Status Codes

Whenever wbs, wnt, wexp, or werr processing occurs, the acquisition condition that initiated that processing is available from the parameter acqstatus. This acquisition condition is represented by two numbers, a "done" code and an "error" code. The done code is set in acqstatus[1] and the error code is set in acqstatus[2]. Macros can take different actions depending on the acquisition condition.

The done codes and error codes are listed in Table 5 and in the file acq_errors in / vnmr/manual. For example, a werr command could specify special processing if the maximum number of transients is accumulated. The appropriate test would be the following:

if (acqstatus[2] = 200) then
"do special processing, e.g. dp='y' au"
endif

These codes apply to all systems, except codes marked with an asterisk (*) are not used on *MERCURY* and *GEMINI 2000* systems.

Codes marked with a double asterisk (**) apply only to UNITY INOVA Whole Body Imaging systems.

Table 5. Acquisition Status Codes

Done	11. FID complete
codes:	12. Block size complete (error code indicates bs number completed)
	13. Soft error
	14. Warning
	15. Hard error
	16. Experiment aborted
	17. Setup completed (error code indicates type of setup completed)
	101. Experiment complete
	102. Experiment started
Error	Warnings
codes:	101. Low-noise signal
	102. High-noise signal
	103. ADC overflow occurred
	104. Receiver overflow occurred*
	Soft errors
	200. Maximum transient completed for single precision data
	201. Lost lock during experiment (LOCKLOST)
	300. Spinner errors:
	301. Sample fails to spin after 3 attempts to reposition (BUMPFAIL)
	302. Spinner did not regulate in the allowed time period (RSPINFAIL)*
	303. Spinner went out of regulation during experiment (SPINOUT)*
	395. Unknown spinner device specified (SPINUNKNOWN)*
	396. Spinner device is not powered up (SPINNOPOWER)*
	397. RS-232 cable not connected from console to spinner (SPINRS232)*
	398. Spinner does not acknowledge commands (SPINTIMEOUT)*
	400. VT (variable temperature) errors:
	400. VT did not regulate in the given time vttime after being set
	401. VT went out of regulation during the experiment (VTOUT)
	402. VT in manual mode after auto command (see Oxford manual)*
	403. VT safety sensor has reached limit (see Oxford manual)*
	404. VT cannot turn on cooling gas (see Oxford manual)*
	405. VT main sensor on bottom limit (see Oxford manual)*
	406. VT main sensor on top limit (see Oxford manual)*
	407. VT sc/ss error (see Oxford manual)*
	408. VT oc/ss error (see Oxford manual)*
	495. Unknown VT device specified (VTUNKNOWN)*
	496. VT device not powered up (VTNOPOWER)*
	497. RS-232 cable not connected between console and VT (VTRS232)*
	498. VT does not acknowledge commands (VTTIMEOUT)
	500. Sample changer errors:
	501. Sample changer has no sample to retrieve
	502. Sample changer arm unable to move up during retrieve
	503. Sample changer arm unable to move down during retrieve
	504. Sample changer arm unable to move sideways during retrieve

- 505. Invalid sample number during retrieve
- 506. Invalid temperature during retrieve
- 507. Gripper abort during retrieve
- 508. Sample out of range during automatic retrieve
- 509. Illegal command character during retrieve*
- 510. Robot arm failed to find home position during retrieve*
- 511. Sample tray size is not consistent*
- 512. Sample changer power failure during retrieve*
- 513. Illegal sample changer command during retrieve*
- 514. Gripper failed to open during retrieve*
- 515. Air supply to sample changer failed during retrieve*
- 525. Tried to insert invalid sample number*
- 526. Invalid temperature during sample changer insert*
- 527. Gripper abort during insert*
- 528. Sample out of range during automatic insert
- 529. Illegal command character during insert*
- 530. Robot arm failed to find home position during insert*
- 531. Sample tray size is not consistent*
- 532. Sample changer power failure during insert*
- 533. Illegal sample changer command during insert*
- 534. Gripper failed to open during insert*
- 535. Air supply to sample changer failed during insert*
- 593. Failed to remove sample from magnet*
- 594. Sample failed to spin after automatic insert
- 595. Sample failed to insert properly
- 596. Sample changer not turned on
- 597. Sample changer not connected to RS-232 interface
- 598. Sample changer not responding*
- 600. Shimming errors:
- 601. Shimming user aborted*
- 602. Lost lock while shimming*
- 604. Lock saturation while shimming*
- 608. A shim coil DAC limit hit while shimming*
- 700. Autolock errors:
- 701. User aborted (ALKABORT)*
- 702. Autolock failure in finding resonance of sample (ALKRESFAIL)
- 703. Autolock failure in lock power adjustment (ALKPOWERFAIL)*
- 704. Autolock failure in lock phase adjustment (ALKPHASFAIL)*
- 705. Autolock failure, lost in final gain adjustment (ALKGAINFAIL)*
- 800. Autogain errors.
- 801. Autogain failure, gain driven to 0, reduce pw (AGAINFAIL)

Hard errors

- 901. Incorrect PSG version for acquisition
- 902. Sum-to-memory error, number of points acquired not equal to np

903. FIFO underflow error (a delay too small?)*
904. Requested number of data points (np) too large for acquisition*
905. Acquisition bus trap (experiment may be lost)*
1000. SCSI errors:
1001. Recoverable SCSI read transfer from console*
1002. Recoverable SCSI write transfer from console**
1003. Unrecoverable SCSI read transfer error*
1004. Unrecoverable SCSI write transfer error*
1100. Host disk errors:
1101. Error opening disk file (probably a UNIX permission problem)*
1102. Error on closing disk file*
1103. Error on reading from disk file*
1104. Error on writing to disk file*
1400–1500. RF Monitor errors:
1400. An RF monitor trip occurred but the error status is OK **
1401. Reserved RF monitor trip A occurred **
1402. Reserved RF monitor trip B occurred **
1404. Excessive reflected power at quad hybrid **
1405. STOP button pressed at operator station **
1406. Power for RF Monitor board (RFM) failed **
1407. Attenuator control or read back failed **
1408. Quad reflected power monitor bypassed **
1409. Power supply monitor for RF Monitor board (RFM) bypassed **
1410. Ran out of memory to report RF monitor errors **
1411. No communication with RF monitor system **
1431. Reserved RF monitor trip A1 occurred on observe channel **
1432. Reserved RF monitor trip B1 occurred on observe channel **
1433. Reserved RF monitor trip C1 occurred on observe channel **
1434. RF Monitor board (PALI/TUSUPI) missing on observe channel **
1435. Excessive reflected power on observe channel **
1436. RF amplifier gating disconnected on observe channel **
1437. Excessive power detected by PALI on observe channel **
1438. RF Monitor system (TUSUPI) heartbeat stopped on observe channel **
1439. Power supply for PALI/TUSUPI failed on observe channel **
1440. PALI asserted REQ_ERROR on observe channel (should never occur) $\ast\ast$
1441. Excessive power detected by TUSUPI on observe channel **
1442. RF power amp: overdrive on observe channel **
1443. RF power amp: excessive pulse width on observe channel **
1444. RF power amp: maximum duty cycle exceeded on observe channel **
1445. RF power amp: overheated on observe channel **
1446. RF power amp: power supply failed on observe channel **
1447. RF power monitoring disabled on observe channel **
1448. Reflected power monitoring disabled on observe channel **
1449. RF power amp monitoring disabled on observe channel **

1451. Reserved RF monitor trip A2 occurred on decouple channel ** 1452. Reserved RF monitor trip B2 occurred on decouple channel ** 1453. Reserved RF monitor trip C2 occurred on decouple channel ** 1454. RF Monitor board (PALI/TUSUPI) missing on decouple channel ** 1455. Excessive reflected power on decouple channel ** 1456. RF amplifier gating disconnected on decouple channel ** 1457. Excessive power detected by PALI on decouple channel ** 1458. RF Monitor system (TUSUPI) heartbeat stopped on decouple channel ** 1459. Power supply for PALI/TUSUPI failed on decouple channel ** 1460. PALI asserted REQ_ERROR on decouple channel (should never occur) ** 1461. Excessive power detected by TUSUPI on decouple channel ** 1462. RF power amp: overdrive on decouple channel ** 1463. RF power amp: excessive pulse width on decouple channel ** 1464. RF power amp: maximum duty cycle exceeded on decouple channel ** 1465. RF power amp: overheated on decouple channel ** 1466. RF power amp: power supply failed on decouple channel ** 1467. RF power monitoring disabled on decouple channel ** 1468. Reflected power monitoring disabled on decouple channel ** 1469. RF power amp monitoring disabled on decouple channel ** 1501. Quad reflected power too high ** 1502. RF Power Monitor board not responding ** 1503. STOP button pressed on operator's station ** 1504. Cable to Operator's Station disconnected ** 1505. Main gradient coil over temperature limit ** 1506. Main gradient coil water is off ** 1507. Head gradient coil over temperature limit ** 1508. RF limit read back error ** 1509. RF Power Monitor Board watchdog error ** 1510. RF Power Monitor Board self test failed ** 1511. RF Power Monitor Board power supply failed ** 1512. RF Power Monitor Board CPU failed ** 1513. ILI Board power failed ** 1514. SDAC duty cycle too high ** 1515. ILI Spare #1 trip ** 1516. ILI Spare #2 trip ** 1517. Quad hybrid reflected power monitor BYPASSED ** 1518. SDAC duty cycle limit BYPASSED ** 1519. Head Gradient Coil errors BYPASSED ** 1520. Main Gradient Coil errors BYPASSED ** 1531. Channel 1 RF power exceeds 10s SAR limit ** 1532. Channel 1 RF power exceeds 5min SAR limit ** 1533. Channel 1 peak RF power exceeds limit ** 1534. Channel 1 RF Amp control cable error ** 1535. Channel 1 RF Amp reflected power too high **

1536. Channel 1 RF Amp duty cycle limit exceeded **
1537. Channel 1 RF Amp temperature limit exceeded **
1538. Channel 1 RF Amp pulse width limit exceeded **
1539. Channel 1 RF Power Monitoring BYPASSED **
1540. Channel 1 RF Amp errors BYPASSED **
1551. Channel 2 RF power exceeds 10s SAR limit **
1552. Channel 2 RF power exceeds 5 min SAR limit **
1553. Channel 2 RF power exceeds 5 min SAR limit **
1554. Channel 2 RF Amp control cable error **
1555. Channel 2 RF Amp reflected power too high **
1556. Channel 2 RF Amp duty cycle limit exceeded **
1557. Channel 2 RF Amp temperature limit exceeded **
1558. Channel 2 RF Amp pulse width limit exceeded **
1559. Channel 2 RF Amp pulse width limit exceeded **

2.3 Spectrometer Control

More than 200 pulse sequence statements are available for pulse sequence generation (PSG). This section starts the discussion of each statement by covering statements intended primarily for spectrometer control. For discussion purposes, the statements in this section are divided into categories: delay-related, observe transmitter pulse-related, decoupler transmitter pulse-related, simultaneous pulses, transmitter phase control, small-angle phase shift, frequency control, power control, and gating control.

Creating a Time Delay

The statements related to time delays are delay, hsdelay, idelay, vdelay, initdelay, and incdelay. Table 6 summarizes these statements.

delay(time) hsdelay(time)	Delay specified time Delay specified time with possible hs pulse
<pre>idelay(time,string)</pre>	Delay specified time with IPA
<pre>incdelay(count,index)</pre>	Set real-time incremental delay
<pre>initdelay(time_increment,index)</pre>	Initialize incremental delay
<pre>vdelay(timebase,count)</pre>	Set delay with fixed timebase and real-time count

Table 6. Delay-Related Statements

The main statement to create a delay in a pulse sequence for a specified time is the statement delay(time), where time is a real number (e.g., delay(d1)). The hsdelay and idelay statements are variations of delay:

• To add a possible homospoil pulse to the delay, use hsdelay(time). If the homospoil parameter hs is set to 'y', then at the beginning of the delay, hsdelay inserts a homospoil pulse of length hst seconds. Although homospoil is not available

on the *GEMINI 2000*, the hsdelay statement can still be used for a delay on *GEMINI 2000* systems.

• To cause interactive parameter adjustment (IPA) information to be generated when gf or go('acqi') is entered, use idelay(time,string), where string is the label used in acqi. If go is entered, idelay is the same as delay. See "Using Interactive Parameter Adjustment," page 120, for details on IPA. IPA and idelay are not available on the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

To set a delay to the product of a fixed timebase and a real-time count, use vdelay(timebase,count), where timebase is NSEC (defined below), USEC (microseconds), MSEC (milliseconds), or SEC (seconds) and count is one of the real-time variables (v1 to v14). For predictable acquisition, the real-time variable should have a value of 2 or more. If timebase is set to NSEC, the delay depends on the type of acquisition controller board (see page 72 for a list) in the system:

- On systems with a Data Acquisition Controller board, the minimum delay is a count of 0 (100 ns), and a count of *n* corresponds to a delay of (100 + (12.5*n)) ns.
- On systems with a Pulse Sequence Controller board or an Acquisition Controller board, the minimum delay is a count of 2 (200 ns), and a count greater than 2 is the minimum delay plus the resolution (25 ns) of the board.
- On systems with Output boards, the minimum delay is a count of 2 (200 ns), and a count greater than 2 is the minimum delay plus the resolution (100 ns) of the board.

The vdelay statement is not available on the *MERCURY-VX*, *MERCURY*, and *GEMINI* 2000.

Use initdelay(time_increment, index) or incdelay(count, index) to enable a real-time incremental delay. A maximum of five incremental delays (set by index) can be defined in one pulse sequence. The following steps are required to set up an incremental delay (initdelay and incdelay are not available on the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*):

1. Enter initdelay(time_increment, index) to initialize the time increment and delay.

The argument time_increment is the time increment that will be multiplied by the count (a real-time variable) for the delay time, and index is one of the indices DELAY1, DELAY2, ..., DELAY5 (e.g., initdelay(1.0/sw, DELAY1) or initdelay(1.0/sw1, DELAY2)).

Set the increment delay by specifying its index and the multiplier count using incdelay(count, index) (e.g., for incdelay(v3, DELAY2), when v3=0, the delay is 0*(1/sw1)).

Pulsing the Observe Transmitter

Statements related to pulsing the observe transmitter are rgpulse, irgpulse, pulse, ipulse, obspulse, and iobspulse. Table 7 summarizes these statements.

Use rgpulse(width, phase, RG1, RG2) as the main statement to pulse the observe transmitter in a sequence, where width is the pulse width, phase (a real-time variable) is the pulse phase, and RG1 and RG2 are defined according to system type:

• On the UNITY *INOVA* and *GEMINI 2000*, RG1 is the delay during which the linear amplifier is gated on and then allowed to stabilize prior to executing the rf pulse, and RG2 is the delay after the pulse after gating off the amplifier. Thus, receiver gating is

<pre>iobspulse(string) ipulse(width,phase,string)</pre>	Pulse observe transmitter with IPA Pulse observe transmitter with IPA
<pre>irgpulse(width,phase,RG1,RG2,string)</pre>	Pulse observe transmitter with IPA
obspulse()	Pulse observe transmitter with amp. gating
<pre>pulse(width,phase).</pre>	Pulse observe transmitter with amp. gating
<pre>rgpulse(width,phase,RG1,RG2)</pre>	Pulse observe transmitter with amp. gating

Table 7.	Observe	Transmitter	Pulse-	Related	Statements
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a misnomer: RG1 and RG2 set amplifier gating, as shown in Figure 3. The receiver is off during execution of the pulses and is only gated on immediately before acquisition.

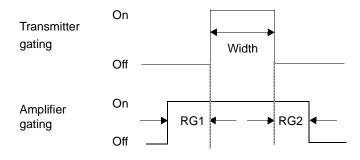


Figure 3. Amplifier Gating

• On the *MERCURY-VX*, *MERCURY*, UNITY*plus*, UNITY, and VXR-S, the receiver and amplifiers are tied together such that when the amplifier is on, the receiver is automatically turned off and when the receiver is on, the amplifier is off.

Some further information about RG1 and RG2:

- Typically, RG1 is 10 μs for $^{1}H/^{19}F$ and 40 μs for other nuclei. A typical value for RG2 is 10 to 20 $\mu s.$
- The phase of the pulse is set at the beginning of RG1. The phase requires about 0.2 μ s to settle on UNITY*INOVA* and UNITY*plus*, 10 μ s on *GEMINI 2000* ¹H/¹³C and broadband decouplers, 1.0 μ s on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* broadband, 0.5 to 1.0 μ s on other systems with direct synthesis rf, and twice as long for rf types A and B.
- A transmitter gate is also switched during RG1. The switching time for this gate is 100 ns for UNITY *INOVA* and UNITY *plus* systems or 1 to 3 μs for *GEMINI 2000* and UNITY systems.

For systems with linear amplifiers, an rf pulse can be unexpectedly curtailed if the amplifier goes into thermal shutdown. Thermal shutdown can be brought about if the amplifier duty cycle becomes too large for the average power output. In addition, on *GEMINI 2000*, *MERCURY-VX*, and *MERCURY* systems, the pulse length is limited to 1 ms.

The remaining statements for pulsing the observe transmitter are variations of rgpulse:

• To pulse the observe transmitter the same as rgpulse but with RG1 and RG2 set to the parameters rof1 and rof2, respectively, use pulse(width,phase). Thus, pulse(width,phase) and rgpulse(width,phase,rof1,rof2) are exactly equivalent.

- To pulse the observe transmitter the same as pulse but with width preset to pw and phase preset to oph, use obspulse(). Thus, obspulse() is exactly equivalent to rgpulse(pw, oph, rof1, rof2).
- To pulse the observe transmitter with rgpulse, pulse, or obspulse, but generate interactive parameter adjustment (IPA) information when gf or go('acqi') is entered, use irgpulse(width, phase, RG1, RG2, string), ipulse(width, phase, string), or iobspulse(string), respectively. The string argument is used as a label in acqi. If go is entered, the IPA information is not generated. For details on IPA, see "Using Interactive Parameter Adjustment," page 120. IPA is not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems.

On UNITY*INOVA* and UNITY*plus* systems, the ampmode parameter gives override capability over the default selection of amplifier modes. Unless overridden, the observe channel is set to the pulse mode, other used channels are set to the CW (continuous wave) mode, and any unused channels are set to the idle mode. By using values of d, p, c, and i for the default, pulse, CW, and idle modes, respectively, ampmode can override the default modes. For example, ampmode='ddp' selects default behavior for the first two amplifiers and forces the third channel amplifier into the pulse mode.

The selection of rf channels on UNITY*INOVA* and UNITY*plus* systems also can be independently controlled with the rfchannel parameter. You do not need rfchannel if you have a single-channel broadband system and you set up a normal HMQC experiment (tn='H1', dn='Cl3'). The software recognizes that you cannot do this experiment and swaps the two channels automatically to make the experiment possible.

The rfchannel parameter becomes important if, for example, you have a three-channel spectrometer and you want to do an HMQC experiment with the decoupler running through channel 3. Instead of rewriting the pulse sequence, you can create rfchannel (by entering create('rfchannel', 'flag')), and then set, for example, rfchannel='132'. Now channels 2 and 3 are effectively swapped, without any changes in the sequence.

Similarly, if you want simply to observe on channel 2 (as in the pulse sequence S2PULR), you just run S2PUL with rfchannel='21'.

The rfchannel mechanism only works for pulse sequences that eliminate all references to the constants TODEV, DO2DEV, and DO3DEV. To take advantage of rfchannel, you must remove statements, such as power and offset, that use these constants and replace them with the corresponding statements, such as obspower and decoffset, that do not contain the constants.

On UNITYINOVA, all standard pulse sequences have been edited to take advantage of the rf channel independence afforded by the rfchannel parameter. This parameter makes it a simple matter to redirect, for example, the dn nucleus to use the third or fourth rf channel.

On *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*, there are only two channels. The software automatically determines which channel is observe or decouple based on tn and dn.

Pulsing the Decoupler Transmitter

Statements related to decoupler pulsing are decpulse, decrgpulse, idecpulse, idecrgpulse, dec2rgpulse, and dec3rgpulse. Table 8 summarizes these statements.

<pre>decpulse(width,phase) decrgpulse(width,phase,RG1,RG2)</pre>	Pulse decoupler transmitter with amp. gating Pulse first decoupler with amplifier gating	
<pre>dec2rgpulse(width,phase,RG1,RG2)</pre>	Pulse second decoupler with amplifier gating	
<pre>dec3rgpulse(width,phase,RG1,RG2)</pre>	Pulse third decoupler with amplifier gating	
<pre>dec4rgpulse(width,phase,RG1,RG2)</pre>	Pulse deuterium decoupler with amplifier gating	
<pre>idecpulse(width,phase,string)</pre>	Pulse first decoupler transmitter with IPA	
idecrgpulse*	Pulse first decoupler with amplifier gating and IPA	
<pre>* idecrgpulse(width,phase,RG1,RG2,string)</pre>		

Table 8. Decoupler Transmitter Pulse-Related Statements

Use decpulse(width, phase) to pulse the decoupler in the pulse sequence at its current power level. width is the time of the pulse, in seconds, and phase is a real-time variable for the phase of the pulse (e.g., decpulse(pp, v3)).

The amplifier is gated on during decoupler pulses as it is during observe pulses. The amplifier gating times (see RG1 and RG2 for decrgpulse below) are internally set to zero. The decoupler modulation mode parameter dmm should be 'c' during any period of time in which decoupler pulses occur.

To pulse the decoupler at its current power level and have user-settable amplifier gating times, use decrgpulse(width, phase, RG1, RG2), where width and phase are the same as used with decpulse, and RG1 and RG2 are the same as used with the rgpulse statement for observe transmitter pulses. In fact, decrgpulse is syntactically equivalent to rgpulse and functionally equivalent with two exceptions:

- The decoupler is pulsed at its current power level (instead of the transmitter).
- If homo='n', the slow gate (100 ns switching time on UNITYINOVA or UNITYplus, 1 to 3 µs switching time on other systems) on the decoupler board is always open and therefore need not be switched open during RG1. In contrast, if homo='y', the slow gate on the decoupler board is normally closed and must therefore be allowed sufficient time during RG1 to switch open (homo is not used on the *MERCURY-VX*, *MERCURY*, or *GEMINI 2000*).

For systems with linear amplifiers, RG1 for a decoupler pulse is important from the standpoint of amplifier stabilization under either of the following conditions:

- When tn and dn both equal 3 H, 1 H, or 19 F (high-band nuclei).
- When tn and dn are less than or equal to ^{31}P (low-band nuclei).

For these conditions, the "decoupler" amplifier module is placed in the pulse mode, in which it remains blanked between pulses. In this mode, RG1 must be sufficiently long to allow the amplifier to stabilize after blanking is removed: 2 μ s on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems, or 5 to 10 μ s for high-band nuclei and 10 to 20 μ s for low-band nuclei on other systems. On 500-MHz systems that use the ENI-5100 class A amplifier for low-band nuclei on the observe channel, RG1 should be set for 40 to 60 μ s.

If the tn nucleus and the dn nucleus are in different bands, such as tn is ¹H and dn is ¹³C, the "decoupler" amplifier module is placed in the continuous wave (CW) mode, in which it is always unblanked regardless of the state of the receiver. In this mode, RG1 is unimportant with respect to amplifier stabilization prior to the decoupler pulse, but with respect to phase setting, it must be set.

The remaining decoupler transmitter pulse-related statements are variations of decpulse and decrgpulse:

- To pulse the decoupler the same as decpulse or decrgpulse, but generate interactive parameter adjustment (IPA) information when gf or go('acqi') is entered, use idecpulse(width,phase,string) or idecrgpulse(width,phase,RG1,RG2,string), respectively, where string is used as a label in acqi. If go is entered instead, the IPA information is not generated. For details on IPA, see "Using Interactive Parameter Adjustment," page 120. IPA is not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems.
- To pulse the second decoupler, use dec2rgpulse(width, phase, RG1, RG2). To pulse the third decoupler, use dec3rgpulse(width, phase, RG1, RG2). To pulse UNITY INOVA systems with a deuterium decoupler installed as the fifth channel, use dec4rgpulse(width, phase, RG1, RG2). The width, phase, RG1, and RG2 arguments have the same meaning as used with decrgpulse and rgpulse. The homo parameter has no effect on the gating on the second decoupler board. On UNITY INOVA and UNITY plus systems only, homo2 controls the homodecoupler gating of the second decoupler, homo3 does the same on the third decoupler, and homo4 does the same on the fourth decoupler when it is used as a deuterium channel (on the MERCURY-VX, MERCURY, and GEMINI 2000, dec2rgpulse, dec3rgpulse, and dec4rgpulse have no meaning and homo is not used).

Pulsing Channels Simultaneously

Statements for controlling simultaneous, non-shaped pulses are simpulse, sim3pulse, and sim4pulse. Table 9 summarizes these statements. Simultaneous pulses statements using shaped pulses are covered in a later section.

simpulse*	Pulse observe and decoupler channels simultaneously	
sim3pulse*	Pulse simultaneously on two or three rf channels	
sim4pulse*	Simultaneous pulse on four channels	
<pre>* sim3pulse(pw1,pw2,pw3,phase1,phase2,phase3,RG1,RG2)</pre>		
<pre>sim3pulse(pw1,pw2,pw3,phase1,phase2,phase3,RG1,RG2)</pre>		
<pre>sim4pulse(pw1,pw2,pw3,pw4,phase1,phase2,phase3,phase4,RG1,RG2)</pre>		

Table 9.	Simultaneous Pulses Statements
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Use simpulse(obswidth, decwidth, obsphase, decphase, RG1, RG2) to simultaneously pulse the observe and first decoupler rf channels with amplifier gating (e.g., simpulse(pw, pp, v1, v2, 0.0, rof2)).

Figure 4 illustrates the action of simpulse on UNITY INOVA, MERCURY-VX MERCURY, GEMINI 2000, UNITY plus, UNITY, and VXR-S systems.

The shorter of the two pulses is centered on the longer pulse, while the amplifier gating occurs before the start of the longer pulse (even if it is the decoupler pulse) and after the end of the longer pulse. The absolute difference in the two pulse widths must be greater than or equal to $0.2 \ \mu s$ ($0.4 \ \mu s$ on the *MERCURY-VX*, *MERCURY*, UNITY*plus*, and *GEMINI 2000*); otherwise, a timed event of less than the minimum value ($0.1 \ \mu s$ on UNITY*INOVA*, $0.2 \ \mu s$ on other systems) would be produced. In such cases, a short time ($0.2 \ \mu s$ on UNITY*INOVA*, $0.4 \ \mu s$ on other systems) is added to the longer of the two pulse widths to remedy the problem, or the pulses are made the same if the difference is less than half the minimum (less than $0.1 \ \mu s$ on UNITY*INOVA*, less than $0.2 \ \mu s$ on other systems).

sim3pulse(pw1,pw2,pw3,phase1,phase2,phase3,RG1,RG2) performs a simultaneous, three-pulse pulse on three independent rf channels, where pw1, pw2, and pw3 are the pulse durations on the observe transmitter, first decoupler, and second decoupler, respectively.phase1, phase2, and phase3 are real-time variables for the

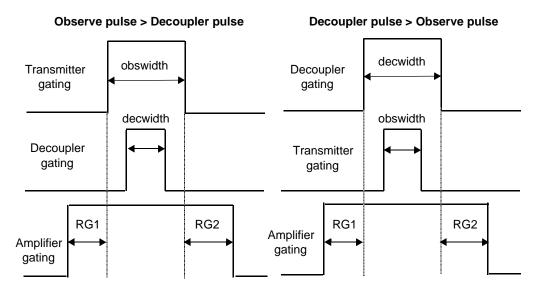


Figure 4. Pulse Observe and Decoupler Channels Simultaneously

phases of the corresponding pulses, for example, sim3pulse(pw,p1,p2,oph, v10,v1,rof1,rof2).

A simultaneous, two-pulse pulse on the observe transmitter and the second decoupler can be achieved by setting the pulse length for the first decoupler to 0.0; for example, sim3pulse(pw, 0.0, p2, oph, v10, v1, rof1, rof2).(sim3pulse has no meaning on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*).

Use sim4pulse(pw1,pw2,pw3,pw4,phase1,phase2,phase3,phase4, RG1,RG2) to perform simultaneous pulses on as many as four different rf channels. Except for the added arguments pw4 and phase4 for a third decoupler, the arguments in sim4pulse are defined the same as sim3pulse. If any pulse is set to 0.0, no pulse is executed on that channel (sim4pulse has no meaning on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*).

Setting Transmitter Quadrature Phase Shifts

The statements txphase, decphase, dec2phase, dec3phase, dec4phase control transmitter quadrature phase (multiple of 90∞). Table 10 summarizes these statements.

decphase(phase)	Set quadrature phase of first decoupler
<pre>dec2phase(phase)</pre>	Set quadrature phase of second decoupler
<pre>dec3phase(phase)</pre>	Set quadrature phase of third decoupler
<pre>dec4phase(phase)</pre>	Set quadrature phase of fourth decoupler

Table 10. Transmitter Quadrature Phase Control Statements

To set the transmitter phase, use txphase(phase), where phase is a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.) that references the desired phase. This enables changing the transmitter phase independently from a pulse.

txphase(phase)

Set quadrature phase of observe transmitter

Chapter 2. Pulse Sequence Programming

For example, knowing that the transmitter phase takes a finite time to shift (as much as 10 μ s on a *GEMINI 2000* ¹H/¹³C system, about 1 μ s on a *MERCURY-VX*, *MERCURY*, or *GEMINI 2000* broadband system, about 400 ns for rf type C, less than 200 ns for rf type D used on UNITY*plus*, and longer for types A and B), you may wish to "preset" the transmitter phase at the beginning of a delay that precedes a particular pulse. The "normal" pulse sequences use an rof1 time preceding the pulse to change the transmitter phase and do not need to "preset" the phase. The phase change will occur at the start of the next event in the pulse sequence.

The other phase control statements are variations of txphase:

- To set the decoupler phase, use decphase(phase). The decphase statement is syntactically and functionally equivalent to txphase. decphase is useful for a decoupler pulse in all cases where txphase is useful for a transmitter pulse.
- To set the quadrature phase of the second decoupler rf or third decoupler rf, use dec2phase(phase) or dec3phase(phase), respectively.

On UNITY *INOVA*, *MERCURY-VX*, *MERCURY*, *GEMINI 2000*, and UNITY *plus*, the hardware WALTZ decoupling lines are XORed with the decoupler phase control. The performance of the WALTZ decoupling should not be affected by the decoupler phase setting. On UNITY and VXR-S systems, however, the hardware WALTZ decoupling lines are ORed with the decoupler phase control. As a consequence, the decoupler phase *must* be set to 0 for WALTZ to function properly.

When using pulse sequences with implicit acquisition, the decoupler phase is set to 0 automatically (within the test4acq procedure in the module hwlooping.cin / vnmr/psg), so under most circumstances no problems are seen. But if you are using explicit acquisition or if you are trying to perform WALTZ decoupling during a period other than acquisition, you must use a decphase(zero) statement in the pulse sequence before the relevant time period.

Setting Small-Angle Phase Shifts

Setting the small-angle phase of rf pulses is implemented by three different methods:

- Fixed 90° settings
- · Direct synthesis hardware control
- Phase-pulse phase shifting

The statements related to these methods are summarized in Table 11. None of these statements apply to the *GEMINI 2000*.

<pre>dcplrphase(multiplier) dcplr2phase(multiplier)</pre>	Set small-angle phase of first decoupler, rf type C or D Set small-angle phase of second decoupler, rf type C or D	
<pre>dcplr3phase(multiplier)</pre>	Set small-angle phase of third decoupler, rf type C or D	
<pre>decstepsize(base)</pre>	Set step size of first decoupler	
<pre>dec2stepsize(base)</pre>	Set step size of second decoupler	
<pre>dec3stepsize(base)</pre>	Set step size of third decoupler	
<pre>obsstepsize(base)</pre>	Set step size of observe transmitter	
phaseshift*	Set phase-pulse technique, rf type A or B	
<pre>stepsize(base,device)</pre>	Set small-angle phase step size, rf type C or D	
<pre>xmtrphase(multiplier)</pre>	Set small-angle phase of observe transmitter, rf type C	
<pre>* phaseshift(base,multiplier,device)</pre>		

Table 11. Phase Shift Statements

Fixed 90° Settings

The first method is the hardwired 90° (or quadrature) phase setting. For both the observe and the decoupler transmitters, phases of 0°, 90°, 180°, and 270° are invoked instantaneously using the obspulse, pulse, rgpulse, simpulse, decpulse, decrgpulse, dec2rgpulse, dec3rgpulse, dec4rgpulse, txphase, decphase, dec2phase, dec3phase, and dec4phase statements.

The receiver phase is actually fixed but is "shifted" by setting the oph variable, which changes the "mode" of the receiver. A 180° receiver "phase" sets the system to subtract instead of add the data—a 90° receiver phase swaps the two channels of the receiver.

Hardware Control

A second method of small-angle phase selection is implemented only on spectrometers with direct synthesis. This method uses hardware that sets transmitter phase in 0.25° increments on UNITY *INOVA* and UNITY *plus* systems, 0.5° increments on UNITY and VXR-S systems, or 1.41° on *MERCURY-VX* and *MERCURY* systems, independently of the phase of the receiver. Unlike the phase-pulse technique (described below), this method is an absolute technique (e.g., if a phase of 60° is invoked twice, the second phase selection does nothing).

The obsstepsize(base) statement sets the step size of the small-angle phase increment to base for the observe transmitter. Similarly, decstepsize(base), dec2stepsize(base), and dec3stepsize(base) set the step size of the smallangle phase increment to base for the first decoupler, second decoupler, and third decoupler, respectively (assuming that system is equipped with appropriate hardware). The base argument is a real number or variable.

The base phase shift selected is active only for the xmtrphase statement if the transmitter is the requested device, only for the dcplrphase statement if the decoupler is the requested device, only for the dcplr2phase statement if the second decoupler is the requested device, or only for the dcplr3phase if the third decoupler is the required device, that is, every transmitter has its own "base" phase shift. Phase information into pulse, rgpulse, decpulse, decrgpulse, dec2rgpulse, dec3rgpulse, and simpulse is still expressed in units of 90°.

The statements xmtrphase(multiplier), dcplrphase(multiplier), dcplr2phase(multiplier), and dcplr3phase(multiplier) set the phase of transmitter, first decoupler, second decoupler, or third decoupler, respectively, in units set by stepsize. If stepsize has not been used, the default step size is 90°. The argument multiplier is a small-angle phaseshift multiplier. The small-angle phaseshift is a product of the multiplier and the preset stepsize for the rf device (observe transmitter, first decoupler, second decoupler, or third decoupler). multiplier must be an real-time variable.

The decstepsize, dec2stepsize, dec3stepsize, and obsstepsize statements are similar to the stepsize statement but have the channel selection fixed. Each of the following pairs of statements are functionally the same:

- obsstepsize(base) and stepsize(base,OBSch).
- decstepsize(base) and stepsize(base, DECch).
- dec2stepsize(base) and stepsize(base,DEC2ch).
- dec3stepsize(base) and stepsize(base,DEC3ch).

On systems with Output boards only (see page 72 for the types of boards), if the product of the base and multiplier is greater than 90°, the sub-90° part is set by the

xmtrphase, dcplrphase, dcplr2phase, or dcplr3phase statements. Carryovers that are multiples of 90° are automatically saved and added in at the time of the next 90° phase selection (e.g., at the time of the next pulse or decpulse). This is true even if stepsize has not been used and base is at its default value of 90°. The following example may help you to understand this question of "carryovers":

On systems with Acquisition Controller boards or Pulse Sequence Controller boards, the 90° multiples are set by the call to xmtrphase, dcplrphase, dcplr2phase, and dcplr3phase.

If xmtrphase, dcplrphase, dcplr2phase, or dcplr3phase is used to set the phase for some pulses in a pulse sequence, it is often necessary to use xmtrphase(zero), dcplrphase(zero), dcplr2phase(zero), or dcplr3phase(zero) preceding other pulses to ensure that the phase specified by a previous xmtrphase, dcplrphase, dcplr2phase, or dcplr3phase does not carry-over into an unwanted pulse or decpulse statement.

Phases specified in txphase, pulse, rgpulse, decphase, decpulse, decrgpulse, dec2phase, dec2rgpulse, dec3rgpulse, and dec4rgpulse statements change the 90° portion of the phase shift only. This feature provides a separation between the small-angle phase shift and the 90° phase shifts, and facilitates programming phase cycles or additional coherence transfer selective phase cycling "on top of" small-angle phase shifts.

Be sure to distinguish xmtrphase from txphase. txphase is optional and rarely needed; xmtrphase is needed any time the transmitter phase shift is to be set to a value not a multiple of 90°. The same distinction can be made between dcplrphase and decphase, dcplr2phase and dec2phase, and dcplr3phase and dec3phase.

Phase-Pulse Technique

The third method is a phase-shifting technique called the *phase-pulse*, described by Lallemand and co-workers (E. Guittet, D. Piveteau, M.-A. Delsuc, and J.-Y. Lallemand, *J. Magn. Reson.*, **62**, 336-339 (1985)) and also discovered independently at Varian (D. Iverson and S.L. Patt, Varian Owners Conference, April, 1985). This method is applicable only to systems lacking hardware small-angle phase shift, which is the case on UNITY and VXR-S spectrometers with type A or B rf.

This method involves shifting the frequency of the transmitter (observe or decoupler) for a brief time at a point in the pulse sequence when no pulse is required, and then returning the frequency to its original value. If this change of frequency can be accomplished with phase continuity (the case on VNMR spectrometers), the temporary shift of transmitter frequency has the effect of producing an apparent phase shift in the transmitter that is the product of the time during which the frequency was changed and the period of the difference frequency. For example, if the frequency is increased by 1000 Hz, the phase will "get

ahead" at a rate of 360° in 1 ms. If this frequency difference is left in effect for 100 μ s, the phase shift is (360°/1 ms) × 100 μ s = 36°.

Since the frequency difference and the time for this shift are under computer control, tremendous flexibility is possible. The larger the frequency shift, the smaller the time for a particular phase shift but also the less the precision in specifying the shift; the smaller the shift, the larger the time for a particular phase shift but the greater the precision in generating that shift. The technique as described by Lallemand required a minimum time of 1 ms to perform the phase pulse; the Varian implementation uses a time of 30 μ s and a resolution of 1.44°.

Use the statement phaseshift(base, multiplier, device) to implement the phase-pulse technique on systems with rf type A or B (for type C, see the next section). base is a real number, expression, or variable representing the base phase shift in degrees. Any value is acceptable. multiplier is the name of a real-time variable (ct, v1 to v14, etc.). The value must be positive. The phase shift will be ((base × multiplier) mod 360). device specifies if the transmitter, first decoupler, second decoupler, or third decoupler will be phase shifted. Values can be OBSch, DECch, DEC2ch, or DEC3ch, respectively (e.g., phaseshift(60.0, ct, OBSch)).

An important point to understand about using the phase-pulse technique is that it is a cumulative technique. That is, a phase shift of 60° followed by another phase shift of 60° results in a total phase shift of 120° . If one pulse requires a 60° phase and a subsequent pulse requires a 0° phase, a -60° phase shift will need to be used after the first pulse.

Another important point is that the frequency that is shifted is the local oscillator (L.O.) frequency. For the observe channel, this means that the phase of the transmitter and the receiver are linked. That is, a 60° phase shift of the observe transmitter during the course of the pulse sequence will also shift the receiver by 60° . If this is not desirable, it would again be possible simply to shift the phase by -60° after the last pulse but before the start of the acquisition.

A third point about phaseshift is the time factor. The phase shift is created by shifting the frequency by a fixed amount for a variable time. However, the introduction of a time delay into a pulse sequence whose length would be variable depending upon the phase shift chosen would be in most cases undesirable. Thus what we have done is to shift the frequency for a variable time, then shift the frequency back, followed by waiting for another variable time at the original frequency, such that the total time of this combined operation is a constant. This time has been chosen to be 30 μ s. Thus, whenever the pulse sequence statement phaseshift is encountered in a pulse sequence, an implicit delay of 30 μ s occurs. In many pulse sequences, this has little consequence. In cases involving spin echoes, however, it will be important to correct for this time.

The final point to understand is the step size. Because of limitations on the timing in the system (25 ns for systems with the Acquisition Controller board or Pulse Sequence Controller board, 0.1 μ s time resolution for systems with the Output board), there is an effective resolution of the phase shift (for the type of board on your system, see "Types of Acquisition Controller Boards," page 72). The implementation as provided gives phase steps of 0.36° (Acquisition Controller board or Pulse Sequence Controller board) or 1.44° (Output board). Thus, for any particular phase shift, there may be a roundoff of ±0.18° (Acquisition Controller board or Pulse Sequence Controller board) or ±0.72° (Output board). This is not a real error because you know exactly what the phase shift is, but are not able to set it with any finer resolution.

On systems with an Output board only (see page 72 for a list of boards), a 0.2 µs delay internally precedes the AP (analog port) bus statements xmtrphase, dcplrphase, and dcplr2phase. The apovrride() statement prevents this 0.2 µs delay from being

inserted prior to the next (and only the next) occurrence of one of the these AP bus statements.

Controlling the Offset Frequency

Statements for frequency control are decoffset, dec2offset, dec3offset, dec4offset, obsoffset, offset, and ioffset. Table 12 summarizes these statements.

<pre>decoffset(frequency) dec2offset(frequency)</pre>	Change offset frequency of first decoupler Change offset frequency of second decoupler
<pre>dec3offset(frequency)</pre>	Change offset frequency of third decoupler
<pre>dec4offset(frequency)</pre>	Change offset frequency of fourth decoupler
<pre>obsoffset(frequency)</pre>	Change offset frequency of observe transmitter
<pre>offset(frequency,device)</pre>	Change offset frequency of transmitter or decoupler
<pre>ioffset(frequency,device,string)</pre>	Change offset frequency with IPA

 Table 12.
 Frequency Control Statements

The main statement to set the offset frequency of the observe transmitter (parameter tof), first decoupler (dof), second decoupler (dof2), or third decoupler (dof3) is the statement offset(frequency,device), where frequency is the new value of the appropriate parameter and device is OBSch (observe transmitter), *DECch* (first decoupler), *DEC2ch* (second decoupler), or DEC3ch (third decoupler). For example, use offset(to2,OBSch) to set the observe transmitter offset frequency. DEC2ch can be used only on systems with three rf channels. Likewise, *DEC3ch* is used only on systems with four rf channels.

- For systems with rf types A or B, the frequency typically changes in 10 to 30 µs, but 100 µs is automatically padded into the sequence by the offset statement so that the time duration of the offset statement is constant and not frequency-dependent.
- For systems with rf type C, which necessarily use PTS frequency synthesizers, the frequency shift time is shown in Table 32. No 100-µs delay is padded into the sequence for systems with rf type C or D. Offset frequencies are not automatically returned to their "normal" values before acquisition—this must be done explicitly.
- For systems with rf type D (UNITY*plus*), the frequency shift time is 14.95 µs (latching with or without over-range). No 100-µs delay is inserted into the sequence by the offset statement. Offset frequencies are not returned automatically to their "normal" values before acquisition; this must be done explicitly, as in the example below.
- For UNITY *INOVA* systems, the frequency shift time is $4 \mu s$.
- For *GEMINI 2000* systems (rf types F or E): on broadband systems, only the decoupler can be shifted (8.6 μ s); on ¹H/¹³C systems, observe (6.48 μ s), decoupler (8.6 μ s), and homodecoupler (8.6 μ s) can be set.
- For *MERCURY-VX* and *MERCURY* systems, the setup time is 86.4 µs and the shift time is 1 µs.
- On systems with the Output board only, all offset statements by default are preceded internally by a 0.2-µs delay.

Other frequency control statements are variations of offset:

• To set the offset frequency of the observe transmitter the same as offset but generate interactive parameter adjustment (IPA) information when gf or go('acqi') is

entered, use ioffset(frequency, device, string), where string is used as a label for the slider in acqi. If go is entered instead, the IPA information is not generated. For details on IPA, see "Using Interactive Parameter Adjustment," page 120. IPA is not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems.

- To set the offset frequency of the observe transmitter (parameter tof), use obsoffset(frequency), which functions the same as offset(frequency,OBSch).
- To set the offset frequency of the first decoupler (parameter dof), use decoffset(frequency), which functions the same as offset(frequency, DECch).
- To set the offset frequency of the second decoupler (parameter dof2), use dec2offset(frequency), which functions the same as offset(frequency,DEC2ch).
- To set the offset frequency of the third decoupler (parameter dof3), use dec3offset(frequency), which functions the same as offset(frequency, DEC3ch).
- To set the offset frequency of the deuterium decoupler used as the fifth channel (parameter dof4), use dec4offset(frequency), which functions the same as offset(frequency, DEC4ch)

Controlling Observe and Decoupler Transmitter Power

Statements to control power by adjusting the coarse attenuators on linear amplifier systems are power, obspower, decpower, dec2power, dec3power, and dec4power. Statements to control fine power are pwrf, pwrm, rlpwrm, obspwrf, decpwrf, dec2pwrf, and dec3pwrf. Statements to control decoupler power level switching are declvlon, declvloff, and decpwr. The apovrride statement overrides an AP bus delay (the delay before AP bus access). Table 13 summarizes these statements. Only the declvloff, declvlon, obspower, and decpower statements apply to the *GEMINI 2000*, and only coarse power can be controlled on *MERCURY-VX* and *MERCURY* systems.

Table 13. Power Control Statement	ïS
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apovrride()	Override internal software AP bus delay
declvloff()	Return first decoupler back to "normal" power
declvlon()	Turn on first decoupler to full power
<pre>decpower(value)</pre>	Change first decoupler power, linear amplifier
<pre>dec2power(value)</pre>	Change second decoupler power, linear amplifier
<pre>dec3power(value)</pre>	Change third decoupler power, linear amplifier
<pre>dec4power(value)</pre>	Change deuterium decoupler power, linear amplifier
<pre>decpwr(level)</pre>	Set decoupler high-power level, class C amplifier
<pre>decpwrf(value)</pre>	Set first decoupler fine power
<pre>dec2pwrf(value)</pre>	Set second decoupler fine power
<pre>dec3pwrf(value)</pre>	Set third decoupler fine power
<pre>ipwrf(value,device,string)</pre>	Change transmitter or decoupler fine power with IPA
<pre>ipwrm(value,device,string)</pre>	Change transmitter or decoupler linear mod. with IPA
<pre>obspower(value)</pre>	Change observe transmitter power, linear amplifier
<pre>obspwrf(value)</pre>	Set observe transmitter fine power
<pre>power(value,device)</pre>	Change transmitter or decoupler power, linear amplifier
<pre>pwrf(value,device)</pre>	Change transmitter or decoupler fine power
<pre>pwrm(value,device)</pre>	Change transmitter or decoupler linear mod. power
<pre>rlpwrm(rlvalue,device)</pre>	Set transmitter or decoupler linear mod. power

Coarse Attenuator Control

On UNITY *INOVA*, UNITY *plus*, and UNITY systems with linear amplifiers, the statement power (value, device) changes transmitter or decoupler power by adjusting the coarse attenuators from 0 (minimum power) to 63 (maximum power) on channels with a 63-dB attenuator, or from -16 (minimum power) to 63 (maximum power) on channels with a 79-dB attenuator.

- value must be stored in a real-time variable such as v2; the actual value cannot be placed directly in the power statement. This allows the attenuators to be changed in real-time or from pulse to pulse.
- device is OBSch to change the transmitter power, DECch to change the first decoupler power, DEC2ch to change the second decoupler power, or DEC3ch to change the third decoupler power (e.g., power (v2,OBSch)).

To avoid using a real-time variable, the fixed-channel statements obspower(value), dec2power(value), and dec3power(value) can be used in place of the power statement, for example, obspower(63.0). For all of these statements, value is either a real number or a variable.

The power and associated fixed-channel statements allow configurations such as the use of the transmitter at a low power level for presaturation followed by a higher power for uniform excitation. The phase of the transmitter is specified as being constant to within 5° over the whole range of transmitter power. Therefore, if you pulse at low power with a certain phase and later at high power with the same phase, the two phases are the "same" to within 5° (at any one power level, the phase is constant to considerably better than 0.5°). The time of the power change is specified in Table 32. On UNITY and VXR-S systems, the power change is somewhat discontinuous and it is advisable, although not strictly necessary, to change the power level at a time when the observe pulse is not turned on, then to allow a minimum of 4 μ s before using a transmitter pulse.

On systems with an Output board only (see page 72 for the types of acquisition controller board), the power and associated statements are preceded internally by a 0.2 µs delay by default (see the apovrride pulse statement for more details).

CAUTION: On systems with linear amplifiers, be careful when using values of power, obspower, decpower, dec2poser, and dec3power greater than 49 (about 2 watts). Performing continuous decoupling or long pulses at power levels greater than this can result in damage to the probe. Use config to set a safety maximum for the tpwr, dpwr, dpwr2, and dpwr3 parameters.

Fine-Power Control

To change the fine power of a transmitter or decoupler by adjusting the optional linear fine attenuators, use pwrf(value,device) or pwrm(value,device). The value argument is real-time variable, which means it cannot be placed directly in the pwrf or pwrm statement, and can range from 0 to 4095 (60 dB on UNITY *INOVA* or UNITY *plus*, about 6 dB on other systems). device is OBSch (for the observe transmitter) or DECch (first decoupler). On UNITY *INOVA* and UNITY *plus* only, device can also be *DEC2ch* (second decoupler) or DEC3ch (third decoupler). *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems do no have fine-power control.

You can use the fixed-channel statement obspwrf(value), decpwrf(value), dec2pwrf(value), and dec3pwrf, or rlpwrm(value, device) to avoid arguments using real-time variables. These statements change transmitter or decoupler

power on systems with linear amplifiers, but value is either a real number or a variable and is stored in a C variable of type double.

The ipwrf(value, device, string) and ipwrm(value, device, string) statement changes interactively the transmitter or decoupler fine power or linear modulators by adjusting the optional fine attenuators. The value and device arguments are the same as pwrf.string can be any string; the first six letters are used in acqi. This statement will generate interactive parameter adjustment (IPA) information only when the command gf or go('acqi') is typed. When the command go is typed, this statement is ignored by the pulse sequence. Use the pwrf pulse statement for this purpose. Do not execute pwrf and ipwrf in the same pulse sequence, as they cancel each other's effect.

On systems with an Output board only (see page 72 for types of boards), a 0.2 µs delay internally precedes the AP (analog port) bus statements power, obspower, decpower, and dec2power. The apovrride() statement prevents this 0.2 µs delay from being inserted prior to the next (and only the next) occurrence of one of the these AP bus statements.

Decoupler Power-Level Switching

On UNITY *INOVA*, UNITY *plus*, and UNITY systems with class C or linear amplifiers, declvlon() and declvloff() switch the decoupler power level between the power level set by the high-power parameter(s) to the *full* output of the decoupler. The statement declvlon() gives full power on the decoupler channel; declvloff switches the decoupler to the power level set by the appropriate parameters defined by the amplifier type: dhp for class C amplifiers or dpwr for a linear amplifiers. If dhp='n', these statements do not have any effect on systems with class C amplifiers, but still function for systems with linear amplifiers.

If declvlon is used, make sure declvloff is used prior to time periods in which normal, controllable power levels are desired, for example, prior to acquisition. Full decoupler power should only be used for decoupler pulses or for solids applications.

On *GEMINI 2000* broadband systems, declvlon sets the power of the decoupler to the level set by the parameter pplvl. This is an important distinction—decoupler pulse power on the *GEMINI 2000* broadband is controlled by the value in pplvl, and declvlon does *not* set the power to "full" output. On *GEMINI 2000* ¹H/¹³C systems, however, declvlon does set the decoupler to full power.

MERCURY-VX and *MERCURY* systems do not use declvlon or declvloff. To distinguish between *GEMINI 2000* and *MERCURY-VX* and *MERCURY*, use declvlflag (e.g., see /vnmr/psglab/dept.c.)

On UNITY systems with a class C amplifier, decpwr(level) changes the decoupler high-power level to the value set by level, which can assume real values from 0 (lowest) to 255 (full power); these units are monotonically increasing but neither linear nor logarithmic. To reset the power back to the "standard" dhp level, use decpwr(dhp).

On *GEMINI 2000* ¹H/¹³C systems, the power is fixed. decpwr has no meaning.

Controlling Status and Gating

Statements to control decoupler and homospoil status are status and setstatus. Explicit transmitter and receiver gating control statements are xmtroff, xmtron, decoff, decon, dec2off, dec2on, dec3off, dec3on, rcvroff, and rcvron. Statements for amplifier blanking and unblanking are obsblank, obsunblank, decblank, decunblank, dec2blank, dec2unblank, dec3blank, dec3unblank, blankingoff, and blankingon. Finally, statements for userdedicated lines are sp#off and sp#on. Table 14 summarizes these statements.

<pre>blankingoff()</pre>	Unblank amplifier channels and turn amplifiers on
blankingon()	Blank amplifier channels and turn amplifiers off
decblank()	Blank amplifier associated with the 1st decoupler
dec2blank()	Blank amplifier associated with the 2nd decoupler
dec3blank()	Blank amplifier associated with the 3rd decoupler
<pre>decoff()</pre>	Turn off first decoupler
<pre>dec2off()</pre>	Turn off second decoupler
<pre>dec3off()</pre>	Turn off third decoupler
decon()	Turn on first decoupler
dec2on()	Turn on second decoupler
dec3on()	Turn on third decoupler
decunblank()	Unblank amplifier associated with the 1st decoupler
dec2unblank()	Unblank amplifier associated with the 2nd decoupler
dec3unblank()	Unblank amplifier associated with the 3rd decoupler
dhpflag=TRUE FALSE	Switch decoupling between high- and low-power levels
<pre>initparms_sis()</pre>	Initialize parameters for spectroscopy imaging sequences
obsblank()	Blank amplifier associated with observe transmitter
obsunblank()	Explicitly enables the amplifier for the observe transmitter
<pre>rcvroff()</pre>	Turn off receiver gate and amplifier blanking gate
rcvron()	Turn on receiver gate and amplifier blanking gate
recoff()	Turn off receiver gate only
recon()	Turn on receiver gate only
setstatus*	Set status of observe transmitter or decoupler transmitter
<pre>status(state)</pre>	Change status of decoupler and homospoil
<pre>statusdelay(state,time)</pre>	Execute status statement with given delay time
<pre>xmtroff()</pre>	Turn off observe transmitter
<pre>xmtron()</pre>	Turn on observe transmitter
* setstatus(channel,on,mo	de,sync,mod_freq)

Table 14.	Gating	Control	Statements
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Gating States

Use status(state) to control decoupler and homospoil gating in a pulse sequence, where state is A to Z (e.g., status(A) or status(B)). Parameters controlled by status are dm (first decoupler mode), dmm (first decoupler modulation mode), and hs (homospoil). For systems with a third or fourth rf channel, dm2 and dm3 (second and third decoupler modes) and dmm2 and dmm3 (second and third decoupler modulation mode) are also under status control. For systems with a deuterium decoupler channel as the fourth decoupler, dm4 and dmm4 are under status control.

Each of these parameters can have multiple states: status(A) sets each parameter to the state described by the first letter of its value, status(B) uses the second letter, etc. If a pulse sequence has more status statements than there are status modes for a particular parameter, control reverts to the last letter of the parameter value. Thus, if dm = 'ny', status(C) will look for the third letter, find none, and then use the second letter (y) and turn the decoupler on. (The status statement is available on the *GEMINI 2000* although homospoil is not possible on *GEMINI 2000* systems.)

Use setstatus(channel, on, mode, sync, mod_freq)to control decoupler gating as well as decoupler modulation modes (GARP, CW, WALTZ, etc.). channel is

OBSch, DECch, DEC2ch, or DEC3ch, on is TRUE or FALSE, mode is a decoupler mode ('c', 'g', 'p', etc.), sync is TRUE or FALSE, and mod_freq is the modulation frequency (e.g., setstatus (DECch, TRUE, 'w', FALSE, dmf). (The setstatus statement is not available on the *MERCURY-VX*, *MERCURY*, or *GEMINI 2000*.)

setstatus provides a way to set transmitters independent of the parameters, one channel at a time. For example, setstatus (OBSch, TRUE, 'g', TRUE, obs_mf), turns the observe transmitter (OBSch) on (TRUE), using GARP modulation ('g') in synchronized mode (TRUE) with a modulation frequency of obs_mf. (The obs_mf parameter will need to be calculated from a parameter set with an appropriate getval statement.)

Note: Be sure to set the power to a safe level before calling setstatus.

Timing for setstatus is the same as for the status statement except that only one channel needs to be taken into account. To ensure that the timing is constant for the status, use the statusdelay statement (e.g., statusdelay(A, 2.0e-5)).

Homospoil gating is treated somewhat differently than decoupler gating. If a particular homospoil code letter is 'y', delays coded as hsdelay that occur when the status corresponds to that code letter will begin with a homospoil pulse, the duration of which is determined by the parameter hst. Thus if hs='ny', all hsdelay delays that occur during status(B) will begin with a homospoil pulse. The final status always occurs during acquisition, at which time a homospoil pulse is not permitted. Thus, if a particular pulse sequence uses status(A), status(B), and status(C), dm and other decoupler parameters may have up to three letters, but hs will only have two, since hs='y' during status(C) would be meaningless and is ignored.

Transmitter Gating

On all systems, transmitter gating is handled as follows:

- Explicit transmitter gating in the pulse sequence is provided by xmtroff() and xmtron(). Transmitter gating is handled automatically by obspulse, pulse, rgpulse, simpulse, sim3pulse, shaped_pulse, simshaped_pulse, sim3shaped_pulse, and spinlock. The obsprgon statement should generally be enabled with an explicit xmtron statement, followed by xmtroff.
- Explicit gating of the first decoupler in the pulse sequence is provided by decoff() and decon(). First decoupler gating is handled automatically by decpulse, decrgpulse, declvlon, declvloff, simpulse, sim3pulse, decshaped_pulse, sim3haped_pulse, sim3shaped_pulse, and decspinlock. The decprgon function should generally be enabled with explicit decon statement and followed by a decoff call.
- Explicit gating of the second decoupler in the pulse sequence is provided by dec2off and dec2on. Second decoupler gating is handled automatically by dec2pulse, dec2rgpulse, sim3pulse, dec2shaped_pulse, sim3shaped_pulse, and dec2spinlock. The dec2prgon function should generally be enabled with an explicit d2con statement, followed by dec2off.
- Likewise, explicit gating of the third decoupler in the pulse sequence is provided by dec3off and dec3on. Third decoupler gating is handled automatically by dec3pulse, dec3rgpulse, dec3shaped_pulse, and dec3spinlock. The dec3prgon function should generally be enabled with an explicit dec3con statement, followed by dec3off.

On the *GEMINI 2000*, all amplifier types are handled internally in declvlon() and declvloff(). No explicit declaration is needed (as described above). declvlon and declvloff have no effect on *MERCURY-VX* and *MERCURY* systems. The variable

declvlflag is added to *GEMINI 2000*, *MERCURY-VX*, and *MERCURY* pulse sequence programming to distinguish between the two within a pulse sequence (declvlflag is TRUE for *GEMINI 2000*, and FALSE for *MERCURY-VX* and *MERCURY*). See dept.c for an example.

On UNITY and VXR-S systems with class C amplifiers, to switch from low-power to highpower decoupling, insert the statement dhpflag=TRUE or the statement dhpflag=FALSE in a pulse sequence just before a status statement (correct use of upper and lower case letters is necessary). dhpflag=TRUE switches the system to highpower decoupling, and dhpflag=FALSE switches to low-power decoupling.

Receiver Gating

Explicit receiver gating in the pulse sequence is provided by the rcvroff(), rcvron(), recoff(), and recon() statements. These statements control the receiver gates except when pulsing the observe channel (in which case the receiver is off) or during acquisition (in which case the receiver is on). The recoff and recon statements (available only on UNITY *INOVA* systems) affect the receiver gate only and do not affect the amplifier blanking gate, which is the role of rcvroff and rcvron.

- On UNITY INOVA and GEMINI 2000, the receiver is on only during acquisition except for certain imaging pulse sequences that have explicit acquires (such as SEMS, MEMS, and FLASH), and for the initparms_sis() statement that defaults the receiver gate to on.
- On *MERCURY-VX*, *MERCURY*, UNITY, and VXR-S, receiver gating is tied to the amplifier blanking and is normally controlled automatically by the pulse statements rgpulse, pulse, obspulse, decrgpulse, decpulse, and dec2rgpulse.
- On UNITY*plus*, the observe amplifier blanking and the receiver gate are tied together. Because the decouplers do not affect the receiver (and vice versa), only the rgpulse, pulse, and obspulse statements and a shaped pulse statement gate the receiver.

Amplifier Channel Blanking and Unblanking

Amplifier channel blanking and unblanking methods depend on the system.

• On UNITY *INOVA*, the receiver and amplifiers are not linked. To explicitly blank and unblank amplifiers, the following statements are provided:

For the amplifier associated with the observe transmitter: obsblank() and obsunblank().

For the amplifiers associated with the first, second, and third decouplers: decblank() and decunblank(), dec2blank() and dec2unblank(), and dec3blank() and dec3unblank(), respectively.

These statements replace blankon and blankoff, no longer in VNMR.

- On *MERCURY-VX* and *MERCURY*, the receiver and amplifier are linked. At the end of each pulse statement, the receiver is automatically turned back on and the amplifier blanked. Immediately prior to data acquisition, the receiver is implicitly turned back on.
- On UNITY*plus*, the receiver is linked to the observe amplifier. The statements to blank and unblank amplifiers on the UNITY*INOVA* also apply to the UNITY*plus*.
- On UNITY and VXR-S, the receiver is linked to both amplifiers. At the end of each pulse statement, *if and only if the receiver has not been previously turned off explicitly by a* rcvroff() *statement*, the receiver is automatically turned back on and the amplifier blanked. Immediately prior to data acquisition, the receiver is implicitly turned back

on and the amplifier off. UNITY and VXR-S systems use the obsunblank() and decunblank() statements to unblank the amplifiers.

• On *GEMINI 2000*, the receiver and amplifier are not linked. The receiver is turned on just before the acquisition and turned off during the rest of the pulse sequence; however, the blankingon() and blankingoff() statements blank and unblank both amplifier channels, as well as turn the amplifiers off and on.

Interfacing to External User Devices

All consoles provide some means of interfacing to external user devices. Table 15 lists the statements available for this feature.

Table 15.	Interfacing	to External	User Devices	
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<pre>readuserap(rtvalue) setuserap(value,nreg)</pre>	Read input from user AP register Set user AP register
<pre>sp#off(), sp#on()</pre>	Turn off and on specified spare line
<pre>vsetuserap(rtvalue,nreg)</pre>	Set user AP register using real-time variable

User-Dedicated Spare Lines

One or more user-dedicated spare lines are available for high-speed device control:

- UNITY *INOVA* consoles have five spare lines in the Breakout panel on the rear of the left cabinet. Each spare line is a BNC connector. The sp#on() and sp#off() statements control specified SPARE lines.
- GEMINI 2000 consoles have a single user-dedicated spare line.
- UNITY*plus* consoles have two spare line on the front panel of the Pulse Sequence Controller board in the digital cardcage. Each spare line is a SMB connector. The sp#on() and sp#off() statements control specified SPARE lines. LEDs between the two connectors indicate activity on each line.
- UNITY and VXR-S consoles have spare lines on the Interface board.

User AP (Analog Port) Lines

UNITY *INOVA* consoles have two 24-pin user AP connectors, J8212 and J8213, in the Breakout panel on the rear of the left cabinet. Each connector has 16 user-controllable lines coinciding with two 8-bit AP bus registers. All four of the AP bus registers are writeable but only one register is readable.

lines 17 to 25 are ground lines.	Register	Connector	Lines	Function
User AP lines allow the	0	J8213	9 to 16	output
synchronous access by users to external services while running a	1	J8213	1 to 8	output
pulse sequence. The statements	2	J8212	9 to 16	output
<pre>setuserap(value,reg),</pre>	3	J8212	1 to 8	input/output

Table 16 shows the mapping of theuser AP lines. On both connectors,lines 17 to 25 are ground lines.

vsetuserap(rtvar, reg),
and readuserap(rtvar) provide access to these lines.

The setuserap and vsetuserap statements enable writing 8-bit information to one of four registers. Each write takes one AP bus cycle, which is 0.5 μ s for the UNITY *INOVA*. The

 Table 16.
 Mapping of User AP Lines

only difference between setuserap and vsetuserap is that vsetuserap uses a real-time variable to set the value.

The readuserap statement lets you read 8-bit information from the register into a realtime variable. You can then act on this information using real-time math and real-time control statements while the pulse sequence is running; however, because the system has to wait for the data to be read before it can continue parsing and stuffing the FIFO, a significant amount of overhead is involved in servicing the read and refilling the FIFO. The readuserap statement takes 500 μ s to execute. The readuserap statement puts in a 500 μ s delay immediately after reading the user AP lines in order for the parser to parse and stuff more words into the FIFO before it underflows. However, this time may not be long enough and you may want to pad this time with a delay immediately following the readuserap statement to avoid FIFO underflow. Depending on the actions in the pulse sequence, your delay may need to be a number of milliseconds. If there is an error in the read, a warning message is sent to the host and a -1 is returned to the real-time variable.

2.4 Pulse Sequence Statements: Phase and Sequence Control

As explained previously, a series of internal variables, named v1, v2, ..., v14, are provided to perform calculations during "real-time" (while the pulse sequence is executing). All realtime variables are pointers to particular memory locations in the acquisition computer. You do not change a real-time variable, rather you change the value in the memory location to which that real-time variable points.

For example, when we speak of v1 being set equal to 1, what we really means is that the value in the memory location pointed to by the real-time variable v1 is 1. The actual value of v1, a pointer, is not changed. The two ideas are interchangeable as long as we recognize exactly what is happening at the level of the acquisition computer.

These internal, real-time variables can be used for a number of purposes, but the two most important are control of the pulse sequence execution (for looping and conditional execution, for example) and calculation of phases. For each pulse in the sequence, the phase is calculated dynamically (at the start of each transient) rather than entirely at the start of this experiment. This allows phase cycles to attain essentially unlimited length, because only one number must be calculated for each phase during each transient. By contrast, attempting to calculate in advance a phase cycle with a cycle of 256 transients and different phases for each of 5 different pulses would require storing 256×5 or 1280 different phases.

Real-Time Variables and Constants

The following variables and constants can be used for real-time calculations:

- v1 to v14Real-time variables, used for calculations of loops, phases, etc. They
are at the complete disposal of the user. The variables point to 16-bit
integers, which can hold values of -32768 to +32767.ctCompleted transient counter, points to a 32-bit integer that is
incremented after each transient, starting with a value of 0 prior to the
 - first experiment. This pattern (0,1,2,3,4,...) is the basis for most calculations. Steady-state transients, invoked by the ss parameter, do not change ct.

Block size counter, points to a <i>16-bit integer</i> that is decremented from bs to 1 during each block of transients. After completing the last transient in the block, bsctr is set back to a value of bs. Thus if bs=8, bsctr has successive values of 8,7,6,5,4,3,2,1,8,7,
Real-time variable that controls the phase of the receiver in 90° increments (0=0°, 1=90°, 2=180°, and 3=270°). Prior to the execution of the pulse sequence itself, oph is set to 0 if parameter cp is set to 'n', or to the successive values $0, 1, 2, 3, 0, 1, 2, 3,$ if cp is set to 'y'. The value of oph can be changed explicitly in the pulse sequence by any of the real-time math statements described in the next section (assign, add, etc.) and is also changed by the setreceiver statement.
Pointers to constants set to select constant phases of 0° , 90° , 180° , and 270° . They <i>cannot</i> be replaced by numbers 0, 1, 2, and 3.
Real-time variables described in "Manipulating Acquisition Variables," page 102.
Pointers (or indexes) to constants identifying the current increment in multidimensional experiments. $id2$ is the current d2 increment. Its value ranges from 0 to the size of the d2 array minus 1, which is typically 0 to ($ni-1$). $id3$ corresponds to current index of the d3 array in a 3D experiment. Its range is 0 to ($ni2-1$). $id4$ corresponds to the current index of the d4 array. Its range is 0 to ($ni3-1$).

Calculating in Real-Time Using Integer Mathematics

A series of special integer mathematical statements are provided that are fast enough to execute in real-time: add, assign, dbl, decr, divn, hlv, incr, mod2, mod4, modn, mult, and sub. These statements are summarized in Table 17.

<pre>add(vi,vj,vk)</pre>	Add integer values: set vk equal to vi + vj
assign(vi,vj)	Assign integer values: set vj equal to vi
<pre>dbl(vi,vj)</pre>	Double an integer value: set vj equal to 2•vi
<pre>decr(vi)</pre>	Decrement an integer value: set vi equal to vi -1
<pre>divn(vi,vj,vk)</pre>	Divide integer values: set vk equal to vi div vj
<pre>hlv(vi,vj)</pre>	Find half the value of an integer: set vj to integer part of 0.5•vi
<pre>incr(vi)</pre>	Increment an integer value: set vi equal to vi + 1
<pre>mod2(vi,vj)</pre>	Find integer value modulo 2: set vj equal to vi modulo 2
<pre>mod4(vi,vj)</pre>	Find integer value modulo 4: set vj equal to vi modulo 4
<pre>modn(vi,vj,vk)</pre>	Find integer value modulo n: set vk equal to vi modulo vj
<pre>mult(vi,vj,vk)</pre>	Multiply integer values: set vk equal to vi•vj
<pre>sub(vi,vj,vk)</pre>	Subtract integer values: set vk equal to vi – vj

 Table 17. Integer Mathematics Statements

Remember that integer mathematics does not include fractions. If a fraction appears in a result, the value is truncated; thus, one-half of 3 is 1, not 1.5.

Integer statements also use the *modulo*, which is the number that remains after the modulo number is divided into the original number. For example, the value of 8 modulo 2 (often abbreviated "8 mod 2") is found by dividing 2 into 8, giving an answer of 4 with a remainder of 0, so 8 mod 2 is 0. Similarly, 9 mod 2 is 1, since 2 into 9 gives 4 with a

remainder of 1. The modulus of a negative number is not defined in VNMR software and should not be used.

Each statement performs one calculation at a time. For example, hlv(ct, vl) takes half the current value of ct and places it in the variable v1. Before each transient, ct has a given value (e.g., 7), and after this calculation, v1 has a certain value (e.g., 3 if ct was 7).

To visualize the action of a statement over the course of a number of transients, pulse sequences typically document this action explicitly as part of their comments. The comment v1=0, 0, 1, 1, ... (or v1=001122...) means that v1 assumes a value of 0 during the first transient, 0 during the second, 1 during the third, etc.

The following series of examples illustrates the action of integer mathematics statements and how comments are typically used:

~ 1	•	
hlv(ct,v1); /*	v1=0011223344	*/
dbl(v1,v1); /*	v1=0022446688	*/
mod4(v1,v1); /*	v1=0022002200	*/
mod2(ct,v2); /*	v2=010101	*/
dbl(v2,v3); /*	v3=020202	*/
/*	v1=00112233	*/
hlv(v1,v2); /*	v2=00001111	*/
dbl(v1,v1); /*	v1=00224466	*/
add(v1,v2,v3); /*	v3=00225577	* /
	VJ=00225577	/
mod4(v3,oph); /*		receiver phase cycle */

Note that the same variable can be used as the input and output of a particular statement (e.g., dbl(vl,vl)) is fine so it is not necessary to use dbl(vl,v2)). Note also that although the mod4 statement is used in several cases, it is never necessary to include it, even if appropriate, because an implicit modulo 4 is always performed on all phases (except when setting small-angle phase shifts).

The division provided by the divn statement is integer division, thus remainders are ignored. vj in each case must be a real-time variable and not a real number (like 6.0) or even an integer constant (like 6). To perform, for example, a modulo 6 operation, something like the following is required:

Controlling a Sequence Using Real-Time Variables

In addition to being used for phase calculations, real-time variables can also be used for pulse sequence control. Table 18 lists pulse sequence control statements.

elsenz(vi) endif(vi)	Execute succeeding statements if argument is nonzero End ifzero statement
<pre>endloop(index)</pre>	End loop
ifzero(vi)	Execute succeeding statements if argument is zero
<pre>initval(realnumber,vi)</pre>	Initialize a real-time variable to specified value
<pre>loop(count,index)</pre>	Start loop

Table 18. Pulse Sequence Control Statements

By placing pulse sequence statements between a loop(count, index) statement and an endloop(index) statement, the enclosed statements can be executed repeatedly.

The count argument used with loop is a real-time variable that specifies the number of times to execute the enclosed statements. count can be any positive number, including zero. index is a real-time variable used as a temporary counter to keep track of the number of times through the enclosed statements, and must not be altered by any of the statements. An example of using loop and endloop is the following:

```
mod4(ct,v5); /* times through loop: v5=01230123... */
loop(v5,v3); /* v3 is a dummy to keep track of count */
delay(d3); /* variable delay depending on the ct */
endloop(v3);
```

Statements within the pulse sequence can be executed conditionally by being enclosed within ifzero(vi), elsenz(vi), and endif(vi) statements. vi is a real-time variable used as a test variable, to be tested for either being zero or non-zero. The elsenz statement may be omitted if it is not desired. It is also not necessary for any statements to appear between the ifzero and the elsenz or the elsenz and the endif statements. The following code is an example of a conditional construction:

A syntactical difference exists between the *ifzero* statement on the *MERCURY* and *GEMINI 2000* systems compared to other Varian spectrometers. On the *MERCURY* and *GEMINI 2000*, the sequence above must be written as follows:

```
mod2(ct,v1);
ifzero(1,v1); /* note different syntax on GEMINI 2000 */
pulse(pw,v2);
delay(d3);
elsenz(1); /* note different syntax on GEMINI 2000 */
pulse(2.0*pw,v2);
delay(d3/2.0);
endif(1); /* note different syntax on GEMINI 2000 */
```

If numbers other than those easily accessible in integer math (such as ct, oph, three) are needed, any variable can be initialized to a value with the initval(number, vi) statement (e.g., initval(4.0, v9). The real number input is rounded off and placed in the variable vi. This statement, unlike the statements such as add and sub described above, is executed once and *only once* at the start of a non-arrayed 1D experiment or at the start of each increment in a 2D experiment or an arrayed 1D experiment, not at the start of each transient.

Real-Time vs. Run-Time—When Do Things Happen?

It may help to explain the pulse sequence execution process in more detail. When you enter go, the go program is executed. This program looks up the various parameters, examines the name of the current pulse sequence, and looks in seqlib for a file of that name. The file in seqlib is a compiled C program, which was compiled with the seqgen command. This program, which is run by the go program, combines the parameters supplied to it by go together with a series of instructions that form the pulse sequence.

Chapter 2. Pulse Sequence Programming

The output of the pulse sequence program in seqlib is a table of numbers, known as the *code table* (generally referred to as *Acodes* or *Acquisition codes*), which contains instructions for executing a pulse sequence in a special language. The pulse sequence program sends a message to the acquisition computer to begin operation, informing it where the code table is stored. This code table is downloaded into the acquisition computer and processed by an interpreter, which is executing in the acquisition computer and which controls operation during acquisition. If after entering go or su, etc., the message that PSG aborted abnormally appears, run the psg macro to help identify the problem.

A pulse sequence can intermix statements involving C, such as d2=1.0/(2.0*J), with special statements, such as hlv(ct, v2). These two statements are fundamentally different kinds of operations. When you enter go, all higher-level expressions are evaluated, once for each increment. Thus in d2=1.0/(2.0*J), the value of J is looked up, d2 is calculated as one divided by 2*J, and the value of d2 is fixed. Statements in this category are called run-time, since they are executed when go is run. The hlv statement, however, is executed every transient. Before each transient, the system examines the current value of ct, performs the integer hlv operation, and sets the variable v2 (used for phases, etc.) to that value. On successive transients, v2 has values of 0,0,1,1,2,2, etc. Statements like these are called *real-time*, because they execute during the real-time operation of the pulse sequence.

Run-time statements, then, are statements that are evaluated and executed in the host computer by the pulse sequence program in seqlib when you enter go. Real-time statements are statements that are repeatedly (every transient) executed by the code program run in the acquisition computer. Therefore, it is not possible to include a statement like d2=1.0+0.33*ct. The variable ct is a real-time variable (it is actually an integer pointer variable), while "C-type" mathematics are a run-time operation. Only the special real-time statements included in this section can be executed on a transient-by-transient basis.

Manipulating Acquisition Variables

Certain acquisition parameters, such as ss (steady-state pulses) and bs (block size), cannot be changed in a pulse sequence with a simple C statement. The reason is that by the time the pulsesequence function is executed, the values of these variables are already stored in a region of the host computer memory that will subsequently form the "low-core" portion of the acquisition code in the acquisition computer. These memory locations can be accessed and modified, however, by using real-time math functions with the appropriate real-time variables.

The value of ss in low core is associated with real-time variables ssval and ssctr:

- ssval is never modified by the acquisition computer unless specifically instructed by statements within the pulse sequence.
- ssctr is automatically initialized to ssval.

For the first increment *only*, if ssval is greater than zero, or else before every increment in a arrayed 1D or 2D experiment, ssctr is decremented after each steady-state transient until it reaches 0. When ssctr is 0, all subsequent transients are collected as data.

The value of bs in low core is associated with real-time variables bsval and bsctr:

- bsval is never modified by the acquisition computer unless specifically instructed by statements within the pulse sequence.
- bsctr is automatically initialized to bsval after each block of transients has been completed.

During the acquisition of a block of transients, bsctr is decremented after each transient. If bsval is non-zero, a zero value for bsctr signals that the block of transients is complete.

The ability within a pulse sequence to modify the values of these low core acquisition variables can be used to add various capabilities to pulse sequences. As an example, the following pulse sequence illustrates the cycling of pulse and receiver phases during steady-state pulses:

```
#include <standard.h>
pulsesequence()
{
    /* Implement steady-state phase cycling */
    sub(ct,ssctr,v10);
    initval(16.0,v9);
    add(v10,v9,v10);
    /* Phase calculation statements follow,
        using v10 in place of ct as the starting point */
    /* Actual pulse sequence goes here */
}
```

Intertransient and Interincrement Delays

When running arrayed or multidimensional experiments (using ni, ni2, etc.), certain operations are done preceding and following the pulse sequence for every array element, the same as there are operations preceding and following the pulse sequence for every transient. These overhead operations take up time that may need to be accounted for when running a pulse sequence. This might be especially important if the repetition time of a pulse sequence has to be maintained across every element and every scan during an arrayed or multidimensional experiment.

These overhead times between increments (array elements) and transients on UNITY INOVA systems are deterministic (i.e., both known and constant); however, the time between increments, which we will call x, is longer than the time between transients, which we will call y. Also, the time between increments will change depending on the number of rf channels.

To maintain a constant repetition time for UNITY *INOVA* systems, a parameter called d0 (for d-zero) can be created so that x=y+d0. Because the interincrement overhead time will differ with different system configurations—and to keep the d0 delay consistent across systems—if d0 is set greater than the overhead delay, the inter-FID delay x is padded such that y+d0=x+(d0-(x-y)). In other words, d0 is used to set a standard delay so the interincrement delay and the intertransient delay are the same when executing transient scans within an array element. The delay is inserted at the beginning of each scan of a FID after the first scan has completed. The d0 delay can be set by the user or computed by PSG (if d0 is set to 'n'). When d0 does not exist, no delay is inserted.

Another factor to consider when keeping a consistent timing in the pulse sequence is the status statement. The timing of this statement varies depending on the number of channels and the type of decoupler modulation. To keep this timing constant, there is the pulse sequence statement statusdelay that allows the user to set a constant delay time for changing the status. For this to work, the delay time has to be longer than the time it takes to set the status. For timing and more information, see the description of statusdelay in Chapter 3.

The overhead operations preceding every transient are resetting the DTM (data-tomemory) control information. The overhead operations following every transient are error detection for number of points and data overflow; detection for blocksize, end of scan, and stop acquisition; and resetting the decoupler status. d0 does not take these delays into account.

The overhead operations preceding every array element are initializing the rf channel settings (frequency, power, etc.), initializing the high-speed (HS) lines, initializing the DTM, and if arrayed, setting the receiver gain. d0 does not take into account arraying of decoupler status shims, VT, or spinning speed.

Controlling Pulse Sequence Graphical Display

The dps_off, dps_on, dps_skip, and dps_show statements, summarized in Table 19, can be inserted into a pulse sequence to control the graphical display of the pulse sequence statements by the dps command:

- To turn off dps display of statements, insert dps_off() into the sequence. All pulse sequences following dps_off will not be shown.
- To turn on dps display of statements, insert dps_on() into the sequence. All pulse sequences following dps_on will be shown.
- To skip dps display of the next statement, insert dps_skip() into the sequence. The next pulse sequence statement will not be displayed.
- To draw pulses for dps display, insert dps_show(options) statements into the pulse sequence. The pulses will appear in the graphical display of the sequence. Many options to dps_show are available. These options enable drawing a line to represent a delay, drawing a pulse picture and displaying the channel name below the picture, drawing shaped pulses with labels, drawing observe and decoupler pulses at the same time, and much more. Refer to Chapter 3, "Pulse Sequence Statement Reference," for a full description of dps_show, including examples.

 Table 19. Statements for Controlling Graphical Display of a Sequence

<pre>dps_off() dps_on()</pre>	Turn off graphical display of statements Turn on graphical display of statements
<pre>dps_show(options)*</pre>	Draw delay or pulses in a sequence for graphical display
dps_skip()	Skip graphical display of next statement
* dps_show has many options. See Chapter 3, "Pulse Sequence Statement Reference," for the syntax and examples of use.	

2.5 Real-Time AP Tables

Real-time acquisition phase (AP) tables can be created under pulse sequence control on all systems except *GEMINI 2000*. These tables can store phase cycles, an array of attenuator values, etc. In the pulse sequence, the tables are associated with variables t1, t2, ... t60.

The following pulse sequence statements accept the table variables t1 to t60 at any place where a simple AP variable, such as v1, can be used:

pulse	rgpulse	decpulse
decrgpulse	dec2rgpulse	dec3rgpulse
simpulse	txphase	decphase
dec2phase	dec3phase	xmtrphase
dcplrphase	dcplr2phase	dcplr3phase

phaseshift	spinlock	decspinlock
dec2spinlock	dec3spinlock	shaped_pulse
decshaped_pulse	dec2shaped_pulse	dec3shaped_pulse
simshaped_pulse	sim3shaped_pulse	power
pwrf		

For example, the statement rgpulse(pw,t1,rof1,rof2) performs an observe transmitter pulse whose phase is specified by a particular statement in the real-time AP table t1, whereas rgpulse(pw,v1,rof1,rof2) performs the same pulse whose phase is specified by the real-time variable v1. The real-time math functions add(), assign(), etc. listed in Table 17 cannot be used with tables t1-t60. The appropriate functions to use are given in Table 20.

Statements using a table can occur anywhere in a pulse sequence except in the statements enclosed by an ifzero-endif pair.

Loading AP Table Statements from UNIX Text Files

Table statements can be loaded from an external UNIX text file with the loadtable statement or can be set directly within the pulse sequence with the settable statement. The values stored must be integral and must lie within the 16-bit integer range of -32768 to 32767.

The AP table file must be placed in the user's private directory tablib, which might be, for example, /home/vnmr1/vnmrsys/tablib, or in the system directory for table files, /vnmr/tablib. The software looks first in the user's personal tablib directory for a table of the specified name, then in the system directory. The format for the table file is quite flexible, comments are allowed, and several special notations are available.

Table Names and Statements

Entries in the table file are referred to as *table names*. Each table name must come from the set t1 to t60 (e.g., t14 is a table name). A table name may be used only once within the table file. If a table name is used twice within the table file, an error message is displayed and pulse sequence generation (PSG) aborts.

Each table statement must be written as an integer number and separated from the next statement by some form of "white" space, such as a blank space, tab, or carriage return. The maximum number of statements per table is 8192. For the average pulse sequence, the maximum number of table statements per *experiment is* approximately 10,000.

The table name is separated from the table statements by an = or a += sign (the += sign is explained below), and there must be a space between the table name and either of these two signs. For example, if a table file contains the table name t1 with statements 0, 1, 2, 3, 2, 3, 0, 1, it would be written as t1 = 0 1 2 3 2 3 0 1.

The index into a table can range from 0 to 1 less than the number of statements in the table. Note that an index of 0 will access the *first* statement in the table. Unless the autoincrement attribute (described below) is imparted to the table, the index into the table is given by ct, the completed transient counter.

If the number of transients exceeds the length of the table, access to the table begins again at the beginning of the table. Thus, given a table of length n with statements numbered 0 through n-1 (this numbering is strictly a way to think about the numbering and does not imply the statements are actually numbered), then when the transient number is ct, the

number of the statement of the table that will be used is ct mod n (remember that ct starts at 0 on the first transient, since ct represents the number of *completed* transients).

AP Table Notation

Special notation is available within the table file to simplify entering the table statements and to impart specific attributes to any table within that file:

- (...)# Indicates the table segment within the parentheses is to be replicated in its entirety # times (where # ranges from 1 to 64) before preceding to any succeeding statements or segments. Do not include any space after ")". For example, t1=(0 1 2)3 /* t1 table=012012012 */.
- [...]# Indicates *each* statement in the table segment within square brackets is to be replicated # times (where # ranges from 1 to 64) before going to the *next* statement in that segment. Do not include any space after "]". For example,

t1=[0 1 2]3 /* t1 table=000111222 */.

- {...}# Imparts the "divn-return" attribute to the table and indicates that the
 actual index into the table is to be the index divided by the number
 # (where # ranges from 1 to 64). # is called the *divn factor* and can
 be explicitly set within a sequence for any table (see
 setdivnfactor). This attribute provides a #-fold level of table
 compaction to the acquisition processor. The { } notation *must*enclose *all* of the table statements for a given table. This notation
 should not be used if this table will be subject to table operations
 such as ttadd (see below)—in this case use []#, which is
 equivalent except for table compression. In entering the { }#
 notation, do not include any space after "}".
- += Indicates that the index into the table starts at 0 for each new FID in an array or 2D experiment, is incremented after *each* access of the table and is therefore independent of ct. This is the *autoincrement* attribute, which can delimit the table name from the table statements. It can be explicitly set within a pulse sequence for any table (see setautoincrement). Tables using the autoincrement feature cannot be accessed within a hardware loop.

The $(\ldots) \#$ and $[\ldots] \#$ notations are expanded by PSG at run-time and, therefore, offer no degree of table compaction to the acquisition processor. Nesting of (\ldots) and $[\ldots]$ expressions is not allowed. The autoincrement += attribute can be used in conjunction with the divn-return attribute and with the (\ldots) and $[\ldots]$ notations.

Multiple $\{\ldots\}$ expressions within one table are not allowed, but (\ldots) and $[\ldots]$ expressions can be placed within a $\{\ldots\}$ expression.

The following examples illustrate combining the notation:

incremented at each reference to table, not at each ct */

Handling AP Tables

Table 20 lists statements for handling AP tables. None of these statements apply to *GEMINI* 2000 systems.

<pre>getelem(tablename,APindes,APdest) loadtable(file)</pre>	Retrieve an element from an AP table Load AP table elements from table text file	
<pre>setautoincrement(tablename)</pre>	Set autoincrement attribute for an AP table	
<pre>setdivnfactor(tablename,divnfactor)</pre>	Set divn-return attribute and divn-factor	
<pre>setreceiver(tablename)</pre>	Associate rcvr. phase cycle with AP table	
settable*	Store array of integers in real-time AP table	
<pre>tsadd(tablename,scalarval,moduloval)</pre>	Add an integer to AP table elements	
<pre>tsdiv(tablename,scalarval,moduloval)</pre>	Divide an AP table into a second table	
<pre>tsmult(tablename,scalarval,moduloval)</pre>	Multiply an integer with AP table elements	
<pre>tssub(tablename,scalarval,moduloval)</pre>	Subtract an integer from AP table elements	
ttadd*	Add an AP table to a second table	
ttdiv*	Divide an AP table into a second table	
ttmult*	Multiply an AP table by a second table	
ttsub*	Subtract an AP table from a second table	
<pre>* settable(tablename,numelements,intarray) ttadd(tablenamedest,tablenamemod,moduloval) ttdiv(tablenamedest,tablenamemod,moduloval) ttmult(tablenamedest,tablenamemod,moduloval) ttdiv(tablenamedest,tablenamemod,moduloval)</pre>		

 Table 20.
 Statements for Handling AP Tables

The loadtable(file) statement loads AP table statements from table text file. file specifies the name of the table file (a UNIX text file) in the user's personal tablib directory or in the VNMR system tablib directory. loadtable can be called multiple times within a pulse sequence. Care should be taken to ensure that the same table name is not used more than once by the pulse sequence.

The settable(tablename, numelements, intarray) statement stores an array of integers in a real-time AP table. tablename specifies the name of the table (t1 to t60). numelements specifies the size of the table. intarray is a C array that contains the table elements. These elements can range from -32768 to 32767. The user must predefine and predimension this array in the pulse sequence using C language statements prior to calling settable.

The getelem(tablename, APindex, APdest) statement retrieves an element from an AP table. tablename specifies the name of the Table (t1 to t60). APindex is an AP variable (v1 to v14, oph, ct, bsctr, or ssctr) that contains the index of the desired table element. Note that the first element of an AP table has an index of 0. APdest is also an AP variable (v1 to v14 and oph) into which the retrieved table element is placed. For tables for which the autoincrement feature is set, APindex, the second argument to getelem, is ignored and can be set to any AP variable name; each element in such a table is by definition always accessed sequentially.

The setautoincrement (tablename) statement sets the autoincrement attribute for an AP table. tablename specifies the name of the table (t1 to t60). The index into the table is set to 0 at the start of an FID acquisition and is incremented after each access into the table. Tables using the autoincrement feature cannot be accessed within a hardware loop.

Chapter 2. Pulse Sequence Programming

The setdivnfactor(tablename, divnfactor) statement sets the divn-return attribute and the divn-factor for an AP table. tablename specifies the name of the table (t1 to t60). The actual index into the table is now set to (index/divnfactor). {0 1}2 is therefore translated by the acquisition processor, not by pulse sequence generation (PSG), into 0 0 1 1. The divn-return attribute results in a divn-factor-fold compression of the AP table at the level of the acquisition processor.

The setreceiver(tablename) statement assigns the ctth element of the AP table tablename to the receiver variable oph. If multiple setreceiver statements are used in a pulse sequence, or if the value of oph is changed by real-time math statements such as assign, add, etc., the last value of oph prior to the acquisition of data determines the value of the receiver phase.

To perform run-time scalar operations of an integer with AP table elements, use the following statements:

```
tsadd(tablename,scalarval,moduloval)
tssub(tablename,scalarval,moduloval)
tsmult(tablename,scalarval,moduloval)
tsdiv(tablename,scalarval,moduloval)
```

where tablename specifies the name of the table (t1 to t60) and scalarval is added to, subtracted from, multiplied with, or divided into each element of the table. The result of the operation is taken modulo moduloval (if moduloval is greater than 0). tsdiv requires that scalarval is not equal to 0; otherwise, an error is displayed and PSG aborts.

To perform run-time vector operations of one AP table with a second table, use the following table-to-table statements:

```
ttadd(tablenamedest,tablenamemod,moduloval)
ttsub(tablenamedest, tablenamemod, moduloval)
ttmult(tablenamedest,tablenamemod,moduloval)
ttdiv(tablenamedest, tablenamemod,moduloval)
```

where tablenamedest and tablenamemod are the names of tables (t1 to t60). Each element in tablenamedest is modified by the corresponding element in tablenamemod. The result, stored in tablenamedest, is taken modulo moduloval (if moduloval is greater than 0). The number of elements in tablenamedest must be greater than or equal to the number of elements in tablenamemod. ttdiv requires that no element in tablenamemod equal 0.

Examples of Using AP Tables

This section contains a two-pulse sequence and a homonuclear J-resolved experiment as examples of using AP tables.

Two-Pulse Sequence

Listing 7 is the contents of the files /home/vnmr1/vnmrsys/psglib/t2pul.c and /home/vnmr1/vnmrsys/tablib/t2pul associated with a hypothetical two-pulse sequence T2PUL.

Notice that t2 and t3 are identical. The pulse sequence could have used just one phase for both the observe pulse and the receiver, but using two separate phases in this way provides more flexibility for allowing run-time modification of all phases independently (e.g., a cancellation experiment can be run by changing line 2 in the tablib file to t2 = 0 or by changing line 3 to t3 = 0).

```
#include <standard.h>
                                    t1 = 0
                                      /* 0000 */
                                    t2 = 0 2 1 3
pulsesequence()
                                      /* 0213 */
{
                                    t3 = 0 2 1 3
   loadtable("t2pul");
                                      /* 0213 */
   status(A);
     hsdelay(d1);
   status(B);
      pulse(p1,t1);
      hsdelay(d2);
   status(C);
      pulse(pw,t2);
      setreceiver(t3);
}
```

Listing 7. Two-Pulse Sequence t2pul.c with Phase Tables

Homonuclear J-Resolved Experiment

Listing 8 lists files /home/vnmr1/vnmrsys/psglib/hom2djt.c and /home/ vnmr1/vnmrsys/tablib/hom2djt associated with a hypothetical homonuclear J-resolved sequence HOM2DJT.

Listing 8. Homonuclear J-Resolved Sequence hom2djt.c with Phase Tables

```
#include <standard.h>
                                    t1 = [0]16
                                      /*000000000000000 */
pulsesequence()
{
                                    t2 = (1 \ 2 \ 3 \ 0)4
   loadtable("hom2djt");
                                      /*1230123012301230 */
   ttadd(t1,t4,4);
                                    t3 = (0 \ 2)8
   ttadd(t2,t4,4);
                                      /*0202020202020202 */
   ttadd(t3,t4,4);
                                    t4 = [0 \ 2 \ 1 \ 3]4
   status(A);
                                      /* 0000222211113333 */
     hsdelay(d1);
   status(B);
      pulse(pw,t1);
      delay(d2/2);
      pulse(p1,t2);
      delay(d2/2);
   status(C);
      setreceiver(t3);
}
```

This sequence uses "conventional" phase cycling, completely different than the pulse cycling in the standard HOM2DJ sequence found in psglib. The phase cycling, contained here in t4, is added to the phases by the pulse sequence itself with the series of three ttadd statements. This can also be done in the table itself, for example, by replacing the t2 line in the tablib file with t2 = 1 2 3 0 3 0 1 2 2 3 0 1 0 1 2 3, which is the completely "spelled out" phase cycle for the second pulse.

When using a table to be referenced with a ttadd statement, you *cannot* compress the table by using $t4 = \{0 \ 2 \ 1 \ 3\}4$. You must use square brackets, which are exactly equivalent to the curly brackets but without achieving table compression at the level of the acquisition processor.

2.6 Accessing Parameters

The getval and getstr statement look up the value of parameters, providing access to parameters. Table 21 summarizes these statements.

Table 21. Parameter Value Lookup Statements

<pre>getstr(parametername,internalname)</pre>	Look up value of string parameter
internalname= <mark>getval</mark> (parametername)	Look up value of numeric parameter

Parameters are defined by the user in particular experiment files (exp1, exp2, etc.) in which the operation is occurring. These parameters are not the same as the parameters that are accessible to the pulse sequence during its execution, although they are at least potentially the same.

Categories of Parameters

Parameters can be divided into three categories:

• Parameters used in a pulse sequence exactly as in the parameter set; in other words, the name of the parameter (d1, for example) is the same in both places. Thus, a statement like delay(d1); is legitimate. Table 22 lists VNMR parameter names and corresponding pulse sequence generation (PSG) variable names and types. Table 23 summarizes VNMR parameter names used primarily for imaging. (Not available on the *GEMINI 2000* are d3, d4, dfrq2, dfrq3, dm2, dm3, dm4, dmf2, dmf3, dmm2, dmm3, dmm4, dof2, dof3, dof4, dpwr2, dpwr3, dpwr4, dres, dres2, dres3, dres4, dseq, dseq2, dseq3, homo, homo2, homo3, inc2D, inc3D, inc4D, nf, phase2, phase3, pwx, satdly, satpwr, and satmode.)

Acquisit	ion		
extern	char	il[MAXSTR]	interleaved acquisition parameter, ' y ' , ' n ' , c
extern	double	inc2D	t1 dwell time in a 3D/4D experiment
extern	double	inc3D	t2 dwell time in a 3D/4D experiment
extern	double	SW	Sweep width
extern	double	nf	Number of FIDs in pulse sequence /
extern	double	np	Number of data points to acquire
extern	double	nt	Number of transients
extern	double	sfrq	Transmitter frequency mix
extern	double	dfrq	Decoupler frequency MHz
extern	double	dfrq2	2nd decoupler frequency MHz
extern	double	dfrq3	3rd decoupler frequency MHz
extern	double	dfrq4	4th decoupler frequency MHz
extern	double	fb	Filter bandwidth
extern	double	bs	Block size
extern	double	tof	Transmitter offset
extern	double	dof	Decoupler offset
extern	double	dof2	2nd decoupler offset
extern	double	dof3	3rd decoupler offset
extern	double	dof4	4th decoupler offset
extern	double	gain	Receiver gain value, or 'n' for autogain
extern	double	dlp	Decoupler low power value
extern	double	dhp	Decoupler low power value
extern	double	tpwr	Transmitter pulse power
extern	double	tpwrf	Transmitter fine linear attenuator for pulse
extern	double	dpwr	Decoupler pulse power
extern	double	dpwrf	Decoupler fine linear attenuator for pulse
extern	double	dpwrf2	2nd decoupler fine linear attenuator
extern	double	dpwrf3	3rd decoupler fine linear attenuator
extern	double	dpwrf4	4th decoupler fine linear attenuator
extern	double	dpwr2	2nd decoupler pulse power
extern	double	dpwr3	3rd decoupler pulse power
extern	double	dpwr4	4th decoupler pulse power
extern	double	filter	Pulse amp filter setting
extern	double	xmf	Transmitter modulation frequency
extern	double	dmf	Decoupler modulation frequency
extern	double	dmf2	Decoupler modulation frequency
extern	double	fb	Filter bandwidth
extern	double	vttemp	VT temperature setting
extern	double	vtwait	VT temperature time-out setting
extern	double	vtc	VT temperature cooling gas setting
extern	double	cpflag	Phase cycling; 1=no cycling, 0=quad detect
extern	double	dhpflag	Decoupler high power flag

	Table 22.	Global]	PSG	Parameters
--	-----------	----------	-----	------------

Pulse W	ïdths		
extern	double	рw	Transmitter modulation frequency
extern	double	pl	A pulse width
extern	double	pw90	90° pulse width
extern	double	hst	Time homospoil is active
Delays			
extern	double	alfa	Time after receiver is turned on that acquisition begins
extern	double	beta	Audio filter time constant
extern	double	dl	Delay
extern	double	d2	A delay, used in 2D experiments
extern	double	d3	A delay, used in 3D experiments
extern	double	d4	A delay, used in 4D experiments
extern	double	pad	Preacquisition delay
extern	double	padactive	Preacquisition delay active parameter flag
extern	double	rofl	Time receiver is turned off before pulse
extern	double	rof2	Time receiver is turned on before receiver is turned on
Total Tin	ne of Exper	iment	
extern	double	totaltime	Total timer events for an experiment duration estimate
extern	int	phasel	2D acquisition mode
extern	int	phase2	3D acquisition mode
extern	int	phase3	4D acquisition mode
extern	int	d2_index	d2 increment (from 0 to ni-1)
extern	int	d3_index	d3 increment (from 0 to ni2-1)
extern	int	d4_index	d4 increment (from 0 to ni3-1)
Program	ımable Dec	oupling Sequences	
extern	char	xseq[MAXSTR]	
extern	char	dseq[MAXSTR]	
extern	char	dseq2[MAXSTR]	
	cilui	USEYZ[MAASIR]	
extern	char	dseq3[MAXSTR]	
extern extern			
	char	dseq3[MAXSTR]	Digit resolution prg dec
extern	char char	dseq3[MAXSTR] dseq4[MAXSTR]	Digit resolution prg dec Digit resolution prg dec
extern extern	char char double	dseq3[MAXSTR] dseq4[MAXSTR] xres	
extern extern extern	char char double double	dseq3[MAXSTR] dseq4[MAXSTR] xres dres	Digit resolution prg dec
extern extern extern extern	char char double double double	dseq3[MAXSTR] dseq4[MAXSTR] xres dres dres2	Digit resolution prg dec Digit resolution prg dec
extern extern extern extern extern	char char double double double double	dseq3[MAXSTR] dseq4[MAXSTR] xres dres dres2 dres3	Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec
extern extern extern extern extern extern	char char double double double double	dseq3[MAXSTR] dseq4[MAXSTR] xres dres dres2 dres3	Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec
extern extern extern extern extern extern <i>Status C</i>	char char double double double double double	dseq3[MAXSTR] dseq4[MAXSTR] xres dres dres2 dres3 dres4	Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec
extern extern extern extern extern <i>Status C</i> extern	char char double double double double double	dseq3[MAXSTR] dseq4[MAXSTR] xres dres dres2 dres3 dres4 xm[MAXSTR]	Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec Transmitter status control
extern extern extern extern extern <i>Status C</i> extern extern	char char double double double double double control char char	dseq3[MAXSTR] dseq4[MAXSTR] xres dres dres2 dres3 dres4 xm[MAXSTR] xmm[MAXSTR]	Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec Digit resolution prg dec Transmitter status control Transmitter modulation type control

Table 22. Global PSG Parameters (continued)

extern	char	dmm2[MAXSTR]	2nd decoupler modulation type control
extern	char	dm3[MAXSTR]	3rd decoupler status control
extern	char	dmm3[MAXSTR]	3rd decoupler modulation type control
extern	char	dm4[MAXSTR]	4th decoupler status control
extern	char	dmm4[MAXSTR]	4th decoupler modulation type control
extern	char	homo[MAXSTR]	1st decoupler homo mode control
extern	char	homo2[MAXSTR]	2nd decoupler homo mode control
extern	char	homo3[MAXSTR]	3rd decoupler homo mode control
extern	char	homo4[MAXSTR]	4th decoupler homo mode control
extern	int	xmsize	Number of characters in xm
extern	int	xmmsize	Number of characters in xmm
extern	int	dmsize	Number of characters in dm
extern	int	dmmsize	Number of characters in dmm
extern	int	dm2size	Number of characters in dm2
extern	int	dmm2size	Number of characters in dmm2
extern	int	dm3msize	Number of characters in dm3
extern	int	dmm3msize	Number of characters in dmm3
extern	int	dm4size	Number of characters in dm4
extern	int	dmm4msize	Number of characters in dmm4
extern	int	homosize	Number of characters in homo
extern	int	homo2size	Number of characters in homo2
extern	int	homo3size	Number of characters in homo3
extern	int	homo4size	Number of characters in homo4
extern	int	hssize	Number of characters in hs

Table 22. Global PSG Parameters (continued)

Table 23. Imaging Variables

RF Puls	ses		
extern	double	p2	Pulse length
extern	double	р3	Pulse length
extern	double	p4	Pulse length
extern	double	р5	Pulse length
extern	double	pi	Inversion pulse length
extern	double	psat	Saturation pulse length
extern	double	pmt	Magnetization transfer pulse length
extern	double	pwx	X-nucleus pulse length
extern	double	pwx2	X-nucleus pulse length
extern	double	psl	Spin-lock pulse length
extern	char	pwpat[MAXSTR]	Pattern for pw, tpwr
extern	char	pwlpat[MAXSTR]	Pattern for p1, tpwr1
extern	char	pw2pat[MAXSTR]	Pattern for p2, tpwr2
extern	char	pw3pat[MAXSTR]	Pattern for pw3, tpwr3
extern	char	pw4pat[MAXSTR]	Pattern for pw4, tpwr4

extern	char	pw5pat[MAXSTR]	Pattern for pw5, tpwr5
extern	char	pipat[MAXSTR]	Pattern for pi, tpwri
extern	char	satpat[MAXSTR]	Pattern for pw, tpwr
extern	char	mtpat[MAXSTR]	Pattern for psat, satpat
extern	char	ps1pat[MAXSTR]	Pattern for spin-lock
extern	double	tpwrl	Transmitter pulse power
extern	double	tpwr2	Transmitter pulse power
extern	double	tpwr3	Transmitter pulse power
extern	double	tpwr4	Transmitter pulse power
extern	double	tpwr5	Transmitter pulse power
extern	double	tpwri	Inversion pulse power
extern	double	satpwr	Saturation pulse power
extern	double	mtpwr	Magnetization transfer pulse power
extern	double	pwxlvl	pwx pulse level
extern	double	pwxlvl2	pwx2 power level
extern	double	tpwrsl	Spin-lock power level
RF Deco	oupler Pul	ses	
extern	char	decpat[MAXSTR]	Pattern for decoupler pulse
extern	char	decpat1[MAXSTR]	Pattern for decoupler pulse
extern	char	decpat2[MAXSTR]	Pattern for decoupler pulse
extern	char	decpat3[MAXSTR]	Pattern for decoupler pulse
extern	char	decpat4[MAXSTR]	Pattern for decoupler pulse
		-	
extern	char	decpat5[MAXSTR]	Pattern for decoupler pulse
extern extern	char char	decpat5[MAXSTR] dpwr1	Pattern for decoupler pulse Decoupler pulse power
		_	
extern	char	dpwr1	Decoupler pulse power
extern extern	char char char	dpwr1 dpwr4	Decoupler pulse power Decoupler pulse power
extern extern extern	char char char	dpwr1 dpwr4 dpwr5	Decoupler pulse power Decoupler pulse power Decoupler pulse power
extern extern extern <i>Gradien</i>	char char char char	dpwr1 dpwr4	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength
extern extern extern <i>Gradien</i> extern	char char char double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3	Decoupler pulse power Decoupler pulse power Decoupler pulse power
extern extern extern <i>Gradien</i> extern extern	char char char <i>tts</i> double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D
extern extern Gradien extern extern extern	char char char double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients
extern extern Gradien extern extern extern extern	char char char <i>ats</i> double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus
extern extern <i>Gradien</i> extern extern extern extern extern extern	char char char <i>tts</i> double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus
extern extern extern extern extern extern extern extern extern extern	char char char double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction
extern extern extern extern extern extern extern extern extern extern extern	char char char <i>tts</i> double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction
extern extern <i>Gradien</i> extern extern extern extern extern extern extern extern extern	char char char double double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf g0, g1, g9	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction Numbered levels
extern extern extern extern extern extern extern extern extern extern extern extern extern	char char char double double double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf g0, g1, g9 gx, gy, gz	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction Slice-select refocus fraction Numbered levels X, Y, and Z levels
extern extern extern extern extern extern extern extern extern extern extern extern extern extern	char char char <i>tts</i> double double double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf g0, g1, g9 gx, gy, gz gvox1, gvox2, gvox3	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction Slice-select refocus fraction Numbered levels X, Y, and Z levels Voxel selection
extern extern extern extern extern extern extern extern extern extern extern extern extern extern extern	char char char double double double double double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf g0, g1, g9 gx, gy, gz gvox1, gvox2, gvox3 gdiff	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction Slice-select refocus fraction Numbered levels X, Y, and Z levels Voxel selection Diffusion encode
extern extern extern extern extern extern extern extern extern extern extern extern extern extern extern	char char char <i>tts</i> double double double double double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf g0, g1, g9 gx, gy, gz gvox1, gvox2, gvox3 gdiff gflow	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction Slice-select refocus fraction Numbered levels X, Y, and Z levels Voxel selection Diffusion encode Flow encode
extern extern extern extern extern extern extern extern extern extern extern extern extern extern extern extern	char char char <i>tts</i> double double double double double double double double double double double double	dpwr1 dpwr4 dpwr5 gro, gro2, gro3 gpe, gpe2, gpe3 gss, gss2, gss3 gror gssr grof gssf g0, g1, g9 gx, gy, gz gvox1, gvox2, gvox3 gdiff gflow gspoil, gspoil2	Decoupler pulse power Decoupler pulse power Decoupler pulse power Readout gradient strength Phase encode for 2D, 3D, and 4D Slice-select gradients Readout focus Slice-select refocus Readout refocus fraction Slice-select refocus fraction Slice-select refocus fraction Numbered levels X, Y, and Z levels Voxel selection Diffusion encode Flow encode Spoiler gradient levels

Table 23. Imaging Variables (continued)

extern	double	gpemult	Shaped phase encode multiplier
extern	double	gradstepsz	Positive steps in the gradient DAC
extern	double	gradunit	Dimensional conversion factor
extern	double	gmax	Maximum gradient value (G/cm)
extern	double	gxmax	X maximum gradient value (G/cm)
extern	double	gymax	Y maximum gradient value (G/cm)
extern	double	gzmax	Z maximum gradient value (G/cm)
extern	double	gtotlimit	Limit combined gradient values (G/cm)
extern	double	gxlimit	Safety limit for X gradient (G/cm)
extern	double	gylimit	Safety limit for Y gradient (G/cm)
extern	double	gzlimit	Safety limit for Z gradient (G/cm)
extern	double	gxscale	X scaling factor for gmax
extern	double	gyscale	Y scaling factor for gmax
extern	double	gzscale	Z scaling factor for gmax
extern	char	gpatup[MAXSTR]	Gradient ramp-up pattern
extern	char	gpatdown[MAXSTR]	Gradient ramp-down pattern
extern	char	gropat[MAXSTR]	Readout gradient pattern
extern	char	gpepat[MAXSTR]	Phase encode gradient pattern
extern	char	gsspat[MAXSTR]	Slice gradient pattern
extern	char	gpat[MAXSTR]	General gradient pattern
extern	char	gpat1[MAXSTR]	General gradient pattern
extern	char	gpat2[MAXSTR]	General gradient pattern
extern	char	gpat3[MAXSTR]	General gradient pattern
extern	char	gpat4[MAXSTR]	General gradient pattern
extern	char	gpat5[MAXSTR]	General gradient pattern
Delays			
extern	double	tr	Repetition time per scan
extern	double	te	Primary echo time
extern	double	ti	Inversion time
extern	double	tm	Mid-delay for STE
extern	double	at	Acquisition time
extern	double	tpe, tpe2, tpe3	Phase encode durations for 2D to 4D
extern	double	tcrush	Crusher gradient duration
extern	double	tdiff	Diffusion encode duration
extern	double	tdelta	Diffusion encode duration
extern	double	tDELTA	Diffusion gradient separation
extern	double	tflow	Flow encode duration

Spoiler duration

Saturation time

General use delay

Physiological trigger hold off

User variable for total experiment time

Gradient coil rise time: sec

Table 23. Imaging Variables (continued)

double

double

double

double

double

double

tspoil

hold

tau

trise

satdly

runtime

extern

extern

extern

extern

extern

extern

Frequencies			
extern	double	resto	Reference frequency offset
extern	double	wsfrq	Water suppression offset
extern	double	chessfrq	Chemical shift selection offset
extern	double	satfrq	Saturation offset
extern	double	mtfrq	Magnetization transfer offset
Physica	l Sizes and	Positions (for slices, voxe	ls, and FOV)
extern	double	pro	FOV position in readout
extern	double	ppe, ppe2, ppe3	FOV position in phase encode
extern	double	pos1, pos2, pos3	Voxel position
extern	double	pss[MAXSLICE]	Slice position array
extern	double	lro	Readout FOV
extern	double	lpe, lpe2, lpe3	Phase encode FOV
extern	double	lss	Dimension of multislice range
extern	double	vox1, vox2, vox3	Voxel size
extern	double	thk	Slice or slab thickness
extern	double	lpe, lpe2, lpe3	Phase encode FOV
extern	double	fovunit	Dimensional conversion factor
extern	double	thkunit	Dimensional conversion factor
Bandwi	dths		
extern	double	sw1, sw2, sw3	Phase encode bandwidths
Counts	and Flags		
extern	double	nD	Experiment dimensionality
extern	double	ns	Number of slices
extern	double	ne	Number of echoes
extern	double	ni	Number of standard increments
extern	double	nv, nv2, nv3	Number phase encode views
extern	double	SSC	Compressed ss transients
extern	double	ticks	External trigger counter
extern	char	ir[MAXSTR]	Inversion recovery flag
extern	char	ws[MAXSTR]	Water suppression flag
extern	char	mt[MAXSTR]	Magnetization flag
extern	char	pilot[MAXSTR]	Auto gradient balance flag
extern	char	seqcon[MAXSTR]	Acquisition loop control flag
extern	char	petable[MAXSTR]	Name for phase encode table
extern	char	acqtype[MAXSTR]	Example: "full" or "half" echo
extern	char	exptype[MAXSTR]	Example: "se" or "fid" in CSI
extern	char	apptype[MAXSTR]	Keyword for parameter init, e.g, "imaging"
extern	char	seqfile[MAXSTR]	Pulse sequence name
extern	char	rfspoil[MAXSTR]	rf spoiling flag
extern	char	satmode[MAXSTR]	Presentation mode
CAUCITI	chai	SACHOUCE[MAASIK]	

 Table 23. Imaging Variables (continued)

extern	char	verbose[MAXSTR]	Verbose mode for sequences and psg
Miscelle	aneous		
extern	double	rfphase	rf phase shift
extern	double	в0	Static magnetic field level
extern	double	slcto	Slice selection offset
extern	double	delto	Slice spacing frequency
extern	double	tox	Transmitter offset
extern	double	toy	Transmitter offset
extern	double	toz	Transmitter offset
extern	double	griserate	Gradient rise rate

Table 23. Imaging Variables (continued)

- Parameters used in the pulse sequence derived from those in the parameter set.
- Parameters unknown to the pulse sequence. This includes parameters created by the user for a particular pulse sequence (such as J or mix) as well as a few surprises, such as at, the acquisition time (the pulse sequence does not know this). The statements getval and getstr are provided for this category.

Looking Up Parameter Values

The statement internalname=getval (parametername) allows the pulse sequence to look up the value of any numeric parameter that it otherwise does not know (parametername) and introduce it into the pulse sequence in the variable internalname. internalname can be any legitimate C variable name that has been defined as type double at the beginning of the pulse sequence (even if it is created as type integer). If parametername is not found in the current experiment parameter list, internalname is set to zero, and PSG produces a warning message. For example, double j;

```
j=getval("j");
```

. . .

The getstr(parametername, internalname) statement is used to look up the value of the string parameter parametername in the current experiment parameter list and introduce it into the pulse sequence in the variable internalname. internalname can be any legitimate C variable name that has been defined as array of type char with dimension MAXSTR at the beginning of the pulse sequence. If the string parameter parametername is not found in the current experiment parameter list,

internalname is set to the null string, and PSG produces a warning message. For example:

```
char coil[MAXSTR];
...
getstr("sysgcoil",coil);
```

Using Parameters in a Pulse Sequence

As an example of using parameters in a pulse sequence, suppose you wish to create a new pulse sequence with new variable names and have it fully functional from VNMR. Usually, the best way to compose a new pulse sequence is to start from a known good pulse sequence

and from a known good parameter set. For many pulse sequences, s2pul.c in /vnmr/psglib and s2pul.par in /vnmr/parlib are a good place to start.

To create a new pulse sequence similar to s2pul but with new variable names and using a shaped pulse, do the following steps:

- 1. In a shell window, enter cd ~/vnmrsys/psglib.
- 2. Use a text editor such as vi to create the file newpul.c shown in Listing 9.

Listing 9. File newpul.c for a New Pulse Sequence

```
/* newpul.c - new pulse sequence */
#include <standard.h>
static int ph2[4] = \{0, 1, 2, 3\};
pulsesequence()
{
  double dlnew, d2new, plnew, pwnew;
  char patnew[MAXSTR];
  dlnew = getval("dlnew");
  d2new = getval("d2new");
  plnew = getval("plnew");
  pwnew= getval("pwnew");
  getstr("patnew",patnew);
  assign(zero,v1);
  settable(t2,4,ph2);
  getelem(t2,ct,v2);
  /* equilibrium period */
  status(A);
  hsdelay(d1new);
  /* --- tau delay --- */
  status(B);
  pulse(plnew,v1);
 hsdelay(d2new);
  /* --- observe period --- */
  status(C);
  shaped_pulse(patnew,pwnew,v2,rof1,rof2);
   /* If you don't have a waveform generator, */
   /* use the following line: */
   /* apshaped_pulse(patnew,pwnew,v2,t4,t5,rof1,rof2); */
}
```

3. After newpul.c is created, in a shell window, enter **seqgen newpul**.

```
The following lines are displayed during pulse sequence generation:
Beginning Pulse Sequence Generation Process...
Adding DPS extensions to Pulse Sequence...
Lint Check of Sequence...
Compiling Sequence...
Link Loading...
Done! Pulse sequence newpul now ready to use.
```

4. To use the pulse sequence in VNMR, add new parameters starting from a known good parameter set (e.g. s2pul.par) by entering from the VNMR command line: s2pul

```
seqfil='newpul'
create('dlnew','delay') dlnew=1
create('d2new','delay') d2new=.001
create('plnew','pulse') plnew=0
create('pwnew','pulse') pwnew=40
create('patnew','string') patnew='square'
```

- 5. The parameters need to be saved as newpul.par in parlib so you can easily retrieve them the next time you run the pulse sequence. Enter: cd cd('vnmrsys/parlib') svp('newpul')
- 6. To access the new parameters and pulse sequence, create a macro by entering, for example:

editmac('newpul')

7. In the pop-up editor window, type editmac('newpul') to enter the insert mode and add the line:

```
psgset('newpul','array','dg','dlnew','d2new','plnew','pwnew','patnew')
```

Save the macro and exit. This macro requires the file newpul.par to be present in parlib.

You can now enter newpul in the VNMR command line any time you wish to use your new pulse sequence. Most of the pulse sequences in /vnmr/psglib are set up in a similar fashion, and so are easily accessible.

The newpul.c pulse sequence also contains examples of phase cycling. There are two basic ways to perform arbitrary user-defined phase cycling:

- Use the real-time variables v1-v14, oph, zero, one, two, and three, and perform math integer operations on them using functions in Table 17.
- Use the real-time AP tables t1-t60, which may be assigned either by static variable declarations and using settable(), or by loading in a table from tablib using loadtable() (see Table 20).

An example of using the real-time variable v1 is given in newpul.c used by assign() and pulse(). An example of using real-time AP tables is given using ph2 and t2. We could also replace v2 with t2 in the shaped_pulse() statement in this particular pulse sequence. In some cases, however, it is necessary to perform further integer math operations on the phase cycle, which is easier to perform on real-time variables than on AP tables, so we give the example using getelem() to assign the table t2 to variable v2. For other examples of phase cycling calculations, see the pulse sequences in /vnmr/psglib.

To add 2D parameters to the newpul.c pulse sequence, make the following changes:

- In step 2, change d2new to d2.
- In step 4, enter par2d set2d('newpul') plnew=40.
- In step 7, add par 2d set 2d('newpul') to the newpul macro after the psgset line.

Also, see the cosyps.c pulse sequence in /vnmr/psglib, section 2.14 "Multidimensional NMR," page 148, and the chapter on Multidimensional NMR in the User Guide: Liquids manual.

2.7 Using Interactive Parameter Adjustment

The section "Spectrometer Control," page 79 included statements for interactive parameter adjustment (IPA). Such routines start with the letter i (e.g., idelay, irgpulse). For users who need added flexibility in programming, this section explains IPA and these routines in more detail. IPA is available on all systems except *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

General Routines

In addition to the statements previously described, PSG has four general routines:

- G_Pulse for generic pulse control
- G_Offset for adjustment of the offset frequency
- G_Delay for generic delay control
- G_Power for fine power control.

Each of these is called with an argument list (described below) specified with attributevalue pairs, terminated by a mandatory zero. *The terminating zero is mandatory. If the zero is left out, the results are unpredictable and can include a core dump of PSG.*

Each attribute has a default value—a pulse can be specified simply as $G_Pulse(0)$, which would produce a transmitter pulse of size pw with rof1 and rof2 set the same as the experiment parameters and phase cycled with the parameter oph.

The attribute SLIDER_LABEL determines whether output is generated for the Acquisition window (opened by the acqi command). If no label is specified, no IPA information is generated by the subroutine. The use of the SLIDER_LABEL with the same value for delays or pulses allows multiple delays or pulses to be controlled via one slider. This is covered later in this section.

As an example of a pulse sequence using the general routines, Listing 10 shows the source code of i2pul.c, which can be compiled and run like S2PUL, but when go('acqi') is typed, IPA information is generated in /vnmr/acqqueue/acqi.IPA.

The command acqi can be used to adjust the pulses and delays in the sequence. Note that G_Pulse covers the statements obspulse, pulse, decpulse, etc.

Macro definitions have been written to cover these:

```
#define obspulse() G_Pulse(0)
#define decpulse(decpulse,phaseptr) \
    G_Pulse (PULSE_DEVICE, DODEV, \
    PULSE_WIDTH, decpulse, \
    PULSE_PHASE, phaseptr, \
    PULSE_PRE_ROFF, 0.0, \
    PULSE_POST_ROFF, 0.0, \
    0)
```

See the file /vnmr/psg/macros.h for a complete list. This file is automatically included when the file standard.h is included in a pulse sequence. Note also that the

Listing 10. Pulse Sequence Listing of File i2pul.c

```
/* I2PUL - interactive two-pulse sequence */
#include <standard.h>
static int phasecycle[4]={0,2,1,3};
pulsesequence()
{
   /* equilibrium period */
  settable(t1,4,phasecycle);
  status(A);
  hsdelay(d1);
  /* --- tau delay --- */
  status(B);
  ipulse(p1,zero,"p1");
  /*
  *
     This ipulse statement is equivalent to
  * the following general pulse statement.
  *
      G_Pulse(PULSE_WIDTH, pl,
              PULSE_PHASE, zero,
  *
   *
              SLIDER_LABEL, "p1",
   *
              0);
  */
  G Delay(DELAY TIME,
                          d2,
          SLIDER_LABEL, "d2",
           SLIDER MAX,
                          10,
           0);
   /* --- observe period --- */
  status(C);
   ipulse(pw,t1,"pw");
  setreceiver(t1);
}
```

same pulse sequence can be used to execute go as well as go('acqi'); however, IPA information is only generated when go('acqi') is used.

Interactive adjustment of *simultaneous* pulses is *not* supported. A limit of 10 has been set on the number of calls with a label. This limits the number of parameters that can be adjusted within one pulse sequence. Note that a subroutine call within a hardware loop is still only one label.

Parameters are adjusted at the end of a sweep. Since this takes a finite amount of time, steady state may be affected. Of course, changing any parameter value also affects the steady state, so this should be of little or no consequence.

pw,

Generic Pulse Routine

The G_Pulse generic pulse routine has the following syntax:

G_Pulse(PULSE_WIDTH,

_ '	T,
PULSE_PRE_ROFF,	rofl,
PULSE_POST_ROFF,	rof2,
PULSE_DEVICE,	TODEV,
SLIDER_LABEL,	NULL,
SLIDER_SCALE,	1,
SLIDER_MAX,	1000,

SLIDER_MIN,	Ο,
SLIDER_UNITS,	1e-6,
PULSE_PHASE,	oph,
0);	

The following table describes the attributes used with G_Pulse:

Attribute	Туре	Default	Description
PULSE_WIDTH	double	pw	As specified in parameter set
PULSE_PRE_ROFF	double	rofl	As specified in parameter se.
PULSE_POST_ROFF	double	rof2	As specified in parameter set
PULSE_DEVICE	int	TODEV	TODEV for observe channel or DODEV for 1st decoupler. On UNITY <i>plus</i> , also DO2DEV or DO3DEV for 2nd/3rd decoupler
SLIDER_LABEL	char *	NULL	Label (1-6 characters) for acqi or NULL for no output to acqi.
SLIDER_SCALE	int	1	Decimal places (0 to 3) on slider
SLIDER_MAX	int	100	Maximum value on the slider
SLIDER_MIN	int	0	Minimum value on the slider
SLIDER_UNITS	double	1e-6	Pulses are in µs, scale factor
PULSE_PHASE	int	oph	Real-time variable

```
Examples of using G_Pulse:
G_Pulse(0); /* equals obspulse(); */
G_Pulse(PULSE_WIDTH, pw, /* equals pulse(pw,vl); */
PULSE_PHASE, vl,
0); /* required terminating zero */
```

Frequency Offset Subroutine

The G_Offset routine adjusts the offset frequency. It has the following syntax: G_Offset(OFFSET_DEVICE, TODEV,

L(OFFSEI_DEVICE,	IODEV,
OFFSET_FREQ,	tof,
SLIDER_LABEL,	NULL,
SLIDER_SCALE,	Ο,
SLIDER_MAX,	1000,
SLIDER_MIN,	-1000,
SLIDER_UNITS,	Ο,
0);	

Attribute	Туре	Default	Description
OFFSET_DEVICE	int	none	Device (or rf channel) to receive frequency offset. <i>This is required! Thus</i> , G_Offset(0) <i>not allowed</i> . TODEV for transmitter channel or DODEV for first decoupler channel. On UNITYplus, DO2DEV for 2nd decoupler channel, or DO3DEV for 3rd decoupler channel.
OFFSET_FREQ	double	*	Offset frequency for selected channel. Default is offset frequency parameter (tof, dof, dof2, dof3) of associated channel.
SLIDER_LABEL	char *	NULL	If no slider label selected, offset cannot be changed in acqi. Otherwise, becomes the label (1-6 characters) in acqi.
SLIDER_SCALE	int	0	Number of decimal places displayed in acqi. Default is 0 because default range is 2000 Hz, so a resolution finer than 1 Hz is not necessary.
SLIDER_MAX	int	*	Maximum value on the slider. Default is 1000 Hz more than the offset frequency.
SLIDER_MIN	int	*	Minimum value on the slider. Default is 1000 Hz less than the offset frequency.
SLIDER_UNITS	double	1.0	Frequencies are in Hz.

The following table describes the attributes used with G_Offset:

* Default value is described in the description column for this attribute.

Examples of using G_Offset:

G_Offset(OFFSET_DEVICE, TODEV, /* equivalent to */
 OFFSET_FREQ, tof, /* offset(tof,TODEV); */
 0); /* required terminating zero */
G_Offset(OFFSET_DEVICE, TODEV, /* basic interactive */
 OFFSET_FREQ, tof, /* offset statement */
 SLIDER_LABEL, "TOF",/* for fine adjustment of */
 0); /* transmitter frequency */

Generic Delay Routine

The G_Delay generic delay routine has the following syntax:

G_Delay(DELAY_TIME,	d1,
SLIDER_LABEL,	NULL,
SLIDER_SCALE,	1,
SLIDER_MAX,	60,
SLIDER_MIN,	Ο,
SLIDER_UNITS,	1.0,
0);	

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Attribute	Туре	Default	Description
DELAY_TIME	double	d1	As specified in parameter set.
SLIDER_LABEL	char *	NULL	Label (1 to 6 characters) for acqi or NULL for no output to acqi.
SLIDER_SCALE	int	1	Decimal places (0 to 3) displayed.
SLIDER_MAX	int	60	Maximum value on the slider.
SLIDER_MIN	int	0	Minimum value on the slider.
SLIDER_UNITS	double	1.0	Delays are in seconds.

The following table describes the attributes used with G_Delay:

Examples of using G_Delay:

<pre>G_Delay(0);</pre>		/* equals delay(d1); *	/
G_Delay(DELAY_TIME,	d2,	/* equals delay(d2); *	/
0);	/* rec	quired terminating zero *	/

IPA allows one slider to control more than one delay or pulse. The maximum number of delays or pulses a slider can control is 32. This multiple control is obtained whenever multiple calls to G_Pulse or G_Delay have the same value for the SLIDER_LABEL attribute.

The first call to G_Pulse in a pulse sequence sets the initial value, the maximum and minimum of the slider, and the scale. Later calls to G_Pulse within that pulse sequence do not alter these. The SLIDER_UNITS attribute are unique to each call to G_Pulse. This allows changing the value seen by a particular event by some multiplication factor. For example, the following two statements create a single slider in the Acquisition window (opened by the acqi command) labeled PW that will control two separate pulses. G Pulse(PULSE DEVICE, TODEV,

G_PUISE(POLSE_DEVICE,	IODEV,
PULSE_WIDTH,	pw,
SLIDER_LABEL,	"PW",
SLIDER_SCALE,	1,
SLIDER_MAX,	1000,
SLIDER_MIN,	Ο,
SLIDER_UNITS,	1.0e-6,
0);	
G_Pulse(PULSE_DEVICE,	TODEV,
PULSE_WIDTH,	pw*2.0,
SLIDER_LABEL,	"PW",
SLIDER_UNITS,	2.0e-6,
0);	

The width of the first pulse will initially be pw, as set by the PULSE_WIDTH attribute for the first G_Pulse call. The width of the second pulse will initially be pw*2.0, as set by the PULSE_WIDTH attribute for the second G_Pulse call.

When the slider is changed in acqi, the amount that the actual pulse width changes is determined by the product of the slider change and the respective multiplicative factors specified by the attribute SLIDER_UNITS. For example, if the slider increased by 3 units, the first pulse width would by increased by 3 * 1.0e-6 seconds and the second pulse would be increased by 3 * 2.0e-6 seconds. In this way, the initial 1 to 2 ratio in pulse widths is maintained while the slider is changed.

Fine Power Subroutine

The G_Power subroutine is used on systems with the optional linear fine attenuators. It has the following syntax:

G_Power(POWER_VALUE,	tpwrf,
POWER_DEVICE,	TODEV,
SLIDER_LABEL,	NULL,
SLIDER_SCALE,	1,
SLIDER_MAX,	4095,
SLIDER_MIN,	Ο,
SLIDER_UNITS,	1.0,
0);	

The following table describes the attributes used with G_Power:

Attribute	Туре	Default	Description
POWER_VALUE	double	tpwrf	As specified in parameter set.
POWER_DEVICE	int	TODEV	TODEV for transmitter channel or DODEV for decoupler channel. On UNITY <i>plus</i> also DO2DEV and DO3DEV for 2nd and 3rd decoupler channels.
SLIDER_LABEL	char *	NULL	Label (1 to 6 characters) for acqi or NULL for no output to acqi.
SLIDER_SCALE	int	1	Decimal places (0 to 3) on slider.
SLIDER_MAX	int	4095	Maximum value on the slider.
SLIDER_MIN	int	0	Minimum value on the slider.
SLIDER_UNITS	double	1.0	Power in arbitrary units.

Examples of using G_Power: G_Power(0);

G_Power(POWER_VALUE,	dpwrf,
POWER_DEVICE,	DODEV,
0);	<pre>/* required terminating zero */</pre>

2.8 Hardware Looping and Explicit Acquisition

The loop and endloop statements described previously generate a *soft loop*, which means that they force the acquisition computer to repeatedly place the information contained within the loop into the pulse program buffer (a FIFO). If this loop must run extremely fast, a condition may arise in which the acquisition computer is not able to provide input to the pulse program buffer as fast as the sequence is required to operate, and this technique does not work.

Because of this problem, a different mode of looping known as *hardware looping* is supported in certain UNITY*INOVA*, *MERCURY-VX*, *MERCURY*, UNITY*plus*, UNITY, and VXR-S systems. In this mode, the pulse program buffer provides its own looping, and the speed can be at the maximum possible rate, with the only limitation being the number of events that can occur during each repetition of the loop. Table 24 lists statements related to hardware looping. Hardware looping is not available on *GEMINI 2000*.

<pre>acquire(num_points,sampling_interval clearapdatatable()</pre>	Explicitly acquire data Zero data in acquisition processor memory
endhardloop()	End hardware loop
<pre>starthardloop(num_repetitions)</pre>	Start hardware loop

Table 24. Hardware Looping Related Statements

Controlling Hardware Looping

Hardware looping capability is determined by the type of acquisition controller board used on the system (see "Types of Acquisition Controller Boards," page 72):

- Data Acquisition Controller boards, Pulse Sequence Controller boards, and Acquisition Controller boards offer expanded capability with respect to hardware looping and timing precision.
- Output boards with Part No. 00-953520-05 or 00-953520-06 have hardware looping capability but are limited in the implementation of hardware loops within a pulse sequence.
- Output boards with Part No. 00-953520-0#, where # is from 0 to 4, have no hardware looping capability and will not be discussed further.
- STM/Output board on *MERCURY-VX* and *MERCURY* systems offers expanded capability with respect to hardware looping.

Use the starthardloop(numrepetitions) and endhardloop() statements start and end a hardware loop. The numrepetitions argument to starthardloop must be a real-time integer variable, such as v2, and *not* a regular integer, a real number, or a variable. The number of repetitions of the hardware loop must be two or more. If the number of repetitions is 1, the hardware looping feature itself is not activated. A hardware loop with a count equal to 0 is not permitted and will generate an error. Depending on the pulse sequence, additional code may be needed to trap for this condition and skip the starthardloop and endhardloop statements if the count is 0.

Only instructions that require no further intervention by the acquisition computer (pulses, delays, acquires, and other scattered instructions) are allowed in a hard loop. Most notably, no real-time math statements are allowed, thereby precluding any phase cycle calculations. Also, no AP table with the autoincrement feature set can be used within a hard loop. The number of events included in the hard loop, including the total number of data points if acquisition is performed, must be as follows:

- 63 or less for Output boards
- 1024 or less for Acquisition Controller boards
- 2048 or less for the *MERCURY-VX* and *MERCURY* STM/Output board, Pulse Sequence Controller board, or Data Acquisition Controller board.

In all cases, the number of events must be greater than 1. No nesting of hard loops is allowed.

For Output boards, a hardware loop must be preceded by some timed event other than an explicit acquisition or another hardware loop. If two hardware loops must follow one another, it will therefore be necessary to insert a statement like delay(0.2e-6) between the first endhardloop and the second starthardloop. With only a single hardware loop, there is no timing limitation on the length of a single cycle of the loop. With two hardware loops (perhaps a loop of pulses and delays followed by an implicit acquisition), the first hardware loop must have a minimum cycle length of approximately 80 μ s. With

three or more hardware loops, loops that are not the first or last must have a minimum cycle length about 100 μ s.

For *MERCURY-VX* and *MERCURY* STM/Output boards, Data Acquisition Controller boards, Acquisition Controller boards, and Pulse Sequence Controller boards, there are no timing restrictions between multiple, back-to-back hard loops. There is one subtle restriction placed on the actual duration of a hard loop if back-to-back hard loops are encountered: the duration of the *i*th hard loop must be N(i+1) * 0.4 ms, where N(i+1) is the number of events occurring in the (i+1)th hard loop.

Number of Events in Hardware Loops

As indicated above, a limit of 63 events can occur in a hardware loop for Output boards, a limit of 1024 events for Acquisition Controller boards, and a limit of 2048 events for the *MERCURY-VX* and *MERCURY* STM/Output, Data Acquisition Controller, and Pulse Sequence Controller boards, with a requirement in all cases that the number of events be greater than 1 (see "Types of Acquisition Controller Boards," page 72, for a description of board types). But what is meant by "an event"?

An *event* is a single activation of the timing circuitry. Pulses, delays, phase shifts, etc., set or reset various gate lines to turn on and off pulses, phase shift lines, etc. but activate the timing circuitry in the same way. Timing is accomplished as follows:

- The Data Acquisition Controller board uses one time base of 12.5 ns.
- Other acquisition controller boards use four time bases: 1 s, 1 ms, 1 µs, and 0.1 µs for Output boards or 25 ns for Acquisition Controller and Pulse Sequence Controller boards. For each time base, the counter can count from 2 to 4095. A maximum of two time bases is used to time any delay, with the smallest time base possible being used.
- *MERCURY-VX* and *MERCURY* uses two time bases: 0.1 µs and 1 ms. As many events as needed are used. Delays greater than 96 seconds use a hard loop.

For example, consider a pulse of 35 μ s on an Output board. This produces a count of 350 in the 0.1 μ s time base and generates a single event in a hardware loop. On the other hand, consider a delay of 542.4 μ s. This time cannot be generated solely in the lowest time base, so it generates two timed events: a count of 542 in the 1 μ s time base and a count of 4 in the 0.1 μ s time base. Thus, 542.4 μ s generates two events in a hardware loop; however, a delay of 542.0 μ s generates only one event, since it can be made fully with the 1 μ s time base.

The final point to understand is that some things that look like one event may actually be more. Consider, for example, the statement rgpulse(pw,v1,rof1,rof2). Does this generate a single event? No, it generates at least three (or more depending on the length of the events). That is because we generate first a time of rof1 with the amplifier unblanked but transmitter off, then a time of pw with the transmitter on, and then a time rof2 with the transmitter off but the amplifier unblanked. Times that are zero generate no events, however. For example, rgpulse(5.0e-6,v1,0.0,0.0) generates only a single event.

Although pulses, delays, and data point acquisitions are the most common things to be in a hardware loop, other choices are possible. Table 25 lists the number of events that may be generated by each statement.

On *MERCURY-VX* and *MERCURY* systems, any delay (pulse, delay, decrgpulse, etc.) is limited to 96 seconds within a hardware loop. In practice, this is not a restriction.

Statement	^{UNITY} INOVA	UNITYplus	UNITY, VXR-S	MERCURY-V X and MERCURY	GEMINI 2000
acquire (Data Acq. Controller board)	1 to 2048	_	_	_	_
acquire (Pulse Seq. Controller board)		1 to 2048		_	_
acquire (Acq. Controller board)			1 to 1024	_	_
acquire (Output board)	—	_	1 to 63	_	_
dcplrphase, dcplr2phase, dcplr3phase	1	4	1	6	_
declvlon, declvloff	1	2	2 (high power)	_	2
decphase, dec2phase, dec3phase	0	0	0	0	0
decpulse	0	1 or 2	1 or 2	1 or 2	5 or 6
decrgpulse, dec2rgpulse, dec3rgpulse	0	3 to 6	3 to 6	3 to 6	7 to 8
delay	1	1 or 2	1 or 2	1 to 5	1 or 2
nsdelay	1	1 or 2	1 or 2	1 to 5	1 or 2
lk_hold, lk_sample	1	2	_	3	—
obspulse	3	3 to 6	3 to 6	3 to 6	5 to 8
offset	9	9 (latching)	7 (standard) 11 (latching)	72	7
power, obspower, decpower, dec2power, dec3power	1	2	2	3	_
pwrf, obspwrf, decpwrf, dec2pwrf, dec3pwrf	1	4	3	_	_
pulse,rgpulse	3	3 to 6	3 to 6	3 to 6	5 to 8
simpulse	3 to 5	3 to 10	3 to 10	3 to 15	7 to 10
sim3pulse	3 to 7	3 to 14	3 to 14	—	
status	0 to 5 times number of channels	0 to 8 times number of channels	0 to 7 per channel	0 to 12	0 to 7
txphase	0	0	0	0	0
xmtrphase	1	4	1	6	

Table 25. N	Number of	Events for	Statements i	n a H	ardware Lo	oop
-------------	-----------	------------	--------------	-------	------------	-----

Explicit Acquisition

Closely related to hardware looping is the *explicit acquisition* feature—the acquisition of one or more pairs of data points explicitly by the pulse sequence. This feature (not available on *MERCURY* and *GEMINI 2000*) lets you intersperse pulses and data acquisition, and allows coding pulse sequences that acquire multiple FIDs during the course of a pulse sequence (such as COCONOSY). It also allows pulse sequences that acquire a single FID one or more points at a time (such as MREV-type sequences).

For Output boards, any sequence that uses hardware looping or explicit acquisition must have parameter dl greater than 0, or at least some delay prior to the start of the hardware loop or explicit acquisition. For Data Acquisition Controller, Acquisition Controller and Pulse Sequence Controller boards, no such restrictions exist.

The acquire(number_points, sampling_interval) statement explicitly acquires data points at the specified sampling interval, where the sequence of events is acquire a pair of points for 200 ns, delay for sampling_interval less 200 ns, then repeat number_points/2 times. For example, acquiring an FID would use acquire(np,1.0/sw).

Both arguments to the acquire statement must be *real* numbers or variables. If an acquire statement occurs outside a hardware loop, the number of complex points to be acquired must be a multiple of 2 for Data Acquisition Controller, Acquisition Controller, and Pulse Sequence Controller boards, or a multiple of 32 for Output boards. Inside a hardware loop, Data Acquisition Controller and Pulse Sequence Controller boards can accept a maximum of 2048 complex points, Acquisition Controller boards can accept a maximum of 1024 complex points, and Output boards can accept a maximum of 63 complex points. number_points must be a multiple of 2, because only *pairs* of points can be acquired (note that this is a different definition than was used on VXR-style systems).

UNITY *INOVA* systems include small overhead delays before and after the acquire statement. The pre-acquire delay takes into account setting the receiver phase (oph) and enabling data overflow detection. Disabling data overflow detection creates a post-acquire delay. These overhead delays and associated functions are placed outside the hardware loop when acquire statements are within a hardware loop, and before the first acquire and after the last acquire, when more than one acquire statement is used to acquire a FID.

Once an explicit acquisition is invoked, even if for one pair of data points, the standard "implicit" acquisition is turned off, and the user is responsible for acquiring the full number of data points. Failure to acquire the correct number of data points before the end of the pulse sequence generates an error. The total number of data points acquired before the end of the sequence must equal the specified number (np). An example of the programming necessary to program a simple explicit acquisition, analogous to the normal implicit acquisition, would look like this:

```
rcvron();
txphase(zero);
decphase(zero);
delay(alfa+(1.0/(beta*fb)));
acquire(np,1.0/sw);
```

Although generally not needed, the clearapdatatable() statement is available to zero the acquired data table at times other than at the start of the execution of a pulse sequence, when the data table is automatically zeroed.

The limitation that multiple hardloops cannot be nested has consequences for the use of the acquire statement inside a hardloop. Depending on its arguments and how it is built into

a pulse sequence, the acquire statement may internally be done as a hardloop by itself. However, a construct like the following does not work:

```
initval(np/2.0, v14);
starthardloop(v14);
    acquire(2.0, 1.0/sw);
endhardloop();
```

A hardloop that consists of a single acquire call are not permitted, but such constructs are not needed because a single statement can be used instead: acquire(np,1.0/sw);

This statement is not equivalent to the first construct because the acquire statement will sample more than just two points (i.e., a complex data point) per loop cycle, thus allowing for np greater than $2.0 \times$ (maximum number of hardloop cycles). Note that the hardloop uses a 16-bit loop counter. Therefore, the maximum number of cycles is 32767 (the largest possible 16-bit number).

On the other hand, a hardloop that contains acquire together with other pulse sequence events works fine as long as the number of complex points to be acquired plus the number of extra FIFO words per loop cycle does not exceed the total number of words in the loop FIFO (63 on Output boards, 1024 on Acquisition Controller boards, or 2048 on Pulse Sequence Controller boards):

```
initval(np/2.0, v14);
starthardloop(v14);
    acquire(2.0, 1.0/sw - (rof1 + pw + rof2));
    rgpulse(pw, v1, rof1, rofr2);
endhardloop;
```

Explicit hardloops with acquire calls are a standard feature in multipulse solids sequences.

Receiver Phase For Explicit Acquisitions

Receiver phase can be changed for explicit acquisitions, the same as for implicit acquisitions, by changing oph or by using the setreceiver statement (setreceiver is not available on *GEMINI 2000*). The value of oph at the time of the acquisition of the first data point is the value that determines the receiver phase setting for the duration of that particular "scan"—the receiver cannot be changed after acquiring some data points and before acquiring the rest.

Multiple FID Acquisition

Explicit acquisition of data can also be used to acquire more than one FID per pulse sequence (simultaneous COSY-NOESY for example). This can be done for 1D or 2D experiments. The parameter nf, for number of FIDs, controls this if it is created and set. To perform such an experiment, enter create('nf', 'integer') to create nf and then set nf equal to an integer such as 2.

Once the data have been acquired, a second new parameter cf (current FID), which must also be created, is used to identify the FID to manipulate. Setting cf=2, for example, would recognize the second FID in the COSY-NOESY experiment (and hence would produce a NOESY spectrum after Fourier transformation). Note that this is distinct from the standard array capability and is, in fact, compatible with the standard arrays. Thus, you can acquire an array of ten experiments, with each consisting of three FIDs that are generated during each pulse sequence. To display the second FID of the seventh experiment, for example, you would type cf=2 dfid(7).

2.9 Pulse Sequence Synchronization

If broken down to its fundamental elements, a pulse sequence is just a set of accurately timed delays in which the appropriate hardware is turned on or off.

External Time Base

For purposes of synchronization, an external timebase halts the pulse sequence until the number of external events in the count field have occurred. The source of events or ticks of this external timebase is up to the user. See your system technical reference for specifics. This feature is not available on *MERCURY-VX*, *MERCURY*, or *GEMINI 2000* systems.

Controlling Rotor Synchronization

Statements for rotor control on systems with solids rotor synchronization hardware are rotorperiod, rotorsync, and xgate. Table 26 summarizes these statements.

Table 26. Rotor Synchronization Control Statements

<pre>rotorperiod(period)</pre>	Obtain rotor period of high-speed rotor
<pre>rotorsync(rotations)</pre>	Gated pulse sequence delay from MAS rotor position
<pre>xgate(events)</pre>	Gate pulse sequence from an external event

- To obtain the rotor period, use rotorperiod (period), where period is a realtime variable into which is the rotor period is placed (e.g., rotorperiod (v5)). The period is placed into the referenced variable as an integer in units of 100 ns.
- To insert a variable-length delay, use rotorsync(rotations), where rotations is a real-time variable that points to the number of rotations to delay, for example, rotorsync(v6). The delay allows synchronizing the execution of the pulse sequence with a particular orientation of the sample rotor. When the rotorsync statement is encountered, the pulse sequence is stopped until the number of rotor rotations has occurred as referenced by the real-time variable given.
- To halt the pulse sequence from an external event, use xgate(events), where events is a double variable (e.g., xgate(2.0)). When the number of external events has occurred, the pulse sequence continues.

Both rotorsync and xgate can be used, but there is a very important distinction between the two—rotorsync synchronizes to the exact position of the rotor, whereas xgate synchronizes to the zero degree position of rotation. For example, if the rotor is at 90°, then for xgate(1.0), the pulse sequence will begin when the rotor is at zero degrees, a rotation of 270°; however, for the equivalent rotorsync, the pulse sequence will begin when the rotor is at 90°, or 360° rotation.

2.10 Pulse Shaping

Waveform generators are an optional piece of equipment available on UNITY *INOVA*, UNITY *plus* and UNITY for controlling rf pulse shapes on one or more rf channels, programmed decoupling patterns, and gradient shapes for imaging applications.

For pulse shaping programming using Pbox, see the manual User Guide: Liquids.

Pulse control of the waveform generators consists of two separate parts:

- A text file describing the shape of a waveform.
- A pulse sequence statement applying that waveform in an appropriate manner.

The power of rf shape or decoupler pattern is controlled by the standard power and fine power control statements for that rf channel. For example, obspower and obspwrf will scale the overall power of a shape on the observe channel.

File Specifications

The macro sh2pul sets up a shaped two-pulse (SH2PUL) experiment. This sequence behaves like the standard two-pulse sequence S2PUL except that the normal hard pulses are changed into shaped pulses from the waveform generator.

To find pulse shape definitions, the pulse sequence generation (PSG) software looks in a user's vnmrsys/shapelib directory and then in the system's shapelib. Each shapelib directory contains files specifying the defined shapes for rf pulses, decoupling, and gradient waveforms. To differentiate the files in a shapelib directory, each type uses a different suffix:

Pattern Type	Suffix	Example
rf pulses	.RF	gauss.RF
decoupling	.DEC	mlev16.DEC
gradient	.GRD	hard.GRD

Each pattern file is a set of element specifications with one element per line. Therefore, a 67 element pattern contains 67 lines. Any blank lines and comments (characters after a # sign on a line) in a specification are ignored.

Shapes can be created by macro, by programs, or by hand. The specifications for each kind of pattern are listed in the following table (if a field is not specified, the default given is used). As an example, an slightly modified excerpt from a file in the system directory shapelib is also shown.

RF Patterns

Column	Description	Limits	Default
1	Phase angle (in degrees) Phase limits	0.5° resolution No limit on magnitude	Required
2	Amplitude	0 to scalable max	max
3	Relative duration	0, or 1 to 255	1
4	Transmitter gate	0, 1	1 (gate on)

For example, the first 8 elements (after the comment lines) of the file sinc.RF:

0.000	0.000	1.000000
0.000	8.000	1.000000
0.000	16.000	1.000000
0.000	24.000	1.000000
0.000	32.000	1.000000
0.000	40.000	1.000000
0.000	48.000	1.000000
0.000	56.000	1.000000

In using the .RF patterns, the actual values for the amplitude are treated as relative values, not as absolute values. All of the amplitudes in the rf shape file are divided by the largest amplitude in the shape file and then multiplied by 1023.0. The net result is that shapes with values of the amplitudes between 0 to 10.0, or between 0 to 1023.0, or between 0 to 100000.0, are effectively all the same shape.

To implement .RF patterns with absolute values for amplitudes, you can use a shape element with 0 duration to fix the scaling factor for the shape. Here is a simple example:

A shape with elements

0.00 10.0 1.0 0.00 100.0 1.0 0.00 20.0 1.0

will result in an actual shape of

0.00	1023.0*10.0/100.0	1.0		0.00	102.30	1.0
0.00	1023.0*100.0/100.0	1.0	or	0.00	1023.0	1.0
0.00	1023.0*20.0/100.0	1.0		0.00	204.60	1.0

A shape with elements

0.001023.00.00.0010.01.00.00100.01.00.0020.01.0

will result in an actual shape of

0.00	1023.0*10.0/1023.0	1.0		0.00	10.0	1.0
0.00	1023.0*100.0/1023.0	1.0	or	0.00	100.0	1.0
0.00	1023.0*20.0/1023.0	1.0		0.00	20.0	1.0

Decoupler Patterns

Column	Description	Limits	Default
1	Tip angle per element (in degrees) Phase limits	0° to 500°, 1° resolution No limit on magnitude	Required
2	RF phase (in degrees)	0.5° resolution	Required
3	Amplitude	0 to scalable max	max
4	Transmitter gate	0, 1	0 (gate off)

For example, the first 8 elements (after the comment lines) of the file waltz16.DEC:

270.0	180.0
360.0	0.0
180.0	180.0
270.0	0.0
90.0	180.0
180.0	0.0
360.0	180.0
180.0	0.0

In using the gate field in . DEC patterns, note the following:

• The waveform generator gate is OR'ed with the output board gate. This means that any time the output board gate is on, the transmitter is on, irrespective of any waveform generator gate.

- If a decoupler pattern is activated under status control (using dmm= 'p'), an implicit output board gate statement is added. In this situation, any 0s or 1s in the gate field of the .DEC pattern are irrelevant because they are overridden (as indicated above).
- If a decoupler pattern is activated by the decprgon statement, the waveform generator gate is the controlling factor. If this gate is specified as 0s or 1s in the .DEC file, that gating will occur. If there is no gate field in the .DEC file, the default occurs—the gate is set to 0 and the decoupler is off. An alternate is to follow the decprgon statement with some kind of gate statement (e.g., decon) to turn on the output board gate (overriding the default of the gate set to 0 from the waveform generator) and to proceed the decprgoff statement with a statement to turn the gate off (for example, decoff).

Gradient Patterns

Column	Description	Limits	Default
1	Output amplitude	-32767 to 32767, 1 unit resolution	Required
2	Relative duration	1 to 255	1

For example, the first 8 elements (after the comment lines) of the file trap.GRD:

1024	1
2048	1
3072	1
4096	1
5120	1
6144	1
7168	1
8192	1

Performing Shaped Pulses

Statements to perform shaped pulses on UNITY *INOVA*, UNITY *plus* and UNITY systems with optional waveform generators are decshaped_pulse, dec2shaped_pulse, dec3shaped_pulse, shaped_pulse, simshaped_pulse, and sim3shaped_pulse. Table 27 provides a summary of these statements.

Table 27. Shaped Pulse Statements

decshaped_pulse*	Perform shaped pulse on first decoupler		
dec2shaped_pulse*	Perform shaped pulse on second decoupler		
dec3shaped_pulse*	Perform shaped pulse on third decoupler		
shaped_pulse*	Perform shaped pulse on observe transmitter		
simshaped_pulse*	Perform simultaneous two-pulse shaped pulse		
<pre>sim3shaped_pulse*</pre>	Perform a simultaneous three-pulse shaped pulse		
<pre>dec2shaped_pulse(shap dec3shaped_pulse(shap simshaped_pulse(obssh obsphase,decphase,R sim3shaped_pulse(obss</pre>			

Shaped Pulse on Observe Transmitter or Decouplers

To perform a shaped pulse on the observe transmitter under waveform generator control, use shaped_pulse(shape,width,phase,RG1,RG2), where shape is the name of a text file in shapelib that stores the rf pattern (leave off the .RF file extension), width is the duration of the pulse; phase is the phase of the pulse (it must be a real-time variable); RG1 is the delay between unblanking the amplifier and gating on the transmitter (the phase shift occurs at the beginning of this delay); and RG2 is the delay between gating off the transmitter and blanking the amplifier (e.g.,

```
shaped_pulse("gauss",pw,v1,rof1,rof2)).
```

If a rf channel does not have a waveform generator, the statements shaped_pulse, decshaped_pulse, and dec2shaped_pulse provide pulse shaping through the linear attenuator and the small-angle phase shifter on the AP bus. This type of pulse shaping is available only on UNITY *INOVA* and UNITY *plus* systems. AP tables for the attenuation and phase values are created on the fly, and the real-time variables v12 and v13 are used to control the execution of the shape. On previous versions of VNMR, this pulse shaping through the AP bus was exclusively controlled by the statements apshaped_pulse, apshaped_decpulse, and apshaped_dec2pulse.

For shaped pulses under waveform generator control, the minimum pulse length is $0.2 \,\mu s$. The overhead at the beginning and end of the shaped pulse varies with the system and the type of acquisition controller board:

- On UNITY INOVA: 0.95 μ s at start, 0 at end.
- On UNITYplus: 6.19 µs at start, 0 at end.
- On systems with an Acquisition Controller board: 10.75 µs at start, 4.3 µs at end.
- On systems with an Output board: 10.95 µs at start, 4.5 µs at end.

If the length is less than $0.2 \,\mu s$, the pulse is not executed and there is no overhead.

The decshaped_pulse, dec2shaped_pulse, and dec3shaped_pulse statements allow a shaped pulse to be performed on the first, second, and third decoupler, respectively. The arguments and overhead used for each is the same as shaped_pulse, except they apply to the decoupler controlled by the statement.

Simultaneous Two-Pulse Shaped Pulse

simshaped_pulse(obsshape,decshape,obswidth,decwidth, obsphase,decphase,RG1,RG2) performs a simultaneous, two-pulse shaped pulse on the observe transmitter and the first decoupler under waveform generator control. obsshape is the name of the text file that contains the rf pattern to be executed on the observe transmitter; decshape is the name of the text file that contains the rf pattern to be executed on the first decoupler; obswidth is the duration of the pulse on the observe transmitter; decwidth is the duration of the pulse on the first decoupler; obsphase is the phase of the pulse on the observe transmitter (it must be a real-time variable); decphase is the phase of the pulse on the first decoupler (it must be a real-time variable); RG1 is the delay between unblanking the amplifier and gating on the first rf transmitter (all phase shifts occur at the beginning of this delay); and RG2 is the delay between gating off

the final rf transmitter and blanking the amplifier; for example: simshaped_pulse("gauss", "hrm180", pw, p1, v2, v5, rof1, rof2)

The overhead at the beginning and end of the simultaneous two-pulse shaped pulse varies with the system and acquisition controller board:

- On UNITY *INOVA*: 1.45 μ s at start, 0 at end.
- On UNITYplus: 11.5 µs at start, 0 at end.

- On systems with an Acquisition Controller board: 21.5 µs at start, 8.6 µs at end.
- On systems with an Output board: 21.7 µs at start, 8.8 µs at end.

These values hold regardless of the values for obswidth and decwidth.

If either obswidth or decwidth is 0.0, no pulse occurs on the corresponding channel. If both obswidth and decwidth are non-zero and either obsshape or decshape is set to the null string (''), then a hard pulse occurs on the channel with the null shape name. If either the pulse width is zero or the shape name is the null string, then a waveform generator is not required on that channel.

Simultaneous Three-Pulse Shaped Pulse

The sim3shaped_pulse statement performs a simultaneous, three-pulse shaped pulse under waveform generator control on three independent rf channels. The arguments to sim3shaped are the same as defined previously for simshaped_pulse, except that dec2shape is the name of the text file that contains the rf pattern to be executed on the second decoupler, dec2width is the duration of the pulse on the second decoupler, and dec2phase is the phase (a real-time variable) of the pulse on the second decoupler (e.g., sim3shaped_pulse("gauss", "hrm180", "sinc", pw, p1, v2, v5, v6, rof1, rof2)).

The overhead at the beginning and end of the simultaneous three-pulse shaped pulse varies with the system and acquisition controller board:

- On UNITY *INOVA*: 1.95 μ s at start, 0 at end.
- On UNITYplus: 17.25 µs at start, 0 at end.
- On systems with an Acquisition Controller board: 32.25 µs at start, 12.9 µs at end.
- On systems with an Output board: 32.45 µs at start, 13.1 µs at end.

These values hold regardless of the values for obswidth, decwidth, and dec2width.

By setting one of the pulse lengths to the value 0.0, sim3shaped_pulse can also perform a simultaneous two-pulse shaped pulse on any combination of three rf channels. (e.g., to perform simultaneous shaped pulses on the first decoupler and second decoupler, but not the observe transmitter, set the obswidth argument to 0.0).

If any of the shape names are set to the null string (''), a hard pulse occurs on the channel with the null shape name. If either the pulse width is zero or the shape name is the null string, a waveform generator is not required on that channel.

Programmable Transmitter Control

Statements related to programmable transmitter control on UNITY*INOVA*, UNITY*plus* and UNITY systems with optional waveform generators are obsprgoff and obsprgon for the observe transmitter, decprgoff and decprgon for the first decoupler, dec2prgoff and dec2prgon for the second decoupler, and dec3prgoffand dec3prgon for the third decoupler. Table 28 provides a summary of these statements.

Programmable Control of Observe Transmitter

Use obsprgon(name, 90_pulselength, tipangle_resoln) to set programmable phase and amplitude control of the observe transmitter. name is the name of the file in shapelib that stores the decoupling pattern, 90_pulselength is the pulse duration for a 90° tip angle, and tipangle_resoln is the resolution in tip-angle degrees to which the decoupling pattern is stored in the waveform generator (e.g.,

<pre>decprgoff()</pre>	End programmable decoupling on first decoupler			
<pre>dec2prgoff()</pre>	End programmable decoupling on second decoupler			
<pre>dec3prgoff()</pre>	End programmable decoupling on third decoupler			
decprgon*	Start programmable decoupling on first decoupler			
dec2prgon*	Start programmable decoupling on second decoupler			
dec3prgon*	Start programmable decoupling on third decoupler			
obsprgoff()	End programmable control of observe transmitter			
obsprgon*	Start programmable control of observe transmitter			
<pre>* decprgon(name,90_pulselength,tipangle_resoln) dec2prgon(name,90_pulselength,tipangle_resoln) dec3prgon(name,90_pulselength,tipangle_resoln) obsprgon(name,90_pulselength,tipangle_resoln)</pre>				

Table 28. Programmable Control Statements

obsprgon("waltz16",pw90,90.0)).

The obsprgon statement returns the number of 50-ns ticks (as an integer value) in one cycle of the decoupling pattern. Explicit gating of the observe transmitter with xmtron and xmtroff is generally required.

To terminate any programmable phase and amplitude control on the observe transmitter under waveform generator control, use <code>obsprgoff()</code>.

Programmable Control of Decouplers

The decprgon, dec2prgon, and dec3prgon statements set programming decoupling on the first, second, and third decouplers, respectively. The arguments for each statement are the same as obsprgon, except they apply to the decoupler controlled by the statement. Each statement returns the number of 50 ns ticks (as an integer value) in one cycle of the decoupling pattern. Similarly, explicit gating of the selected decoupler is generally required, and termination of the control is done by the decprgoff(), dec2prgoff(), and dec3prgoff() statements, respectively.

Arguments to obsprgon, decprgon, dec2prgon, and dec3prgon can be variables (which need the appropriate getval and getstr statements) to permit changes via parameters.

The macro pwsadj(shape_file,pulse_parameter) adjusts the pulse interval time so that the pulse interval for the shape specified by shape_file (a file from shapelib) is an integral multiple of 100 ns. This eliminates a time truncation error in the execution of the shaped pulse by the programmable pulse modulators. pulse_parameter is a string containing the adjusted pulse interval time.

Setting Spin Lock Waveform Control

Statements for spin lock control on UNITY *INOVA*, UNITY *plus* and UNITY systems with optional waveform generators are spinlock, decspinlock, dec2spinlock, and dec3spinlock for the observe transmitter, first decoupler, second decoupler, and third decoupler, respectively. Table 29 provides a summary of these statements.

Spin Lock Waveform Control on Observe Transmitter

To execute a waveform-generator-controlled spin lock on the observe transmitter, use spinlock(name,90_pulselength,tipangle_resoln,phase,ncycles),

decspinlock*	Set spin lock waveform control on first decoupler			
dec2spinlock*	Set spin lock waveform control on second decoupler			
dec3spinlock*	Set spin lock waveform control on third decoupler			
spinlock*	Set spin lock waveform control on observe transmitter			
* decspinlock(name,90_pu	lselength,tipangle_resoln,phase,ncycles)			
	oulselength,tipangle_resoln,phase,ncycles)			
	oulselength,tipangle_resoln,phase,ncycles)			
<pre>spinlock(name,90_pulse</pre>	elength,tipangle_resoln,phase,ncycles)			

Table 29. Spin Lock Control Statements

name is the name of the file in shapelib that stores the decoupling pattern (leave off the .DEC file extension); 90_pulselength is the pulse duration for a 90° tip angle; tipangle_resoln is the resolution in tip-angle degrees to which the decoupling pattern is stored in the waveform generator; phase is the phase angle of the spin lock (it must be a real-time variable); and ncycles is the number of times that the spin-lock pattern is to be executed (e.g., spinlock('mlev16', pw90,90.0,v1,50))

Both rf gating and the mixing delay are handled within this statement.

Spin Lock Waveform Control on Decouplers

The decspinlock, dec2spinlock, and dec3spinlock set spin lock waveform control on the first, second, and third decouplers, respectively. The arguments are the same as used with spinlock, except that 90_pulselength is the pulse duration for a 90° tip angle on the decoupler controlled by the statement.

Arguments to spinlock, decspinlock, dec2spinlock, and dec3spinlock can be variables (which would need the appropriate getval and getstr statements) to permit changes via parameters.

Shaped Pulse Calibration

Macros bandinfo and pulseinfo can be run interactively (without arguments) to give a table with shaped pulse information for calibration. bandinfo takes the name of the shape and the bandwidth desired for the pulse and gives a table containing the duration of that pulse and a predicted 90° pulse power setting. pulseinfo takes the name of the shape and the duration of the pulse and gives the bandwidth of that pulse and a predicted 90° pulse power setting. Both macros can also be called from another macro. For more information, refer to the VNMR Command and Parameter Reference.

2.11 Shaped Pulses Using Attenuators

UNITY INOVA, MERCURY-VX, MERCURY, UNITY plus and UNITY systems are equipped with computer-controlled attenuators (0 dB to 79 dB on UNITY INOVA and UNITY plus, 0 dB to 63 dB on MERCURY-VX, MERCURY, and UNITY) on the observe and decouple channels, linear amplifiers, and T/R (transmit/receive) switch preamplifiers that allow lowlevel transmitter signals to be generated and pass unperturbed into the probe. Similarly, *GEMINI 2000* broadband systems are equipped with 0-dB to 63.5-dB computer-controlled attenuators but without the T/R switch preamplifiers. The combination of these elements means that the capability for performing shaped pulse experiments is inherent in the systems and does not require the more sophisticated waveform generation capability of the optional waveform generators. Hardware differences must be considered between systems, with and without the waveform generators. The attenuators have more limited dynamic range, slower switching time, and fewer pulse programming steps available. Nonetheless, the capability still allows significant experiments using only attenuators.

Two custom (non-standard) configurations also exist on UNITY systems:

- A third (or fourth) 0-dB to 63-dB attenuator can be added.
- One (or both) of the standard attenuators can be replaced with an 79-dB attenuator (whose values run from -16 to 63 for consistency with the 63-dB attenuator).

Three issues affect all shaped pulses, but particularly attenuator-based pulses:

- *Number of steps* The more steps used, the closer the shape approximates a continuous shape. At what level does this become overkill? For the most common shape, Gaussian, as few as 19 steps have been shown to be completely acceptable.
- *Dynamic range* How much dynamic range is required within a shape for proper results. For a Gaussian shape it has been shown that 33 dB is a useful limit; little or no improvement is achieved with more. With a single 63-dB attenuator, then, a Gaussian pulse with 33 dB dynamic range can be superimposed on a level ranging from 0- to 30-dB, more with a 79-dB attenuator.
- Overall power level of the shape A Gaussian pulse has an effective power approximately 8 dB lower than a rectangular pulse with an identical peak power. This means that given a full-power rectangular pulse of, say, 25 kHz, a Gaussian pulse with the same peak power has approximately a 10 kHz strength. Using instead a Gaussian pulse with only 33 dB dynamic range and a peak power 30 dB lower results in a shaped pulse of approximately 312 Hz, which is useful for some applications, like exciting the NH region of a spectrum, but too strong for others.

To increase the dynamic range (and decrease the strength of the shaped pulse) further, we can use one of three approaches:

- Replace the 63-dB attenuator with a 79-dB unit. This adds 16 dB of dynamic range, producing shaped pulses in the range of 50 Hz, suitable for multiplet excitation.
- Add an additional 63-dB attenuator in series with the first. If you use the entire 63 dB of the second attenuator to control the level of the pulse and use the first attenuator only for the shape, you still produce a pulse whose power is (for a Gaussian) 71 dB (63 + 8) below that of the hard pulse. This would produce a 7 Hz pulse, about as weak a pulse as one ever needs (and which could be reduced 30 dB further by only using 33 dB of the first attenuator for the shape). On UNITY*plus* systems, both phase and (linear) amplitude can be controlled over the AP bus, in addition to the 79-dB attenuator. It is possible to use this control to create shaped pulses without a waveform generator.
- Use a time-sharing or "DANTE" approach, applying the shaped pulse in such a way that it is switched on and off with a particular duty cycle during the course of the shape. A 10% duty cycle, for example, reduces the power by a factor of ten.

On UNITY*INOVA* and UNITY*plus* systems, both the phase and linear attenuator on each transmitter can be controlled through pulse sequence statements (see pwrf, obspwrf, decpwrf, dec2pwrf, dec3pwrf, pwrm, rlpwrm, and dcplrphase) so it is possible to create shaped pulses without a waveform generator.

AP Bus Delay Constants

Table 30 lists the most important AP bus delay "constants" (C macros) for the UNITY family of spectrometers (^{UNITY}*INOVA*, UNITY*plus*, UNITY, and VXR-S). The list is

Chapter 2. Pulse Sequence Programming

incomplete, but a complete list can be found at the bottom of the text file /vnmr/psg/apdelay.h.

The constants OFFSET_DELAY and OFFSET_LTCH_DELAY are applicable only to UNITY*INOVA* and UNITY*plus* systems that use PTS synthesizers with latching on the input. Although the constants are identical, use only OFFSET_DELAY on these systems. Most UNITY and VXR-S systems do not have PTS synthesizers with latching, but OFFSET_DELAY can be used on these systems.

Constant	Indicates Duration of
ACQUIRE_START_DELAY*	Overhead at start of acquisition
ACQUIRE_STOP_DELAY*	Overhead at end of acquisition
DECMODFREQ_DELAY	Overhead for setting modulator frequency
GRADIENT_DELAY	rgradient, zgradpulse (two times)
OBLIQUEGRADIENT_DELAY	oblique_gradient (applicable only to imaging)
OFFSET_DELAY**	decoffset, dec2offset, obsoffset, offset
OFFSET_LTCH_DELAY***	decoffset, dec2offset, obsoffset, offset
POWER_DELAY	decpower, dec2power, obspower, power, rlpower, etc.
PRG_OFFSET_DELAY	Time shift of WFG output with obsprgon, etc.
PRG_START_DELAY	decprgon, dec2prgon, obsprgon, etc.
PRG_STOP_DELAY	decprgoff, dec2prgoff, obsprgoff, etc.
PWRF_DELAY	decpwrf, dec2pwrf, obspwrf, pwrf
SAPS_DELAY	dcplrphase,dcplr2phase,dcplr3phase, xmtrphase
SETDECMOD_DELAY	Overhead for setting modulator mode
SPNLCK_START_DELAY	Overhead at start of decspinlock, spinlock, etc.
SPNLCK_STOP_DELAY	Overhead at end of decspinlock, spinlock, etc.
VAGRADIENT_DELAY	vagradpulse (two times)
WFG_OFFSET_DELAY	Time shift of WFG output
WFG_START_DELAY	Overhead at start of decshaped_pulse, shaped_pulse
WFG_STOP_DELAY****	Overhead at end of decshaped_pulse, shaped_pulse
WFG2_START_DELAY	Overhead at start of simshaped_pulse, etc.
WFG2_STOP_DELAY****	Overhead at end of simshaped_pulse, etc.
WFG3_START_DELAY	Overhead at start of sim3shaped_pulse, etc.
WFG3_STOP_DELAY****	Overhead at end of sim3shaped_pulse, etc.

Table 30. AP Bus Delay Constants

* On UNITY *INOVA* systems; on other systems, this constant is zero (no support for FSQ). ** Use OFFSET_DELAY only on UNITY *INOVA* and UNITY *plus* systems. *** Only on systems that use PTS synthesizers with latching.

**** On UNITYplus systems only, this constant is zero.

Controlling Shaped Pulses Using Attenuators

The statements power, obspower, decpower, dec2power, dec3power, and (optionally) pwrf, obspwrf, decpwrf, dec2pwrf, dec3pwrf, pwrm, and rlpwrm are used to change the attenuation (and hence the power level) of either the transmitter or

decouplers. A pulse sequence in which one of these statements is placed in a loop and repeatedly executed with different values for the amount of attenuation therefore results in a shaped pulse. This can be a C loop or a "soft" loop (using the loop statement), but not a "hard" loop. The successive values for the power may be calculated in real-time, read from a table (assuming that only positive numbers are involved), or set up from a static C variable. Although no standard pulse sequences exist that implement this feature, several contributions to the user library provide excellent examples of how to do this.

The statements shaped_pulse, decshaped_pulse, and dec2shaped_pulse provide fine-grained "waveform generator-type" pulse shaping through the AP bus. If an rf channel does not have a waveform generator configured, this is the same type of pulse shaping that statements apshaped_pulse, apshaped_decpulse, and apshaped_dec2pulse provide, and is a simpler implementation.

This type of pulse shaping is available only on UNITY*INOVA* and UNITY*plus* systems. They use the standard pulse shape files, such as gauss.RF, for the waveform generator. *MERCURY-VX* and *MERCURY* systems support these statements, however, only power level is controlled, not phase, making gauss.RF the only shape currently provided.

The apshaped_pulse, apshaped_decpulse, and apshaped_dec2pulse pulse statements use table variables to define the amplitude and phase tables, whereas the standard shaped_pulse, decshaped_pulse, and dec2shaped_pulse statements create and use these tables on the fly. Both types of AP bus waveshaping statements use real-time variables v12 and v13 to control execution of the shape. Table 31 summarizes the statements described in this section.

First decoupler pulse shaping via the AP bus Second decoupler pulse shaping via the AP bus				
Observe transmitter pulse shaping via the AP bus				
Perform shaped pulse on first decoupler				
Perform shaped pulse on second decoupler				
Perform shaped pulse on observe transmitter				
<pre>shape,pulse_width,pulse_phase, se_table,RG1,RG2) shape,pulse_width,pulse_phase, se_table,RG1,RG2) se,pulse_width,pulse_phase,power_table,</pre>				
RG2)				
decshaped_pulse(shape,width,phase,RG1,RG2)				
nape,width,phase,RG1,RG2)				
dec3shaped_pulse(shape,width,phase,RG1,RG2)				
width,phase,RG1,RG2)				

Table 31. Statements for Pulse Shaping Through the AP Bus

Controlling Attenuation

This section describes how to configure and control the system attenuators.

Standard System with Two Attenuators

On UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S systems with two attenuators, connect the two existing attenuators in series, leaving one channel without computer-controlled attenuation. This is often acceptable in homonuclear experiments, while in heteronuclear experiments and some homonuclear experiments it may be desirable to insert a simple fixed attenuator in-line in the channel that isn't being shaped.

If you take this approach, the tpwr and dpwr parameters (or, equivalently, the power(...,OBSch) and power(...,DECch) pulse sequence statements) control the two attenuators. The simplest approach is to use one of the two attenuators to control the shape, while using the second to set the overall level of the pulse. Assuming that there are also hard pulses in the pulse sequence, you'll also need to remember to write your pulse sequence to return both attenuators to values suitable for the hard pulse.

System with a Third Attenuator

On systems specially configured with a third attenuator (not available on UNITY INOVA, MERCURY-VX, MERCURY, UNITY plus, or GEMINI 2000 systems), connect the hardware so that control of the additional attenuator is through one of the two "fine" attenuator controls. Note that if this system also has two "real" fine attenuators (a 0- to 6-dB attenuator used for solid-state NMR applications), one of the fine attenuators will have to be disconnected while the third 0-dB to 63-dB attenuator uses its control circuitry.

In a system configured this way, the pulse sequence statement pwrf or pwrm is used to control the power of the pulse (either pwrf(...,OBSch) or pwrf(...,DECch), depending on how the additional attenuator was connected). If a 0-dB to 63-dB attenuator is connected to the fine attenuator control, the controlling hardware (and software) runs backwards. In other words, 0 gives no attenuation (maximum power), while 63 gives full attenuation (minimum power). This is the opposite of the standard power control.

Pulse sequences can be written that require the user to recognize this difference, or, more elegantly, a mathematical transformation within the pulse sequence can allow the user to enter "normal" values that are then reversed by the pulse sequence. The transformation approach is recommended for writing pulse sequences.

For example, assume that you want to have a parameter shapepwr that sets the overall power of the shaped pulse with the third attenuator, while using the standard attenuator to apply the shape. The relevant part of the pulse sequence might look like this: double shapepwr;

```
shapepwr = 63 - getval("shapepwr");
initval(shapepwr,v10);
pwrf(v10,OBSch);
...
```

This method allows the user to enter 0 to get minimum power and 63 to get maximum power, just as with tpwr and dpwr, and reverses the sense of the parameter within the pulse sequence where the user need not be concerned with it. Notice that the only thing different about this sequence is the "63 –" added before the getval—everything else in this example would be required in any case.

2.12 Internal Hardware Delays

Many pulse sequence statements result in "hidden" delays. These delays are not intrinsic to pulse sequence generation (PSG) software but are rather internal to the hardware.

Each AP bus instruction is considered a FIFO event and incurs the following delay, which is the time it takes to set the hardware on the AP bus:

- On UNITY *INOVA*, 0.5-µs delay (except PFG, which has a 1.0-µs delay).
- On MERCURY-VX and MERCURY, 1.2 µs delay.
- On UNITYplus, 1.15-µs delay.
- On GEMINI 2000, UNITY, and VXR-S, 2.15-µs delay.

Delays from Changing Attenuation

The pulse sequence statement power, which is used to change the level of attenuation produced by a 63-dB rf attenuator in the system, leads to the following values:

- On UNITY INOVA, 1 AP bus instruction, 0.5-μs concomitant internal delay (WFG start takes 1 AP bus instructions at 0.5 μs and extra board delay of 0.75 μs, total 1.25 μs).
- On MERCURY-VX and MERCURY, 4 AP bus instructions, 4.8-µs concomitant internal delay.
- On UNITYplus, 2 AP bus instructions, 2.3-µs concomitant internal delay (WFG start takes 5 AP bus instructions at 5.75 µs).
- On VXR-S and UNITY, 2 AP bus instructions, 4.3-µs concomitant internal delay (WFG start takes 7 AP bus instructions at 15.00 µs).

Table 32 lists all pulse sequence statements that lead to an internal delay and the magnitude of this delay. Similar information to the table is contained in the PSG header file apdelay.h, which resides in the VNMR system PSG directory.

On systems with the Output board, Table 32 indicates that the pulse sequence statement power incurs a 4.5 μ s internal delay, not a 4.3 μ s delay as previously stated. Of the 4.5 μ s delay, 0.2 μ s is to allow any high-speed line, (for example, the transmitter gate control line) that has been turned off in PSG at the end of the preceding delay to actually turn off in hardware before the AP bus instructions have been issued from the FIFO. Otherwise, any such high-speed line would not be turned off in hardware until the end of the series of AP bus instructions. This extra 0.2 μ s delay can be avoided with the apovrride statement.

Delays from Changing Status

Other delays can be incurred with the status and setstatus statements. The first occurrence of the status statement always incurs the full delay. On subsequent occurrences of status, the delay depends on values of the parameters dmm, dmm2, and dmm3. There are three parts that contribute to this delay:

- *Modulation mode* On UNITY*INOVA*, if and only if the modulation mode changes, 1.0 μ s is added to the delay, and the first occurrence of 's' in the dm string (or dm2 or dm3) adds an extra 1.0 μ s. On systems with apinterface=3 or UNITY*plus* systems, if and only if the modulation mode changes, 2.3 μ s is added to the delay on UNITY*plus* (4.3 μ s on other systems). On UNITY*plus* only, if the mode is synchronous, the first occurrence of the 's' in the dm string (or dm2) adds an extra 2.3 μ s when the modulation mode is switched from CW to synchronize the decoupling scheme. Note that the waveform generator (mode 'p') needs CW modulation (mode 'c').
- Waveform generator Starting a waveform generator adds 1.25 μs on UNITYINOVA, 5.75 μs on UNITYplus, and 10.75 μs on other systems. Stopping a waveform generator adds 1 μs on the UNITYINOVA, 2.3 μs on UNITYplus, and 4.3 μs on other systems. (The modulation mode is to or from 'p'.) The waveform generator also has an offset or propagation delay, which is discussed below.
- *Modulation frequency* If the modulation frequency changes, 1 µs is added on the UNITY*INOVA*, 4.6 µs on the UNITY*plus*, and 6.45 µs on other systems. Note that for the UNITY*INOVA*, and UNITY*plus*, this is different for a shaped pulse. The modulation frequency can change if the statement setstatus is called with a modulation frequency different from the parameter corresponding to the transmitter set, or if the modulation mode changes to or from 'g' and 'r'. If the change is to 'g' and 'r', the modulation frequency is internally scaled, changing the frequency.

Pulse Sequence Statements						
	^{UNITY} INOVA	MERCURY- VX and MERCURY	UNITYplus	GEMINI 2000	UNITY, VXR-S	Output Board Systems
acquire	1.0 pre 0.5 post	-	0.0 pre 0.0 post	_	0.0 pre 0.0 post	_
xmtrphase dcphase dcplrphase dcplr2phase dcplr3phase	0.5	7.2	3.45	-	2.15	2.35
power, obspower decpower dec2power dec3power	0.5	4.8	2.3	_	4.3	4.5
pwrf, obspwrf decpwrf dec2pwrf dec3pwrf	0.5	-	4.6	_	6.45	-
offset (S=standard L=latching)	4.0	86.4	10.35	15.25	15.05 S 21.5 L	15.25 21.7
shaped_pulse decshaped_pulse dec2shaped_pulse dec3shaped_pulse	1.25 pre 0.5 post	_	5.75	_	15.05	15.45
simshaped_pulse	*	_	11.5	_	30.1	30.50
sim3shaped_pulse	* *	_	17.25	-	45.15	45.55
obsprgon decprgon dec2prgon dec3prgon	1.25	-	5.75	_	10.75	10.95
obsprgoff decprgoff dec2prgoff dec3prgoff	0.5	-	2.3	_	4.3	4.5
spinlock decspinlock dec2spinlock dec3spinlock	1.25 pre 0.5 post	-	5.75	-	15.05	15.45
rgradient and vgradient with gradtype='p'	4.0	-	6.9	_	12.9	Not a optio
rgradient and vgradient with gradtype='w'	0.5	_	3.45	_	6.9	Not a optio
zgradpulse gradtype='p'	delay + 8.0	-	delay + 13.8	_	delay + 25.8	Not a optio
zgradpulse gradtype='w'	delay + 1.0	_	delay + 6.9	_	delay + 13.8	Not a optio

Table 32. AP Bus Overhead Delays

* simshaped_pulse: 1.75 pre, 0.5 post
** sim3shaped pulse: 2.25 pre, 0.5 post

Finally, these delays are added up for each channel, and this becomes the delay incurred for status or setstatus. For example, if dm = 'nnnss', dmm = 'cpfwp', and dm2 = 'y', then dmm2 = 'cccpc', Table 33 summarizes the internal intervals, assuming

Statement	Delay (µs) ^{UNITY} INOVA	Delay (µs) apinterface=3	Delay (µs) UNITYplus	Reason
status(B)	0	0	0	dmm from 'c' to 'p', WFG not started because dm= 'n' in B
status(C)	1.0	4.3	2.3	dmm from 'p' to 'f', no WFG to stop
status(D)	1.0+1.25	4.3+10.75	4.6+5.75	dmm from 'f' to 'w', ^{UNITY} INOVA and UNITY <i>plus</i> synchronize, dmm2 from 'c' to 'p'
status(E)	1.75+0.5	15.05+4.3	8.05+2.3	dmm from 'w' to 'p' (='c') and start WFG, dmm2 from 'p' to 'c', only stop WFG

Table 33. Example of AP Bus Overhead Delays for status Statement

status(A) is the initial state.

To keep the status timing constant, use the statusdelay statement. This statement allows the user to specify a defined period of time for the status statement to execute. For example, if statusdelay('B', 2.0e-5) is used, as long as the time it takes to execute status for state B is less than 20 microseconds, the statement will always take 20 microseconds. If the time to execute state B is greater than 20 microseconds, the statement still executes, but a warning message is generated.

Waveform Generator High-Speed Line Trigger

Along with the AP bus overhead delay, the waveform generator has an offset delay as a result of high-speed line (WFG) propagation delay. This shifts the rf pattern beyond the AP bus delay. Figure 5 illustrates the delay for UNITY*INOVA*. The time overhead for the AP bus is 1.25 μ s (this includes a 0.5- μ s AP bus delay and a 0.75- μ s board delay). The offset delay is an additional 0.45 μ s, for a total delay of 1.70 μ s. The UNITY*INOVA* WFG also has a post pulse overhead delay.

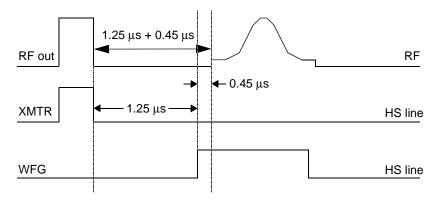


Figure 5. Waveform Generator Offset Delay on UNITY INOVA Systems

On UNITY *plus*, the time overhead for the AP bus is $5.75 \,\mu$ s. The offset delay is an additional 0.45 μ s, for a total delay of 6.20 μ s.

Note that if the shaped pulse is followed by a delay, say d3, then the end of the delay is at 1.7+pshape+0.5+d3. Similarly, on UNITY*plus*, the end of the delay is at 6.20+pshape+d3. On UNITY, it shifts $1.5 \mu s$, so the offset delay depends on the type of system. To obtain the proper offset delay, available in apdelay.h. are macros WFG_OFFSET_DELAY, WFG2_OFFSET_DELAY, and WFG3_OFFSET_DELAY.

Another delay is incurred between transients on systems other than UNITY *INOVA*. At the end of data collection, 3.5 ms is inserted to give the acquisition computer time to check lock, temperature, spin, etc. If the solids ADC is used so that sw is greater than 100000, this delay is extended to 15.5 ms on UNITY *plus* systems or extended by 10 ms per kilobyte points on UNITY and VXR-S systems. The UNITY *INOVA* has a 0.004-ms delay at the start of a transient to initialize the data collection hardware, and a 2.006-ms delay at the end of a transient for data collection error detection. For systems with gradients, the end of scan delays do not include the times to turn off gradients, which is done at the end of every scan.

2.13 Indirect Detection on Fixed-Frequency Channel

Indirect detection experiments, in which the observe nucleus is ¹H and the decouple nucleus is a low-frequency nucleus, usually ¹³C, are easily done on systems with two broadband channels (not available on *GEMINI 2000* systems). Systems with a fixed-frequency decoupler depend on the type of system.

Fixed-Frequency Decoupler

For systems with a fixed-frequency ¹H decoupler, the implementation depends on whether the system is a UNITY *INOVA*, *MERCURY-VX*, *MERCURY*, UNITY*plus*, or *GEMINI 2000*, or instead, is a UNITY or VXR-S.

UNITY INOVA, MERCURY, UNITYplus, GEMINI 2000 Systems

A UNITY *INOVA* or UNITY *plus* system with the label Type of RF set to U+ H1 Only in the CONFIG window, or any *MERCURY-VX*, *MERCURY*, or *GEMINI 2000* broadband system, can use the same parameter sets and pulse sequences as a dual-broadband system (e.g., HMQC) as long as the pulse statements in a sequence do not use the channel identifiers TODEV, DODEV, DO2DEV, and DO3DEV. This restriction is negligible because statements obspower, dec2power, and dec3power are available that specify an rf channel without requiring the these channel identifiers. Each of these statements require only the power level and can be remapped to different rf channels. The rfchannel parameter enables remapping rf channel selection. Refer to the description of rfchannel in the *VNMR Command and Parameter Reference* for details.

Internal logic on this system checks if the first decoupler is U+H1 Only, or the system is a *GEMINI 2000*, tn is set to 'H1', and dn is not set to 'H1'. If this is the case, the parameters and pulse statements for rf channels 1 and 2 are exchanged automatically.

MERCURY-VX, MERCURY, and GEMINI 2000 support automatic channel swapping as well.

UNITY and VXR-S Systems

UNITY and VXR-S fixed-frequency systems present special pulse sequence programming and hardware considerations. The hardware issues are discussed in the operation manuals. In this section, we discuss pulse sequence programming of these systems.

Pulse sequences written to perform indirect detection experiments must use decpulse (and related) statements to pulse the ¹H channel, and pulse statements to pulse the X channel. Having done this, and having set tn='Cl3' and dn='Hl', the software would normally set Channel A (the high-frequency channel) of the pulse amplifier into a CW mode, as appropriate for decoupling, and Channel B (the low-frequency channel) of the amplifier into a pulse mode. Proper operation of the pulse sequence requires that these modes be switched—the low-frequency channel in CW mode and the high-frequency channel in pulse mode.

To accomplish this, the C source file revmode.c is provided, and must be included in any pulse sequence to be run in the "reversed" configuration, as shown here:

```
/* s2pulr - reverse mode s2pul */
#include <standard.h>
#include <revmode.c> /* for reverse configuration */
pulsesequence()
{
    hsdelay(d1); decrgpulse(p1,zero,rof1,rof1);
    delay(d2); decrgpulse(pw,oph,rof1,rof2);
}
```

In addition to setting the proper modes for each channel of the amplifier, the revmode file also configures the local oscillator (L.O.) relay properly so that the local oscillator signal is taken from the "decoupler" board.

When used in the reverse mode, the X nucleus decoupling signal comes from the "observe" board. This board does not contain any of the hardware decoupler modulations such as WALTZ decoupling. Furthermore this decoupling signal is not controlled by the parameter dm, which controls (under "status" control) the ¹H signal. For these reasons any pulse sequence in which X nucleus decoupling is desired during acquisition (on a single-broadband system) must use "programmed" decoupling with explicit acquisition—see the hmqcr.c sequence for an example. Do *not* code sequences in which the status statement is used to switch on the decoupler. If the parameter dm is used, it must be used indirectly, as in hmqcr.c.

The legrelay parameter provides override capability over the magnet leg high band and low (broad) band rf signal routing. This is useful when a probe has a high and low band nucleus double-tuned to a coil and the standard logic would switch to the wrong probe connection. A system has this override capability if it uses N-type connectors instead by BNC connectors on the magnet leg. Valid values of legrelay are the following:

- 'n' means to use normal logic to set the magnet leg relay
- 'h' means to set the leg relay to high band
- 'l' means to set the leg relay to low (broad) band

Any other value will result in an error message and PSG will abort. The legrelay parameter normally does not exist but can be created with the command create('legrelay','string').

2.14 Multidimensional NMR

A standard feature of all pulse sequences is the ability to array acquisition parameters and automatically acquire an array of the corresponding FIDs. For example, arraying the pw parameter and viewing the resulting array of spectra is one way to estimate the 90-degree pulse width. This explicit array feature is automatic, whenever a parameter is set to multiple values, such as pw=5, 6, 7, 8, 9, 10.

A separate type of arrayed data set are the 2D, 3D, and 4D data sets. The distinguishing feature of this type of data set is that the arrayed element has a uniform, automatically calculated increment between values. The ni parameter is set to the number of increments desired in the first indirect dimension of a multidimensional data set. The inverse of the parameter sw1 defines the increment in successive values of the implicitly arrayed delay d2. For example, if ni=8, an implicit d2 array with values d2=0, 1/sw1, 2/sw1, 3/sw1, 4/sw1, 5/sw1, 6/sw1, 7/sw1 is generated. Eight FIDs, each using the corresponding d2 delay, will be acquired.

For the second indirect dimension, the analogous parameters are ni2, sw2, and d3. For the third indirect dimension, the analogous parameters are ni3, sw3, and d4.

When creating a new 2D pulse sequence in standard form, the pulse sequence should contain a d2 delay. To create the appropriate parameters, use the par2d macro. It is usually convenient to call par2d from within the macro used to set up the pulse sequence, and to set the parameters to appropriate values with the set2d macro. Examples of 2D pulse sequences are given in the standard software in /vnmr/psglib and /vnmr/ maclib.

When creating a new 3D pulse sequence in standard form, the pulse sequence should contain the delays d2 and d3, and parameters can be created with the par3d macro. Similarly, a 4D pulse sequence should contain the delays d2, d3, and d4, with parameters created by the par4d macro.

Each indirect dimension of data can be acquired in a phase-sensitive mode. Examples of this include the hypercomplex method and the TPPI method (see the chapter on multidimensional NMR in *User Guide: Liquids NMR* for more details).

For each indirect dimension, a *phase* parameter selects the type of acquisition. For the first indirect dimension, the corresponding phase parameter is phase. For the second indirect dimension, the parameter is phase2. For the third indirect dimension, the parameter is phase3. The total number of FIDs in a given multidimensional data set is stored in the parameter arraydim. For a 2D experiment, arraydim is equal to ni*(number of elements of the phase parameter).

When programming the multidimensional pulse sequences, it is convenient to have access to the current increment in a particular indirect dimension, and to know what the phase element is. Table 34 lists these PSG variables (see Table 22 for the full list of Vnmr parameters and their corresponding PSG variable names and types).

Some pulse sequences, such as heteronuclear 2D-J (HET2DJ), can be used "as is" for phase-sensitive 2D NMR; however, the hypercomplex and TPPI experiments require more information compared to "normal" pulse sequences, and this is presented here.

Hypercomplex 2D

Hypercomplex 2D (States, Haberkorn, Ruben) requires only that a pulse sequence be run using an arrayed parameter that generates the two required experiments. While this can be any parameter, for consistency we recommend the use of a parameter phase, which can

PSG Variable	PSG type	Vnmr parameter	Description
d2_index	int	0 to (ni-1)	Current index of the d2 array
id2	real-time	0 to (ni-1)	Current real-time index of the d2 array
inc2D	double	1.0/sw1	Dwell time for first indirect dimension
phase1	int	phase	Acquisition mode for first indirect dimension
d3_index	int	0 to (ni2-1)	Current index of the d3 array
id3	real-time	0 to (ni2-1)	Current real-time index of the d3 array
inc3D	double	1.0/sw2	Dwell time for second indirect dimension
phase2	int	phase2	Acquisition mode for second indirect dimension
d4_index	int	0 to (ni3-1)	Current index of the d4 array
id4	real-time	0 to (ni3-1)	Current real-time index of the d4 array
inc4D	double	1.0/sw3	Dwell time for third indirect dimension
phase3	int	phase3	Acquisition mode for third indirect dimension
ix	int	l to arraydim	Current element of an arrayed experiment

Table 34. Multidimensional PSG Variable	Table 34.	Multidimensional PSG Variables
---	-----------	--------------------------------

be set by the user to 0 (to give a non-phase-sensitive experiment) or to an array (as in phase=1,2) to generate the two desired experiments. The parameter phase is automatically made available to a pulse sequence as the integer phase1. Typical code as part of the pulse sequence might look like this: pulsesequence()

```
{
   if (phase1==0)
   {
                      /* Phase calculation for */
                       /* 'normal' experiment */
   . . .
   }
  else if (phase1==1)
   {
                       /* Phase calculation for */
                       /* first of two arrays */
   . . .
   }
      else if (phase1==2)
                      /* Phase calculation for */
      {
                       /* second of two arrays */
      . . .
      }
}
```

This code usually can be condensed because the phases are obviously related in the three experiments, and three separate phase calculations are not needed. One possibility is to write down the phase cycle for the entire experiment, interspersing the "real" and "imaginary" experiments, then generate an "effective transient counter" as follows:

Now a single phase cycle can be derived from v10 instead of from ct. If phase1=0, each element of this phase cycle is selected. If phase1=1, only the odd elements are selected (the first, third, fifth, etc. transients for which ct=0, 2, 4,...). If phase1=2, the even elements only are selected (ct odd).

Real Mode Phased 2D: TPPI

For TPPI experiments, the increment index is typically needed at some point in the phase calculation. The simplest way to obtain the index is to use the built-in real-time constant id2. This can be used in a construction such as

```
if (phase1==3)
add(v11,id2,v11);
```

which adds the increment value (which starts at 0) to the phase contained in v11.

2.15 Gradient Control for PFG and Imaging

UNITY INOVA, MERCURY-VX, MERCURY, UNITY plus, UNITY, and GEMINI 2000 systems support gradient control for applications using the optional pulsed field gradient (PFG) and imaging. The configuration parameter gradtype, set by the config program, specifies the presence of gradient hardware and its capabilities. The available gradient control statements are listed in Table 35. MERCURY-VX, MERCURY, and GEMINI 2000 systems use rgradient and vagradient, and MERCURY-VX and MERCURY uses the lk_sample and lk_hold statements

Table 36 lists delays for shaped gradient statements on systems with gradient waveform generators (gradtype='w' or gradtype='q'). The times for the three-axis gradient statements (obl_gradient, oblique_gradient, pe2_gradient, phase_encode3_gradient, etc.) are the overhead times for setting all three gradients. The gradients are always set in sequential 'x', 'y', 'z' order.

It is important to note that starting with VNMR 5.1, some gradient statements use DAC values to set the gradient levels and others use values in gauss/cm. The lower level gradient statements (gradient, rgradient, shapedgradient, etc.) use DAC values, and the obliquing and variable-angle gradient statements use gauss/cm. The gradient statements associated with DAC values are used in single-axis PFG pulse sequences and microimaging pulse sequences and triple-axis PFG pulse sequences.

Setting the Gradient Current Amplifier Level

To set the gradient current amplifier level, use rgradient (channel,value), where channel is 'X', 'x', 'Y', 'Y', 'Z', or 'z' (only 'Z' or 'z' is supported on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*) and value is a real number for the amplifier level (e.g, rgradient ('z', 1327.0)). For the Performa I PFG module, value must be from 2048 to 2047; for Performa II, value must be from -32768.0 to 32767.0.

To set the gradient current amplifier level but determine the value instead by real-time math, use vgradient(channel,intercept,slope,rtval), where channel is used the same as in rgradient, and amplifier level is determined by intercept + slope * rtval (e.g., vgradient('z',-5000.0,2500.0,v10). This statement not available on the Performa I PFG module.

lk_hold()	Set lock correction circuitry to hold
lk_sample()	Set lock correction circuitry to sample
obl_gradient*	Execute an oblique gradient
oblique_gradient*	Execute an oblique gradient
obl_shapedgradient*	Execute a shaped oblique gradient
oblique_shapedgradient*	Execute a shaped oblique gradient
pe_gradient*	Oblique gradient with PE in 1 axis
pe2_gradient*	Oblique gradient with PE in 2 axes
pe3_gradient*	Oblique gradient with PE in 3 axes
<pre>pe_shapedgradient*</pre>	Oblique shaped gradient with PE in 1 axis
pe2_shapedgradient*	Oblique shaped gradient with PE in 2 axes
pe3_shapedgradient*	Oblique shaped gradient with PE in 3 axes
phase_encode_gradient*	Oblique gradient with PE in 1 axis
phase_encode3_gradient*	Oblique gradient with PE in 3 axes
phase_encode_shapedgradient*	Oblique shaped gradient with PE in 1 axis
phase_encode3_shapedgradient*	Oblique shaped gradient with PE in 3 axes
<pre>rgradient(channel,value)</pre>	Set gradient to specified level
<pre>shapedgradient*</pre>	Shaped gradient pulse
<pre>shaped2Dgradient*</pre>	Arrayed shaped gradient function
shapedincgradient*	Dynamic variable gradient function
shapedvgradient*	Dynamic variable shaped gradient function
vgradient*	Set gradient to level determined by real-time math
vagradient*	Variable angle gradient
vagradpulse*	Pulse controlled variable angle gradient
vashapedgradient*	Variable angle shaped gradient
vashapedgradpulse*	Variable angle pulse controlled shaped gradient
<pre>zgradpulse(value,delay)</pre>	Create a gradient pulse on the z channel
<pre>zero_all_gradients*</pre>	Set all gradients to zero
* For the argument list, refer to the statement	reference in Chapter 3

Table 35. Gradient Control Statements

Generating a Gradient Pulse

To create a gradient pulse on the z channel with given amplitude and duration, use zgradpulse(value,delay), where value is used the same as in rgradient and delay is any delay parameter (e.g., zgradpulse(1234.0,d2)).

shapedgradient(pattern,width,amp,channel,loops,wait) generates a shaped gradient, where pattern is a file in shapelib, width is the pulse length, amp is a value that scales the amplitude of the pulse, channel is the same as used with rgradient, loops is the number of times (1 to 255) to loop the waveform, and wait is WAIT or NOWAIT for whether or not a delay is inserted to wait until the gradient is completed before executing the next statement (e.g., shapedgradient("hsine", 0.02, 32676, 'y', 1, NOWAIT))

snapedgradient("fisine",0.02,32676, 'y',1,NOWAIT))

This statement is only available on the Perform II PFG module.

Controlling Lock Correction Circuitry

On *MERCURY-VX*, *MERCURY*, UNITY *INOVA*, and UNITY *plus* systems, lk_sample() and lk_hold() are provided to control the lock correction circuitry. If during the course

-	Delay (µs)		
Pulse Sequence Statements	^{UNITY} INOVA	UNITYplus	UNITY, VXR-S
shapedgradient	0.5	5.75	10.75
shapedvgradient	1.5	14.95	27.95
shapedincgradient	1.5	12.65	23.65
incgradient (gradtype='p', gradtype='q')	4.0	_	_
incgradient (gradtype='w')	0.5	3.45	6.9
obl_gradient, oblique_gradient, pe_gradient, phase_encode_gradient (gradtype='p', gradtype='q')	12.0	20.70	38.70
<pre>obl_gradient, oblique_gradient, pe_gradient, phase_encode_gradient (gradtype='w')</pre>	1.5	10.35	20.70
pe2_gradient, phase_encode3_gradient (gradtype='p', gradtype='q')	12.0	_	_
pe2_gradient, phase_encode3_gradient (gradtype='w')	1.5	10.35	20.70
obl_shapedgradient, oblique_shapedgradient	1.5	17.25	32.25
pe_shapedgradient, phase_encode_shapedgradient	4.5	44.85	83.85
pe2_shapedgradient, pe3_shapedgradient, phase_encode3_shapedgradient	4.5	37.95	70.95

Table 36. Delays for Obliquing and Shaped Gradient Statements

of a pulse sequence the lock signal is disturbed—for instance, with a gradient pulse or pulses at the ²H frequency—the lock circuitry might not be able to hold on to the lock. When this is the case, the correction added in the feedback loop that holds the lock can be held constant by calling $lk_hold()$. At some time after the disturbance has passed (how long depends on the type of disturbance), the statement $lk_sample()$ should be called to allow the circuitry to correct for disturbances external to the experiment.

Programming Microimaging Pulse Sequences

The procedures for programming microimaging pulse sequences for UNITY and UNITY*plus* systems are the same as those used in the programming of spectroscopy sequences, with the exception that additional pulse sequence statements have been added to define the amplitude and timing of the gradient pulses and the shaped rf pulses. For example, in the statement rgradient(name,value) to set a gradient, the argument name is either X, Y, or Z (or alternatively with the connection through the parameter

orient, gread, gphase, or gslice) and value is the desired gradient strength in DAC units at the time the statement is to be implemented.

The basic imaging sequences included with the VNMR software are sequences for which the image data can be acquired, processed, and displayed with essentially the same software tools that are used with 2D spectra. These sequences have been written in a form that provides a great deal of flexibility in adapting them to the different modes of imaging and include the capabilities of multislice and multiecho imaging. Many of the spectroscopic preparation pulse sequences can be linked to the standard imaging sequences to limit the spin population type that is imaged, to provide greater contrast in the image, or to remove artifacts from the image.

For UNITY*plus*, UNITY, and VXR-S systems, configuring the system as an imaging spectrometer has a number of PSG implications. See the next section for more information on the implications relative to PSG, and see the software installation manual for system configuration procedures.

2.16 Programming the Performa XYZ PFG Module

The Performa XYZ pulsed field gradient (PFG) module adds new capabilities to highresolution liquids experiments on Varian spectrometers. The module applies gradients in B_0 along three distinct axes at different times during the course of the pulse sequence. These gradients can perform many functions, including solvent suppression and coherence pathway selection. This section describes pulse sequence programming of the module.

Creating Gradient Tables

In order for the software to have the necessary information on all three axes to convert between gauss/cm and DAC values, the XYZ PFG probe and amplifier combination can be calibrated using the creategtable macro and a gradient table made in /vnmr/imaging/gradtables.

The macro first prompts the user to see if the gradient axes are set to the same gradient strength (horizontal-bore imaging system) or if the axes have different gradient strengths (vertical-bore PFG gradients). Next, the user is prompted for a name for the gradient coil, and that name is then used in the gcoil and sysgcoil parameters in order to correctly translate between DAC and gauss/cm values. Finally, the macro prompts the user for the boresize of the magnet (51 mm), the gradient rise time (40 μ s), and the maximum gradient strength obtainable for each axis. Note that the gradient strengths are not equal and the amplifier does not limit the combined output.

If the parameter gcoil does not exist in a parameter set and must be created, you must set the protection bit that causes the macro_gcoil to be executed when the value for gcoil is changed. Setting the protection bit can be done two ways:

- Use the macro updtgcoil, which will create the gcoil parameter if it does not exist.
- Create gcoil with the following commands: create('gcoil','string') setprotect('gcoil','set',9)

In an experiment that uses gradient coils, the sysgcoil parameter can be set to the coil name specified with the creategtable macro and then the updtgcoil macro can be run to update the local gcoil parameter from the global sysgcoil parameter. When the local gcoil parameter is updated, the local gxmax, gymax, gzmax, trise and

boresize parameters are also updated. Refer to the VNMR Command and Parameter Reference and the User Guide: Imaging for additional information about creategtable.

Pulse Sequence Programming

Table 37 lists the pulse sequence statements related to the XYZ PFG module. The system can be programmed by using the statements rgradient(channel,value) and zgradpulse(value,delay). Pulse sequences g2pul.c and profile.c in /vnmr/psglib are examples of using the gradaxis parameter and the rgradient statement.

<pre>magradient(gradlvl) magradpulse(gradlvl,gradtime)</pre>	Simultaneous gradient at the magic angle Simultaneous gradient pulse at the magic angle
mashapedgradient*	Simultaneous shaped gradient at the magic angle
mashapedgradpulse*	Simultaneous shaped gradient pulse at the magic angle
<pre>rgradient(axis,value)</pre>	Set gradient to specified level
vagradpulse*	Variable angle gradient pulse
vashapedgradient*	Variable angle shaped gradient
vashapedgradpulse*	Variable angle shaped gradient
<pre>zgradpulse(value,delay)</pre>	Create a gradient pulse on the z channel
<pre>* mashapedgradient(pattern,gradlvl,gradtime,theta,phi,loops,wait) mashapedgradpulse(pattern,gradlvl,gradtime,theta,phi) vagradpulse(gradlvl,gradtime,theta,phi) vashapedgradient(pattern,gradlvl,gradtime,theta,phi,loops,wait) vashapedgradpulse(pattern,gradlvl,gradtime,theta,phi)</pre>	

Table 37.	Performa	XYZ	PFG	Module	Statements

To produce a gradient at any angle by the combination of two or more gradients, the vagradpulse(gradlvl,gradtime,theta,phi) statement can be used, and to produce three equal and simultaneous gradients, such that an effective gradient is produced at the magic angle, the magradpulse(gradlvl,gradtime) statement is available. The statements vagradpulse and magradpulse are structured so that the software does all of the calculations to produce the effective gradient desired. Both statements take the argument for the gradient level (gradlvl) in gauss/cm. This is distinctly different from the rgradient and zgradpulse statements, which take the argument for the gradient level (value) in DAC.

With these statements, the gcoil and sysgcoil parameters are required for the software to calculate the correct DAC value for each channel in order to produce the requested effective gradient. After the gradients have each been calibrated and a gradtable has been constructed with the creategtable macro, as described above, then the sysgcoil parameter can be set to that coil name used. The updtgcoil macro can then update the local gcoil parameter from the global sysgcoil parameter.

The vagradpulse statement uses the theta and phi angles to produce an effective gradient at any arbitrary angle. For example, using vagradpulse with theta=54.7 and phi=0.0, an effective gradient is produced at the magic angle by the correct combination of the Z gradient and the Y gradient. Whereas, if theta=54.7 and phi=90, an effective gradient is produced at the magic angle by the correct combination of the Z gradient. Variations on the vagradpulse statement include the capability of shaping the gradient waveform with the vashapedgradient and the vashapedgradpulse statements. For more information about these statements, see their descriptions in Chapter 3.

In addition, the magradpulse statement produces equal and simultaneous gradients on all three axes in order to produce an effective gradient at the magic angle. Variations on the magradpulse statement include the capability of shaping the gradient waveform with the mashapedgradient and the mashapedgradpulse statements. Again, for more information, refer to Chapter 3.

2.17 Imaging-Related Statements

Table 38 summarizes the PSG statements related to imaging. In VNMR 5.1, most of these statements could only be used with the system configured as an imaging spectrometer. With VNMR 5.3 and later software, however, the PSG imaging statements are used whenever their functionality is needed, provided your system does not have a 63-step output board.

Statements related to imaging can be grouped as follows:

- · Real-time gradient statements
- · Oblique gradient statements
- · Global list and position statements
- · Looping statements
- Waveform initialization statements
- Other statements

These statements were developed to support oblique imaging using standard units (gauss/ cm) to set the gradient values and to support the use of real-time variables and loops when constructing imaging sequences. Using real-time variables and loops resulting in "compressed" acquisitions, instead of standard acquisition arrays, reduces the number of acodes sets needed to run the experiment, cutting down significantly on the start-up time of the experiment and removing any inter-FID and intertransient overhead delays. This is not really a problem on UNITY *INOVA* systems, because its small overhead delays and d0 parameter make the inter-FID and intertransient delays consistent, but may make a difference in some applications.

Real-time Gradient Statements

Real-time gradient statements consist of additions to the standard gradient and shapedgradient statements, which provide real-time variable control for the gradient amplitudes. Real-time statements include shapedvgradient, which provides real-time control on one axis, incgradient and shapedincgradient, which support real-time control over three axes. The vgradient statement also belongs to this group.

Oblique Gradient Statements

To support oblique imaging and the imaging interface, oblique gradient statements include oblique_gradient, phase_encode_gradient, pe_gradient, and all of their variations. The inputs to these statements are amplitudes and phases. Amplitudes are expressed in gauss/cm and correspond to the read-out, phase-encode, and slice-select axis in the logical frame. Phase angles correspond to Euler angles psi, phi, and theta and describe the coordinate rotation applied to the input amplitudes. For more information on use, see the manual *User Guide: Imaging*.

create_delay_list*	Create table of delays Create table of frequencies
<pre>create_freq_list* greate_offget_list*</pre>	Create table of frequency offsets
<pre>create_offset_list* endmsloop*/endpeloop*</pre>	Ends a loop started by the msloop/peloop
getarray*	Retrieves all values of arrayed parameter
getorientation*	Read image plane orientation
incgradient*	Dynamic variable gradient function
init_rfpattern*	Create rf pattern file
init_gradpattern*	Create gradient pattern file
init_vscan*	Initialize real-time variable for vscan
obl_gradient*	Execute an oblique gradient
oblique_gradient*	Execute an oblique gradient
obl_shapedgradient*	Execute a shaped oblique gradient
oblique_shapedgradient*	Execute a shaped oblique gradient
msloop*/peloop*	Provides a sequence-switchable loop
pe_gradient*	Oblique gradient with PE in 1 axis
pe2_gradient*	Oblique gradient with PE in 2 axes
pe3_gradient*	Oblique gradient with PE in 3 axes
<pre>pe_shapedgradient*</pre>	Oblique shaped gradient with PE in 1 axis
pe2_shapedgradient*	Oblique shaped gradient with PE in 2 axes
pe3_shapedgradient*	Oblique shaped gradient with PE in 3 axes
phase_encode_gradient*	Oblique gradient with PE in 1 axis
phase_encode3_gradient*	Oblique gradient with PE in 3 axes
phase_encode_shapedgradient*	Oblique shaped gradient with PE in 1 axis
phase_encode3_shapedgradient*	Oblique shaped gradient with PE in 3 axes
<pre>poffset*/position_offset*</pre>	Set frequency based on position
<pre>poffset_list*</pre>	Set frequency from position list
<pre>position_offset_list*</pre>	Set frequency from position list
shapedgradient*	Provide shaped gradient pulse
<pre>shaped2Dgradient*</pre>	Arrayed shaped gradient function
shapedincgradient*	Dynamic variable gradient function
shapedvgradient*	Dynamic variable shaped gradient function
sli*	Set SLI lines
vagradient*	Variable angle gradient
vagradpulse*	Pulse controlled variable angle gradient
vashapedgradient*	Variable angle shaped gradient
vashapedgradpulse*	Variable angle pulse controlled shaped gradient
vdelay*	Select delay from table
vdelay_list*	Get delay value from delay list with real-time index
vfreq*	Select frequency from table
vgradient*	Dynamic variable gradient
voffset*	Select frequency offset from table
vscan*	Dynamic variable scan function
vsli*	Set SLI lines from real-time variable
<pre>zero_all_gradients*</pre>	Sets all gradients to zero
* For the argument list, refer to the statement	0
	*

Table 38. Imaging-Related Statements

Global List and Position Statements

The global list statements support real-time selection of frequencies, offsets, and delays. Global lists are different from AP tables in that the lists are sent down to the acquisition console when the experiment starts up and remain accessible until the experiments completes. The lists can be arrayed parameters (with a protection bit set to prevent an arrayed acquisition) read into the pulse sequence using the getarray statement or standard C language arrays calculated within the pulsesequence. The lists are initialized with the statements create_freq_list, create_offset_list, and create_delay_list, and then selected and set using the vfreq, voffset, and vdelay_list statements; which use a real-time parameter as an index into the list.

The position statements set the rf frequency from a given position or an array of positions. These statements are poffset, poffset_list, position_offset, and position_offset_list. The position list statements use global lists, which initialize the list and select and set the position in a single statement.

When creating global list parameters, create them as acquisition parameters and set protection bit 8 (value 256) or else PSG tries to array them as standard arrayed acquisitions.

Looping Statements

The looping statements msloop and peloop define multislice and phase encode loops when creating imaging pulse sequences. The looping statements also allow selection of a standard "arrayed" acquisition or a "compressed" acquisition using the seqcon parameter.

Waveform Initialization Statements

The waveform initialization statements init_rfpattern and init_gradpattern are available to all configurations and allow the user to calculate and create gradient and rf patterns in PSG.

Other Statements

The init_vscan and vscan statements are used to provide a dynamic scan capability. The sli and vsli statements are used with the Synchronized Line Interface board, which is a SIS specific hardware device used to support interfacing to external devices. The sli and vsli statements are not supported on UNITY *INOVA*. UNITY *INOVA* support for interfacing to an external device is included in the AP User interface.

2.18 User-Customized Pulse Sequence Generation

The complete pulse sequence generation (PSG) source code is supplied in the VNMR system psg directory. This code enables users to create their own libpsglib.so PSG directory for link loading with the pulse sequence object file pulsesequence.o.

The UNIX shell script setuserpsg in the system directory creates the directory vnmrsys/psg for a user, if it does not already exist, and initializes this user PSG directory with the appropriate object libraries from the system PSG directory. The script setuserpsg should only have to be run once by each separate user. setuserpsg places the file libpsglib.a in the user's psg directory.

The UNIX shell script psggen compiles files in the user PSG object directory and places the files in the user PSG directory. When executed, seggen looks first for the user PSG

Chapter 2. Pulse Sequence Programming

library ~/vnmrsys/psg in the user PSG directory, and then in the system library directory /vnmr/lib.

Modifying a PSG source file and subsequently recompiling the user PSG object directory is done as follows:

1. Enter **setuserpsg** from a UNIX shell (done only once).

Typical output from this command is as follows: Creating user PSG directory... Copying User PSG library from system directory...

- 2. Copy the desired PSG source file(s) from \$vnmrsystem/psg to \$vnmruser/psg.
- 3. Modify the PSG source files(s) in the user PSG directory.
- 4. Enter **psggen** from a UNIX shell or from within Vnmr.

Typical output from this command is as follows: Creating additional source links... Compiling PSG Library... PSG Library Complete.

Chapter 3. Pulse Sequence Statement Reference

This chapter contains a detailed reference to the statements used in VNMR pulse sequence programming. For a list of statements, refer to the Table of Contents.

For each statement, the syntax and a description is provided. If the statement contains arguments, a description of each argument and an example showing the use of the arguments is also provided. For most statements, a cross-reference to related statements is provided at the end of the listing. If the statement applies only to certain hardware or system options, an applicability entry is included. A change bar indicates new or changed information since the last version of VNMR.

Α

acquire	Explicitly acquire data
Applicability:	All systems except MERCURY and GEMINI 2000.
Syntax:	<pre>acquire(number_points,sampling_interval) double number_points; /* points to acquire */ double sampling_interval; /* dwell time in sec */</pre>
Description:	Acquire data points where the sequence of events is to acquire a pair of points for 200 ns, delay for sampling_interval minus 200 ns, then repeat for number_points/2 times.
	For UNITY <i>INOVA</i> systems there are small overhead delays before and after the acquire. The pre-acquire delay takes into account setting the receiver phase with oph and enabling data overflow detection. The post-acquire delay is for disabling data overflow detection. When using acquire statements within a hardware loop these overhead delays and the functions associated with them are placed outside the hardware loop. When using multiple acquire statements outside a hardware loop in a pulse sequence setting, the phase and enabling data overflow detection is done before the first acquire statement. Disabling overflow detection is done after the last acquire, so there is no overhead time between acquire statements.
	If an acquire statement occurs outside a hardware loop, the number of complex points to be acquired must be a multiple of 2 on systems with a Digital Acquisition Controller board, an Acquisition Controller board, or a Pulse Sequence Controller board, or must be a multiple of 32 on systems with a Output board (each board is described below).
	Inside a hardware loop, systems with a Digital Acquisition Controller board or a Pulse Sequence Controller board can accept a maximum of 2048 complex points, systems with an Acquisition Controller board can accept a maximum of

1024 complex points, and systems with an Output board can accept a maximum of 63 complex points.

The following list identifies the acquisition controller boards used on Varian NMR spectrometer systems:

- Data Acquisition Controller boards, Part No. 01-902010-00. Started shipping in mid-1995 with the introduction of the UNITYINOVA system.
- Pulse Sequence Controller boards, Part No. 00-992560-00. Started shipping in early 1993 with the introduction of the UNITYplus system.
- Acquisition Controller boards, Part No. 00-969204-00 or 00-990640-00. Started shipping 00-969204-00 in late 1988 as a replacement for the Output boards. Part No. 00-990640-00 replaced 00-969204-00 in mid-1990.
- *Output boards, Part No. 00-953520-0#, where # is an integer.* Shipped with systems prior to 1988.

Arguments: number_points is the number of data point to be acquired.

sampling_interval is the length, in seconds, of the sampling interval.

Examples: acquire(np,1.0/sw);

Related:	endhardloop	End hardware loop
	starthardloop	Start hardware loop

add

Add integer values

Syntax:	add(vi,vj,v codeint vi; codeint vj; codeint vk;	<pre>/* real-time variable vi for addend */ /* real-time variable vj for addend */ /* real-time variable vk for sum */</pre>
Description:	Sets vk equal to	the sum of integer values of vi and vj.
Arguments:	vi, vj, and vk	are real-time variables (v1 to v14, oph, etc.).
Examples:	add(v1,v2,v)	r3);
Related:	assign dbl decr divn hlv incr mod2 mod4 modn mult sub	Assign integer values Double an integer value Decrement an integer value Divide integer values Half the value of an integer Increment an integer value Find integer value modulo 2 Find integer value modulo 4 Find integer value modulo n Multiply integer values Subtract integer values
apovrride	Override inter	nal software AP bus delay
Applicability:	UNITY and VXR-S systems with the 63-step Output board (Part No. 00-953520-0#, where # is an integer). This board shipped prior to 1988.	
Syntax:	apovrride()	
Description:	Systems with the 63-step Output board can use this statement to prevent a delay of 0.2 µs from being inserted prior to the next (and only the next) occurrence of one of the AP (analog port) bus statements dcplrphase, dcplr2phase, dcplr3phase, decprgoff, dec2prgoff, dec3prgoff, dec3prgoff, decprgon,	

dec2prgon, dec3prgon, decshaped_pulse, dec2shaped_pulse, dec3shaped_pulse, decspinlock, dec2spinlock, dec3spinlock, obsprgoff, obsprgon, power, rlpower, shaped_pulse, simshaped_pulse, sim3shaped_pulse, spinlock, and xmtrphase.

apshaped_decpulse First decoupler pulse shaping via AP bus

Applicability:	UNITY <i>INOVA</i> and UNITY <i>plus</i> systems. On <i>MERCURY-VX</i> and <i>MERCURY</i> , only shapes with no phase shifts are supported.
Syntax:	<pre>apshaped_decpulse(shape,pulse_width,pulse_phase, power_table,phase_table,RG1,RG2) char *shape;</pre>
Description:	Provides first decoupler fine-grained "waveform generator-type" pulse shaping through the AP bus. A pulse shape file for the waveform generator (/vnmr/shapelib/*.RF) is used. This statement overrides any existing small-angle phase shifting (i.e., a preceding dcplrphase) and step size setting on the first decoupler channel. After apshaped_decpulse, first decoupler channel small-angle phase shifting is reset to zero and the step size is set to 0.25 degrees.
	apshaped_decpulse capability is now integrated into the statement decshaped_pulse. The decshaped_pulse statement calls apshaped_decpulse without table variables if a waveform generator is not configured on the decoupler channel. decshaped_pulse creates AP tables on the fly for amplitude and phase, and does not use the AP tables allocated for users. It still uses real-time variables v12 and v13.
Arguments:	shape is a shape file (without the .RF extension) in /vnmr/shapelib or in ~/vnmrsys/shapelib. The amplitude and phase fields of the shape file are used. The relative duration field (field 3) should be left at the default value of 1.0 or at least small numbers, and the gate field (field 4) is currently not used because the transmitter is switched on throughout the shape. On <i>MERCURY-VX</i> and <i>MERCURY</i> systems, no phase is changed or set.
	pulse_width is the total pulse width, in seconds, excluding the amplifier gating delays around the pulse.
	pulse_phase is the 90° phase shift of the pulse. For small-angle phase shifting, note that apshaped_decpulse sets the phase step size to the minimum on the one channel that is used.
	power_table and phase_table are two table variables (t1 to t60) used as intermediate storage addresses for the amplitude and phase tables, respectively. If apshaped_decpulse is called more than once, different table names should be used in each call.
	RG1 is the amplifier gating time, in seconds, before the pulse.
	RG2 is the amplifier gating time, in seconds, after the pulse.
Examples:	<pre>apshaped_decpulse("gauss",pw,v1,rof1,rof2);</pre>
Related:	apshaped_dec2pulseSecond decoupler pulse shaping via the AP busapshaped_pulseObserve transmitter pulse shaping via the AP bus

dcplrphase	Set small-angle phase of first decoupler, rf type C or D
decshaped_pulse	Perform shaped pulse on first decoupler

apshaped_dec2pulse Second decoupler pulse shaping via AP bus

Applicability:	UNITY INOVA and UNITY plus systems.	
Syntax:	<pre>apshaped_dec2pulse(shape,pulse_width,pulse_phase, power_table,phase_table,RG1,RG2) char *shape;</pre>	
Description:	Provides second decoupler fine-grained "waveform generator-type" pulse shaping through the AP bus. A pulse shape file for the waveform generator (/ vnmr/shapelib/*.RF) is used. Note that the real-time variables v12 and v13 are used by this statement. apshaped_dec2pulse overrides any existing small-angle phase shifting (i.e., a preceding dcplr2phase) and step size setting on the second decoupler channel. After apshaped_dec2pulse, second decoupler channel small-angle phase	
	shifting is reset to zero and the step size is set to 0.25 degrees. apshaped_dec2pulse capability is now integrated into the statement dec2shaped_pulse. The dec2shaped_pulse statement calls apshaped_dec2pulse without table variables if a waveform generator is not configured on the decoupler channel. dec2shaped_pulse creates AP tables on the fly for amplitude and phase, and does not use the AP tables allocated for users.It still uses real-time variables v12 and v13.	
Arguments:	shape is a shape file (without the .RF extension) in /vnmr/shapelib or in ~/vnmrsys/shapelib. The amplitude and phase fields of the shape file are used. The relative duration field (field 3) should be left at the default value of 1.0 or at least small numbers, and the gate field (field 4) is currently not used because the transmitter is switched on throughout the shape.	
	pulse_width is the total pulse width, in seconds, excluding the amplifier gating delays around the pulse.	
	<pre>pulse_phase is the 90° phase shift of the pulse. For small-angle phase shifting, note that apshaped_dec2pulse sets the phase step size to the minimum on the one channel that is used. power_table and phase_table are two table variables (t1 to t60) used as intermediate storage addresses for the amplitude and phase tables, respectively. If apshaped_dec2pulse is called more than once, different table names should be used in each call.</pre>	
	RG1 is the amplifier gating time, in seconds, before the pulse.	
	RG2 is the amplifier gating time, in seconds, after the pulse.	
Examples:	<pre>apshaped_dec2pulse("gauss",pw,v1,t10,t11,rof1,rof2);</pre>	
Related:	apshaped_decpulseFirst decoupler pulse shaping via the AP busapshaped_pulseObserve transmitter pulse shaping via the AP busdcplr2phaseSet small-angle phase of 2nd decoupler, rf type C or Ddec2shaped_pulsePerform shaped pulse on second decoupler	

apshaped_pulse Observe transmitter pulse shaping via AP bus

Applicability: UNITY INOVA and UNITY plus systems. On MERCURY-VX and MERCURY, only shapes with no phase shifts are supported.

Syntax:	apshaped_pulse(shape	e,pulse_width,pulse_phase,	
	<pre>power_table,phase_</pre>	_table,RG1,RG2)	
	char *shape;	/* name of .RF shape file */	
	double pulse_width;	/* pulse width in sec */	
	codeint pulse_phase;	/* real-time phase of pulse */	
	<pre>codeint power_table;</pre>	/* table variable to store power	*/
	codeint phase_table;	/* table variable to store phase	*/
	double RG1;	/* gating time before pulse in sec	*/
	double RG2;	/* gating time after pulse in sec	*/

Description: Provides observe transmitter fine-grained "waveform generator-type" pulse shaping through the AP bus. A pulse shape file for the waveform generator (/ vnmr/shapelib/*.RF) is used. This statement overrides any existing small-angle phase shifting (i.e., a preceding xmtrphase) and step size setting on the observe transmitter channel. After apshaped_pulse, observe transmitter channel small-angle phase shifting is reset to zero and the step size is set to 0.25 degrees.

apshaped_pulse capability is now integrated into the shaped_pulse statement. The shaped_pulse statement calls apshaped_pulse without table variables if a waveform generator is not configured on the decoupler channel. shaped_pulse creates AP tables on the fly for amplitude and phase, and does not use the AP tables allocated for users. It still uses real-time variables v12 and v13.

Arguments: pattern is a shape file (without the .RF extension) in /vnmr/shapelib or in ~/vnmrsys/shapelib. The amplitude and phase fields of the shape file are used. The relative duration field (field 3) should be left at the default value of 1.0 or at least small numbers, and the gate field (field 4) is currently not used because the transmitter is switched on throughout the shape. On *MERCURY-VX* and *MERCURY* systems, no phase is changed or set.

pulse_width is the total pulse width, in seconds, excluding amplifier gating delays around the pulse.

pulse_phase is the 90° phase shift of the pulse. For small-angle phase shifting, note that apshaped_pulse sets the phase step size to the minimum on the one channel that is used.

power_table and phase_table are two table variables (t1 to t60) used as intermediate storage addresses for the amplitude and phase tables, respectively. If apshaped_pulse is called more than once, different table names should be used in each call.

RG1 is the amplifier gating time, in seconds, before the pulse.

RG2 is the amplifier gating time, in seconds, after the pulse.

Examples: apshaped_pulse("gauss",pw,v1,rof1,rof2);

 Related:
 apshaped_deccpulse
 First decoupler pulse shaping via the AP bus

 apshaped_dec2pulse
 Second decoupler pulse shaping via the AP bus

 shaped_pulse
 Perform shaped pulse on observe transmitter

 xmtrphase
 Set small-angle phase of observe transmitter, rf C or D

assign	Assign intege	r values	
Syntax:		vj) /* real-time variable for starting value */ /* real-time variable for assigned value */	
Description:	Sets vj equal to	o the integer value vi.	
Arguments:	vi and vj are	real-time variables (v1 to v14, oph, etc.).	
Examples:	assign(v3,	v2);	
Related:	add	Add integer values	
	dbl	Double an integer value	
	decr	Decrement an integer value	
	divn	Divide integer values	
	hlv	Half the value of an integer	
	incr	Increment an integer value	
	mod2	Find integer value modulo 2	
	mod4	Find integer value modulo 4	
	modn	Find integer value modulo n	
	mult	Multiply integer values	
	sub	Subtract integer values	

В

blankingoff	Unblank amplifier channels and turn amplifiers on		
Applicability:	MERCURY-VX, MERCURY, and GEMINI 2000 systems only.		
Syntax:	blankingoff()		
Description:	Unblanks, or enables, both amplifier channels.		
Related:	blankingon Blank amplifier channels and turn amplifiers off		
blankingon	Blank amplifier channels and turn amplifiers off		
Applicability:	MERCURY-VX, MERCURY, and GEMINI 2000 systems only.		
Syntax:	blankingon()		
Description:	Blanks, or disables, both amplifier channels.		
Related:	blankingoff Unblank amplifier channels and turn amplifiers on		
	- · · · · · · · · · · · · · · · · · · ·		
blankoff	Stop blanking observe or decoupler amplifier (obsolete)		
Description:	No longer in VNMR. The blankoff statement is replaced by the statements obsunblank, decunblank, dec2unblank, and dec3unblank.		
Related:	decunblank Unblank amplifier associated with first decoupler		
	dec2unblank Unblank amplifier associated with second decoupler		
	dec3unblank Unblank amplifier associated with third decoupler		
	obsunblank Unblank amplifier associated with observe transmitter		

blankon	Start blanking observe or decoupler amplifier (obsolete)		
Description:	No longer in VNMR. The blankon statement is replaced by the statements obsblank, decblank, dec2blank, and dec3blank.		
Related:	decblank dec2blank dec3blank obsblank	Blank amplifier associated with first decoupler Blank amplifier associated with second decoupler Blank amplifier associated with third decoupler Blank amplifier associated with observe transmitter	

С

clearapdatatable Zero all data in acquisition processor memory

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax: clearapdatatable()

Description: Zeroes the acquired data table at times other than at the start of the execution of a pulse sequence, when the data table is automatically zeroed. This statement is generally not needed.

create_delay_list Create table of delays

Applicability: Not applicable on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

Syntax:	create_delay_list(li	st,nvals,list_number)
	double *list;	/*	pointer to list of delays */
	int nvals;	/*	number of values in list */
	<pre>int list_number;</pre>	/*	number 0-255 for each list */

Description: Stores global lists of delays that can be accessed with a real-time variable or table element for dynamic setting in pulse sequences. The lists need to be created in order starting from 0 using the list_number argument, or by setting the list_number argument to -1, which makes the software allocate and create the next free list and give the list number as a return value. Each list must have a unique and sequential list_number. There can be a maximum of 256 lists, depending on the size of the lists. The lists are stored in data memory and compete for space with the acquisition data for each array element. If a list is created, the return value is the number of the list (0 to 255); if an error occurs, the return value is negative.

create_delay_list creates what is called a global list. Global lists are different from AP tables in that the lists are sent down to the acquisition console when the experiment starts up and are accessible until the experiment completes. In working with arrayed experiments, be careful when using a -1 in the list_number argument because a list will be created for *each* array element. In this case, a list parameter can be created as an arrayed parameter with protection bit 8 (256) set. To read in the values of this type of parameter, use the getarray statement. To ensure that the list is only created once, check the global array counter variable ix, and only call create_delay_list to create the list when it equals 1. An example is shown below.

Arguments: list is a pointer to a list of delays.

nvals is the number of values in the list.

```
list_number -1 or a unique number from 0 to 255 for each list.
     Examples: pulsesequence()
                {
                    /* Declare static to save between calls */
                   static int list1, list2;
                   int i, n;
                   double delay1[1024], delay2[1024];
                   n = 1024;
                   if (ix == 1) {
                       for (i=0; i<n; i++) {</pre>
                           ... /* Initialize delay1 & delay2 arrays */
                       }
                       /* First, list1 is set to 0 */
                       list1 = create delay list(delay1,n,0);
                       /* This is list #1 */
                       create_freq_list(freqs,nfreqs,OBSch,1);
                       /* This is list #2 */
                       create_offset_list(freqs,nfreqs,OBSch,2);
                       /* Next, list2 is set to 3 */
                       list2 = create delay list(delay2,n,-1);
                    }
                    . . .
                   vdelay_list(list2,v5); /* Use v5 from list2 */
                   vfreq(1,v2);
                                               /* Use v2 from list #1 */
                   voffset(2,v1);
                                               /* Use v1 from list #2 */
                   vdelay_list(list1,v1); /* Use v1 from list1 */
                    . . .
                }
       Related: create_freq_list
                                      Create table of frequencies
                create_offset_list Create table of frequency offsets
                                      Delay for a specified time
                delay
                getarray
                                      Retrieves all values of an arrayed parameter
                vdelay
                                      Select delay from table
create_freq_list
                       Create table of frequencies
   Applicability: Not applicable on MERCURY and GEMINI 2000.
        Syntax: create freq list(list,nvals,device,list number)
                double *list; /* pointer to list of frequencies */
                int nvals;
                                     /* number of values in list */
                              /* OBSch, DECch, DEC2ch, or DEC3ch */
                int device;
                                    /* number 0-255 for each list */
                int list_number;
    Description: Stores global lists of frequencies that can be accessed with a real-time variable
                or table element for dynamic setting of frequencies. Frequency lists use
                frequencies in MHz (such as from sfrq, dfrq). The lists need to be created in
                order starting from 0 using the list_number argument, or by setting the
                list_number argument to -1, which makes the software allocate and create
                the next free list and give the list number as a return value. Each list must have
                a unique and sequential list_number. There can be a maximum of 256 lists
                depending on the size of the lists. The lists are stored in data memory and
                compete for space with the acquisition data for each array element. If a list is
```

created, the return value is the number of the list (0 to 255); if an error occurs, the return value is negative.

create_freq_list creates what is called a global list. Global lists are different from AP tables in that the lists are sent down to the acquisition console when the experiment starts up and are accessible until the experiment completes. In working with arrayed experiments, be careful when using a -1 in the list_number argument because a list will be created for *each* array element. In this case, a list parameter can be created as an arrayed parameter with protection bit 8 (256) set. To read in the values of this type of parameter, use the getarray statement. To ensure that the list is only created once, check the global array counter variable ix, and only call create_freq_list to create the list when it equals 1. An example is shown in the entry for the create_delay_list statement.

Arguments: list is a pointer to a list of frequencies.

nvals is the number of values in the list.

device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

list_number is -1 or a unique number from 0 to 255 for each list created.

Examples: See the example for the create_delay_list statement.

Related:	create_delay_list	Create table of delays
	create_offset_list	Create table of frequency offsets
	getarray	Retrieves all values of an arrayed parameter
	delay	Delay for a specified time
	vfreq	Select frequency from table

create_offset_list Create table of frequency offsets

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.

create_offset_l	<pre>ist(list,nvals,device,list_number)</pre>
double *list;	<pre>/* pointer to list of frequency offsets */</pre>
int nvals;	/* number of values in list */
int device;	/* OBSch, DECch, DEC2ch, or DEC3ch */
<pre>int list_number;</pre>	/* number 0-255 for each list */
	<pre>double *list; int nvals; int device;</pre>

Description: Stores global lists of frequencies that can be accessed with a real-time variable or table element for dynamic setting of frequency offsets. Offset lists define lists of frequency offsets in Hz (such as from tof, dof). Imaging pulse sequences typically use offset lists, not frequency lists. The lists need to be created in order starting from 0 using the list_number argument, or by setting the list_number argument to -1, which makes the software allocate and create the next free list and give the list number. There can be a maximum of 256 lists depending on the size of the lists. The lists are stored in data memory and compete for space with the acquisition data for each array element. If a list is created, the return value is the number of the list (0 to 255); if an error occurs, the return value is negative.

create_offset_list creates what is called a global list. Global lists are different from AP tables in that the lists are sent down to the acquisition console when the experiment starts up and are accessible until the experiment completes. In working with arrayed experiments, be careful when using a -1 in the list_number argument because a list will be created for *each* array

element. In this case, a list parameter can be created as an arrayed parameter with protection bit 8 (256) set. To read in the values of this type of parameter, use the getarray statement. To ensure that the list is only created once, check the global array counter variable ix, and only call create_offset_list to create the list when it equals 1. An example is shown in the entry for the create_delay_list statement.

Arguments: list is a pointer to a list of frequency offsets.

nvals is the number of values in the list.

device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

 $\texttt{list_number}\ is\ -1\ or\ a\ unique\ number\ from\ 0\ to\ 255\ for\ each\ list\ created.$

Examples:	See the example for the create_delay_list statement.	
Related:	create_delay_list	Create table of delays
	create_freq_list	Create table of frequencies
	getarray	Retrieves all values of an arrayed parameter
	delay	Delay for a specified time
	voffset	Select frequency offset from table

D

dbl	Double an integer value	
Syntax:	dbl(vi,vj) codeint vi; codeint vj;	/* variable for starting value */ /* variable for twice starting value */
Description:	Sets vj equal to	twice the integer value of vi.
Arguments:	vi and vj are r	eal-time variables (v1 to v14, oph, etc.).
Examples:	dbl(v1,v2);	
Related:	add assign decr divn hlv incr mod2 mod4 modn mult sub	Add integer values Assign integer values Decrement an integer value Divide integer values Half the value of an integer Increment an integer value Find integer value modulo 2 Find integer value modulo 4 Find integer value modulo n Multiply integer values Subtract integer values
dcphase	Set decoupler phase (obsolete)	
Description:	No longer suppo statement.	orted. Replace dcphase statements with the decphase
Related:	decphase	Set phase of first decoupler

dcplrphase	Set small-angle phase of 1st decoupler, rf type C or D		
Applicability:	Systems using a first decoupler with rf type C or D and <i>MERCURY-VX</i> and <i>MERCURY</i> . (<i>GEMINI 2000</i> system decouplers are rf type F and E).		
Syntax:	<pre>dcplrphase(multiplier) codeint multiplier; /* real-time phase step multiplier */</pre>		
Description:	Sets first decoupler phase in step size units set by the stepsize statement. The small-angle phaseshift is a product of multiplier and the step size. If stepsize has not been used, default step size is 90°.		
	multiplier is gr Only on systems wi automatically saved (such as at the time of Acquisition Control Acquisition Control	e step size set by the stepsize statement and reater than 90°, the sub-90° part is set by dcplrphase. th an Output board are carryovers that are multiples of 90° and added in at the time of the next 90° phase selection of the next pulse or decpulse). On systems with a Data ler board, a Pulse Sequence Controller board, or an ler board, this is done by dcplrphase (see the description aire statement for further information about these boards).	
	phase shift is to be	e, dcplrphase is needed any time the first decoupler set to a value not a multiple of 90°. decphase sets ift only, which is rarely needed.	
Arguments:	multiplier is a small-angle phaseshift multiplier for the first decoupler. The value must be a real-time variable (v1 to v14, oph, etc.) or real-time constant (zero, one, etc.).		
Examples:	dcplrphase(ze	ro);	
Related:	dcplr2phase dcplr3phase decphase stepsize xmtrphase	Set small-angle phase of second decoupler, rf type C or D Set small-angle phase of third decoupler, rf type C or D Set quadrature phase of first decoupler Set small-angle phase step size, rf type C or D Set small-angle phase of obs. transmitter, rf type C	
dcplr2phase	Set small-angle phase of 2nd decoupler, rf type C or D		
Applicability:			
Syntax:	<pre>dcplr2phase(multiplier) codeint multiplier; /* real-time phase step multiplier */</pre>		
Description:	Sets second decoupler phase in step size units set by the stepsize statement. The small-angle phaseshift is a product of multiplier and the step size. If stepsize has not been used, the default step size is 90°.		
	multiplier is gr Only on systems wi are automatically sa (such as at the time Data Acquisition Control description section these boards).	e step size set by the stepsize statement and reater than 90°, the sub-90° part is set by dcplr2phase. th an Output board are carryovers that are multiples of 90° ved and added in at the time of the next 90° phase selection of the next pulse or dec2pulse). On systems with a pontroller board, a Pulse Sequence Controller board, or an ler board, this is done by dcplr2phase (see the of the acquire statement for further information about	
	phase shift is to be s	e, dcplr2phase is needed any time the second decoupler et to a value that is not a multiple of 90°. dec2phase sets ift only, which is rarely need.	

Arguments:	multiplier is a small-angle phaseshift multiplier for the second decoupler. The value must be a real-time variable (v1 to v14, oph, etc.) or real-time constant (zero, one, etc.).	
Examples:	dcplr2phase(zero);	
Related:	dcplrphase dec2phase stepsize xmtrphase	Set small-angle phase of first decoupler, rf type C or D Set quadrature phase of second decoupler Set small-angle phase step size, rf type C or D Set small-angle phase of obs. transmitter, rf type C
dcplr3phase	Set small-angle p	phase of 3rd decoupler, rf type C or D
Applicability:	Systems using a th	ird decoupler with rf type C or D.
Syntax:	<pre>dcplr3phase(multiplier) codeint multiplier; /* multiplies phase step */</pre>	
Description:	Sets the third decoupler phase in units set by the stepsize statement. If stepsize has not been used, the default step size is 90°. The small-angle phaseshift is a product of multiplier and the preset stepsize. The full small-angle phase is set by dcplr3phase.	
	phase shift is to be	se, dcplr3phase is needed any time the third decoupler set to a value that is not a multiple of 90°. dec3phase sets hift only, which is rarely needed.
Arguments:	multiplier is a small-angle phaseshift multiplier for the third decoupler. The value must be a real-time variable (v1 to v14, oph, etc.) or real-time constant (zero, one, etc.).	
Examples:	dcplr2phase(zero);	
Related:	dcplrphase dec3phase stepsize xmtrphase	Set small-angle phase of first decoupler, rf type C or D Set quadrature phase of third decoupler Set small-angle phase step size, rf type C or D Set small-angle phase of obs. transmitter, rf type C
decblank	Blank amplifier a	ssociated with first decoupler
Applicability:		
Syntax:	decblank()	
Description:	Disables the amplifier for the first decoupler. This is generally used after a call to decunblank.	
Related:	decunblank obsblank obsunblank rcvroff rcvron	Unblank amplifier associated with first decoupler Blank amplifier associated with observe transmitter Unblank amplifier associated with observe transmitter Turn off receiver Turn on receiver
dec2blank	Blank amplifier a	ssociated with second decoupler
Applicability:	All systems with linear amplifiers.	

Syntax: dec2blank()

- Description: Disables the amplifier for the second decoupler. This is generally used after a call to dec2unblank.
 - Related:
 dec2unblank
 Unblank amplifier associated with second decoupler

 rcvroff
 Turn off receiver

 rcvron
 Turn on receiver

dec3blank Blank amplifier associated with third decoupler Applicability: UNITYINOVA and UNITYplus systems with third decoupler.

Syntax: dec3blank()

Description: Disables the amplifier for the third decoupler. This is generally used after a call to dec3unblank.

Related:	dec3unblank	Unblank amplifier associated with third decoupler
	rcvroff	Turn off receiver
	rcvron	Turn on receiver

declvloff Return first decoupler back to "normal" power

Syntax: declvloff()

Description: Switches the decoupler power to the power level set by the appropriate parameters defined by the amplifier type: dhp for class C amplifiers or dpwr for linear amplifiers. If dhp='n', declvloff has no effect on systems with class C amplifiers but still functions for systems with linear amplifiers. (On *GEMINI 2000* systems, dhp='n' has no meaning and the power level is reversed from declvlon.)

Related:	declvlon	Turn on first decoupler to full power
	power	Change transmitter or decoupler power, lin. amp. sys.
	pwrf	Change transmitter or decoupler fine power
	rlpower	Change transmitter or decoupler power, lin. amp. sys.
	rlpwrf	Set transmitter or decoupler fine power

declvlon Turn o

Turn on first decoupler to full power

Syntax: declvlon()

Description:

on: Switches the first decoupler power level between the power level set by the high-power parameter(s) to the *full* output of the decoupler. If dhp='n', declvloff has no effect on systems with class C amplifiers but still functions for systems with linear amplifiers. (On *GEMINI 2000* systems, dhp='n' has no meaning. On *GEMINI 2000* broadband systems, declvlon switches to pplvl (high) from dpwr (low), or on *GEMINI 2000* ¹H/¹³C systems to full pulse power from dhp).

If declvlon is used, make sure declvloff is used prior to time periods in which normal, controllable power levels are desired, such as prior to acquisition. Use full decoupler power only for decoupler pulses or for solids applications.

Related:	declvloff	Return first decoupler back to "normal" power
	power	Change transmitter or decoupler power, lin. amp. sys.
	pwrf	Change transmitter or decoupler fine power
	rlpower	Change transmitter or decoupler power, lin. amp. sys.
	rlpwrf	Set transmitter or decoupler fine power

decoff	Turn off first decoupler		
Syntax:	decoff()		
Description:	Explicitly gates off the first decoupler in the pulse sequence.		
Related:	decon	Turn on first decoupler	
	dec2off	Turn off second decoupler	
	dec3off	Turn off third decoupler	
dec2off	Turn off seco	nd decoupler	
Applicability:	Systems with a	second decoupler.	
Syntax:	dec2off()		
Description:	Explicitly gates	off the second decoupler in the pulse sequence.	
Related:	dec2on	Turn on second decoupler	
1	Turn off third		
dec3off		-	
Applicability:		UNITYplus systems with a third decoupler.	
•	<pre>dec3off()</pre>		
-		off the third decoupler in the pulse sequence.	
Related:	dec3on	Turn on third decoupler	
decoffset	Change offset	t frequency of first decoupler	
Syntax:	decoffset(: double frequ		
Description:	Changes the offset frequency of the first decoupler (parameter dof). It is functionally the same as offset (frequency, DODEV).		
Arguments:	frequency is	s the offset frequency desired, in hertz.	
Examples:	decoffset(do1);	
Related:	dec2offset	Change offset frequency of second decoupler	
	dec3offset	Change offset frequency of third decoupler	
	obsoffset offset	Change offset frequency of observe transmitter Change offset frequency of transmitter or decoupler	
	OIISet	Change offset frequency of transmitter of decoupler	
dec2offset	Change offset	t frequency of second decoupler	
Syntax:	dec2offset double frequ	(frequency) uency; /* offset frequency in Hz */	
Description:	Changes the offset frequency of the second decoupler (parameter dof2). It is functionally the same as offset (frequency, DO2DEV).		
Arguments:	frequency is the offset frequency desired, in hertz.		
Examples:	dec2offset	(do2);	
Related:	decoffset	Change offset frequency of first decoupler	
	dec3offset	Change offset frequency of third decoupler	
	obsoffset	Change offset frequency of observe transmitter	
	offset	Change offset frequency of transmitter or decoupler	

dec3offset	Change offset	frequency of third decoupler	
Syntax:			
	double frequ		
Description:	Changes the offset frequency of the third decoupler (parameter dof3). It is functionally the same as offset (frequency, DO3DEV).		
Arguments:	frequency is the offset frequency desired, in hertz.		
Examples:	dec3offset	(do3);	
Related:	decoffset dec2offset obsoffset offset	Change offset frequency of first decoupler Change offset frequency of second decoupler Change offset frequency of observe transmitter Change offset frequency of transmitter or decoupler	
dec4offset	Change offset	frequency of fourth decoupler	
Applicability:	UNITY <i>INOVA</i> systems with a deuterium decoupler channel as the fourth decoupler.		
Syntax:	<pre>dec4offset(frequency) double frequency; /* offset frequency in Hz */</pre>		
Description:	Changes the offset frequency of the fourth decoupler (parameter dof4). It is functionally the same as offset (frequency, D04DEV).		
Arguments:	frequency is	the offset frequency desired, in hertz.	
Examples:	dec4offset	(do4);	
Related:	decoffset dec2offset obsoffset offset rftype	Change offset frequency of first decoupler Change offset frequency of second decoupler Change offset frequency of observe transmitter Change offset frequency of transmitter or decoupler Type of rf generation	
decon	Turn on first d	lecoupler	
Syntax:	decon()		
Description:			
	decprgon generally needs to be enabled with an explicit decon statement and followed by a decoff call.		
Related:	decoff dec2on dec3on	Turn off first decoupler Turn on second decoupler Turn on third decoupler	
dec2on	Turn on secor	nd decoupler	
Applicability:	Systems with a	second decoupler.	
Syntax:	dec2on()		
Description:	decoupler gatin	on the second decoupler in the pulse sequence. Second g is handled automatically by the statements dec2rgpulse, _pulse, dec2spinlock, sim3pulse, and _pulse.	

dec2prgon generally needs to be enabled with an explicit dec2on statement and followed by a dec2off call.

Turn off second decoupler

dec3on	Turn on third decoupler		
Applicability:	UNITY INOVA and UNITY plus systems with a third decoupler.		
Syntax:	dec3on()		
Description:	Explicitly gates on the third decoupler in the pulse sequence. Third decoupler gating is handled automatically by the statements dec3rgpulse, dec3shaped_pulse, and dec3spinlock		
	dec3prgon generally needs to be enabled with an explicit dec3on statement and followed by a dec3off call.		
Related:	dec3off Turn off third decoupler		
decphase	Set quadrature phase of first decoupler		
Syntax:			
Description:	Sets quadrature phase (multiple of 90°) for the first decoupler rf. decphase is syntactically and functionally equivalent to txphase and is useful for a decoupler pulse in all cases where txphase is useful for a transmitter pulse.		
Arguments:	phase is the quadrature phase for the first decoupler rf. The value must be a real-time variable (v1 to v14, oph, ct, etc.).		
Examples:	decphase(v4);		
Related:	dcplrphaseSet small-angle phase of first decoupler, rf type C or Ddec2phaseSet quadrature phase of second decouplerdec3phaseSet quadrature phase of third decouplertxphaseSet quadrature phase of observe transmitter		
dec2phase	Set quadrature phase of second decoupler		
Applicability:			
Syntax:	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */</pre>		
	dec2phase(phase)		
Description:	dec2phase(phase)		
Description: Arguments:	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */ Sets quadrature phase (multiple of 90°) for the second decoupler rf.</pre>		
Arguments:	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */ Sets quadrature phase (multiple of 90°) for the second decoupler rf. phase is the quadrature phase for the second decoupler rf. The value must be</pre>		
Arguments:	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */ Sets quadrature phase (multiple of 90°) for the second decoupler rf. phase is the quadrature phase for the second decoupler rf. The value must be a real-time variable (v1 to v14, oph, ct, etc.).</pre>		
Arguments: Examples:	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */ Sets quadrature phase (multiple of 90°) for the second decoupler rf. phase is the quadrature phase for the second decoupler rf. The value must be a real-time variable (v1 to v14, oph, ct, etc.). dec2phase(v9); dcplr2phase Set small-angle phase of second decoupler, rf type C or D</pre>		
Arguments: Examples: Related:	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */ Sets quadrature phase (multiple of 90°) for the second decoupler rf. phase is the quadrature phase for the second decoupler rf. The value must be a real-time variable (v1 to v14, oph, ct, etc.). dec2phase(v9); dcplr2phase Set small-angle phase of second decoupler, rf type C or D decphase Set quadrature phase of first decoupler</pre>		
Arguments: Examples: Related: dec3phase	<pre>dec2phase(phase) codeint phase; /* real-time variable for quad. phase */ Sets quadrature phase (multiple of 90°) for the second decoupler rf. phase is the quadrature phase for the second decoupler rf. The value must be a real-time variable (v1 to v14, oph, ct, etc.). dec2phase(v9); dcplr2phase Set small-angle phase of second decoupler, rf type C or D decphase Set quadrature phase of first decoupler Set quadrature phase of third decoupler</pre>		

Arguments:	phase is the quadrature phase for the third decoupler rf. The value must be a real-time variable (v1 to v14, oph, ct, etc.).	
Examples:	dec3phase(v9);	
Related:	dcplr3phase decphase	Set small-angle phase of third decoupler, rf type C or D Set quadrature phase of first decoupler
dec4phase	Set quadrature p	hase of fourth decoupler
Applicability:	UNITY INOVA system decoupler.	s with a deuterium decoupler channel as the fourth
Syntax:	<pre>dec4phase(pha codeint phase;</pre>	ase) /* real-time variable for quad. phase */
Description:	Sets quadrature pha	ase (multiple of 90°) for the fourth decoupler rf.
Arguments:		rature phase for the third decoupler rf. The value must be a v1 to v14, oph, ct, etc.).
Examples:	dec4phase(v9)	;
Related:	rftype decphase	Type of rf generation Set quadrature phase of first decoupler
decpower	Change first deco	oupler power level, linear amp. systems
Applicability:	Systems with linear	r amplifiers.
Syntax:	<pre>decpower(powe double power;</pre>	er) /* new power level for DODEV */
Description:	Changes the first de rlpower(value	ecoupler power. It is functionally the same as e, DODEV).
Arguments:	(maximum power)	wer level by assuming values from 0 (minimum power) to 63 on channels with a 63-dB attenuator, or from -16 (minimum mum power) on channels with a 79-dB attenuator.
CAUTION:	decpower greater decoupling or lor in damage to the	linear amplifiers, be careful when using values of r than 49 (about 2 watts). Performing continuous ng pulses at power levels greater than this can result probe. Use config to set a safety maximum for dpwr, dpwr2, and dpwr3.
Related:	dec3power Ch obspower Ch	hange second decoupler power, linear amplifier systems hange third decoupler power, linear amplifier systems hange observe transmitter power, linear amplifier systems hange power level, linear amplifier systems
dec2power	Change second o	decoupler power level, linear amp. systems
Applicability:	Systems with a sec	ond decoupler.
Syntax:	dec2power(pow double power;	ver) /* new power level for DO2DEV */
Description:	Changes the second rlpower(value	d decoupler power. It is functionally the same as a DO2DEV).

Arguments:	power sets the power level by assuming values from 0 (minimum power) to 63 (maximum power) on channels with a 63-dB attenuator, or from -16 (minimum power) to 63 (maximum power) on channels with a 79-dB attenuator.			
Related:	decpower dec3power obspower rlpower	Change first decoupler power, linear amplifier systems Change third decoupler power, linear amplifier systems Change observe transmitter power, linear amplifier systems Change power level, linear amplifier systems		
dec3power	Change third of	decoupler power level, linear amp. systems		
Applicability:	UNITY INOVA and	UNITYplus systems with a third decoupler.		
Syntax:	dec3power(p double power			
Description:	-	Changes the third decoupler power. It is functionally the same as rlpower(value, DO3DEV).		
Arguments:	power sets the power level by assuming values from 0 (minimum power) to 63 (maximum power) on channels with a 63-dB attenuator, or from -16 (minimum power) to 63 (maximum power) on channels with a 79-dB attenuator.			
Related:	decpower dec2power obspower rlpower	Change first decoupler power, linear amplifier systems Change second decoupler power, linear amplifier systems Change observe transmitter power, linear amplifier systems Change power level, linear amplifier systems		
dec4power	Change fourth	decoupler power level, linear amp. systems		
Applicability:	UNITY INOVA syst decoupler.	tems with a deuterium decoupler channel as the fourth		
Syntax:	dec4power(p double power			
Description:	Changes the third decoupler power. It is functionally the same as rlpower(value, DO4DEV).			
Arguments:	power sets the power level by assuming values from 0 (minimum power) to 63 (maximum power).			
Related:	decpower dec2power obspower rlpower rftype	Change first decoupler power, linear amplifier systems Change second decoupler power, linear amplifier systems Change observe transmitter power, linear amplifier systems Change power level, linear amplifier systems Type of rf generation		
decprgoff	End programm	nable decoupling on first decoupler		
Applicability:	Systems with a	waveform generator on rf channel for the first decoupler.		
Syntax:	decprgoff())		
Description:	•	Terminates any waveform-generator-controlled programmable decoupling on the first decoupler started by the decprogn statement.		
Related:	decprgon dec2prgoff dec3prgoff	Start programmable decoupling on first decoupler End programmable decoupling on second decoupler End programmable decoupling on third decoupler		

dec2prgoff	End programmable decoupling on second decoupler		
Applicability:	Systems with a waveform generator on rf channel for the second decoupler.		
	dec2prgoff()		
Description:	Terminates any waveform-generator-controlled programmable decoupling on the second decoupler set by the dec2prgon statement.		
Related:	dec2prgon Start programmable decoupling on second decoupler		
dec3prgoff	End programmable decoupling on third decoupler		
Applicability:	UNITY <i>INOVA</i> and UNITY <i>plus</i> systems with a waveform generator on rf channel with the third decoupler.		
Syntax:	dec3prgoff()		
Description:	Terminates any waveform-generator-controlled programmable decoupling on the third decoupler set by the dec3prgon statement.		
Related:	dec3prgon Start programmable decoupling on third decoupler		
decprgon	Start programmable decoupling on first decoupler		
Applicability:	Systems with a waveform generator on rf channel for the first decoupler.		
Syntax:	<pre>decprgon(pattern,90_pulselength,tipangle_resoln) char *pattern;</pre>		
Description:	Executes programmable decoupling on the first decoupler under waveform generator control, and returns the number of 50-ns ticks (as an integer value) in one cycle of the decoupling pattern. Explicit gating of the first decoupler with decon and decoff is generally required. Arguments can be variables (which require the appropriate getval and getstr statements) to permit changes by the parameters (see the second example).		
Arguments:	pattern is the name of the text file in the shapelib directory that stores the decoupling pattern (leave off the .DEC file extension).		
	90_pulselength is the pulse duration, in seconds, for a 90° tip angle on the first decoupler.		
	tipangle_resoln is the resolution, in tip-angle degrees, to which the decoupling pattern is stored in the waveform generator.		
Examples:	<pre>decprgon("garp1",1/dmf, 1.0); decprgon(modtype,pwx90,dres); n50ns_ticks = decprgon("waltz16",1/dmf,90.0);</pre>		
Related:	decprgoffEnd programmable decoupling on first decouplerdec2prgonStart programmable decoupling on second decouplerdec3prgonStart programmable decoupling on third decouplerobsprgonStart programmable control of obs. transmitter		
dec2prgon	Start programmable decoupling on second decoupler		
Applicability:	Systems with a waveform generator on rf channel for the second decoupler.		
Syntax:	<pre>dec2prgon(pattern,90_pulselength,tipangle_resoln) char *pattern;</pre>		

double 90_pulselength; /* 900000-deg pulse length in sec
*/
double tipangle_resoln; /* tip-angle resolution */

- Description: Executes programmable decoupling on second decoupler under waveform generator control, and returns the number of 50-ns ticks (as an integer value) in one cycle of the decoupling pattern. Explicit gating of the second decoupler with dec2on and dec2off is generally required. Arguments can be variables (which require the appropriate getval and getstr statements) to permit changes by the parameters (see the second example below).
- Arguments: pattern is the name of the text file in the shapelib directory that stores the decoupling pattern (leave off the .DEC file extension).

90_pulselength is the pulse duration, in seconds, for a 90° tip angle on the second decoupler.

tipangle_resoln is the resolution, in tip-angle degrees, to which the decoupling pattern is stored in the waveform generator.

Examples: (1) dec2prgon("waltz16",1/dmf2,90.0);

- (2) dec2prgon(modtype,pwx290,dres2); n50ns_ticks=dec2prgon("garp1",1/dmf2,1.0);
- Related:
 decprgon
 Start programmable decoupling on first decoupler

 dec2prgoff
 End programmable decoupling on second decoupler

 obsprgon
 Start programmable control of obs. transmitter

dec3prgon Start programmable decoupling on third decoupler

- Applicability: UNITY *INOVA* and UNITY *plus* systems with a waveform generator on rf channel for the third decoupler.
- Description: Executes programmable decoupling on third decoupler under waveform generator control. It returns the number of 50-ns ticks (as an integer value) in one cycle of the decoupling pattern. Explicit gating of the third decoupler with dec3on and dec3off is generally required. Arguments can be variables (which require the appropriate getval and getstr statements) to permit changes by parameters (see second example below).
- Arguments: pattern is the name of the text file in the shapelib directory that stores the decoupling pattern (leave off the .DEC file extension).

90_pulselength is the pulse duration, in seconds, for a 90° tip angle on the third decoupler.

tipangle_resoln is the resolution, in tip-angle degrees, to which the decoupling pattern is stored in the waveform generator.

Examples: (1) dec3prgon("waltz16",1/dmf3,90.0);

(2) dec3prgon(modtype,pwx390,dres3); n50ns_ticks = dec3prgon("garp1",1/dmf3,1.0);

Related:	decprgon	Start programmable decoupling on first decoupler
	dec2prgoff	End programmable decoupling on second decoupler
	obsprgon	Start programmable control of obs. transmitter

decpulse	Pulse first decoupler transmitter with amplifier gating
Syntax:	<pre>decpulse(width,phase) double width; /* width of pulse in sec */ codeint phase; /* real-time variable for phase of pulse */</pre>
Description:	Pulses the first decoupler at its current power level. The amplifier is gated off during decoupler pulses as it is during observe pulses. The amplifier gating times (see <i>RG1</i> and <i>RG2</i> for decrgpulse) are internally set to zero for this statement. dmm should be set to 'c' during any period of time in which decoupler pulses occur.
Arguments:	width is the duration of the pulse, in seconds.
	phase is the phase of the pulse. The value must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).
Examples:	<pre>decpulse(pp,v3); decpulse(2.0*pp,zero);</pre>
Related:	decrgpulsePulse decoupler transmitter with amplifier gatingidecpulsePulse the decoupler transmitter with IPArgpulsePulse observe transmitter with amplifier gatingsimpulsePulse observe, decoupler channels simultaneouslysim3pulseSimultaneous pulse on 2 or 3 rf channels
decpwr	Set first decoupler high-power level, class C amplifier
Applicability:	All systems (except for the GEMINI 2000) with class C amplifiers.
Syntax:	<pre>decpwr(level) double level; /* new power level for DODEV channel */</pre>
Description:	Changes the first decoupler high-power level to the value specified. To reset the power back to the "standard" dhp level, use decpwr(dhp).
	Switching between low power decoupling $(dhp='n')$ and high power decoupling $(dhp=x)$, as well as switching between different levels of low power decoupling, uses relays whose switching time is about 10 ms and are not provided for in the standard pulse sequence capability. Neither function should prove necessary because extremely low levels of decoupling are provided for in dhp mode by using very small (0 to 30) values of dhp.
Arguments:	level specifies the decoupler high-power level, from 0 (lowest) to 255 (full power). These values in this range increase monotonically but are neither linear nor logarithmic
Examples:	<pre>decpwr(255.0); decpwr(level1);</pre>
Related:	declvloff Return first decoupler back to "normal" power
decpwrf	Set first decoupler fine power
Applicability:	Systems with fine power control on the first decoupler. Not available on <i>MERCURY-VX</i> , <i>MERCURY</i> , or <i>GEMINI 2000</i> .
Syntax:	<pre>decpwrf(power) double power; /* new fine power value for DODEV */</pre>
Description:	Changes first decoupler fine power. It is functionally the same as <pre>rlpwrf(value,DODEV).</pre>
Arguments:	power is the fine power desired.

Examples: decpwrf(4.0); Related: dec2pwrf Set second decoupler fine power dec3pwrf Set third decoupler fine power obspwrf Set observe transmitter fine power rlpwrf Set transmitter or decoupler fine power dec2pwrf Set second decoupler fine power Applicability: Systems with fine power control on the second decoupler. Syntax: dec2pwrf(power) /* new fine power value for DO2DEV */ double power; Description: Changes the second decoupler fine power. It is functionally the same as rlpwrf(value,DO2DEV). Arguments: power is the fine power desired. Examples: dec2pwrf(4.0);Related: decpwrf Set first decoupler fine power dec3pwrf Set third decoupler fine power Set observe transmitter fine power obspwrf rlpwrf Set transmitter or decoupler fine power dec3pwrf Set third decoupler fine power UNITY INOVA and UNITY plus systems with fine power control on the third Applicability: decoupler. Syntax: dec3pwrf(power) double power; /* new fine power value for DO3DEV */ Description: Changes third decoupler fine power. It is functionally the same as rlpwrf(value,DO3DEV). Arguments: power is the fine power desired. Examples: dec3pwrf(4.0); Related: decpwrf Set first decoupler fine power dec2pwrf Set second decoupler fine power obspwrf Set observe transmitter fine power rlpwrf Set transmitter or decoupler fine power decr Decrement an integer value Syntax: decr(vi) codeint vi; /* real-time variable for starting value */ Description: Decrements integer value vi by 1 (i.e., vi=vi-1). Arguments: vi is a real-time variable (v1 to v14, oph, etc.). Examples: decr(v5); Related: Add integer values add assign Assign integer values dbl Double an integer value divn Divide integer values

> Half the value of an integer Increment an integer value

Find integer value modulo 2

hlv

incr

mod2

mod4	Find integer value modulo 4
modn	Find integer value modulo n
mult	Multiply integer values
sub	Subtract integer values

decrgpulse	Pulse first decoupler with amplifier gating		
Syntax:	<pre>decrgpulse(width,phase,RG1,RG2) double width; /* width of pulse in sec */ codeint phase; /* real-time variable for phase */ double RG1; /* gating delay before pulse in sec */ double RG2; /* gating delay after pulse in sec */</pre>		
Description:	rgpulse with two exceptions. First, the first decoupler (instead of the transmitter) is pulsed at its current power level. Second, if homo='n', the slow gate (about 100-ns switching time on UNITY <i>plus</i> systems, 1 to 3 μ s switching time on other systems, homo not available on <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> systems) on the first decoupler board is always open and therefore need not be switched open during <i>RG1</i> . In contrast, if homo='y', the slow gate on the first decoupler board is normally closed and must therefore be allowed sufficient time during <i>RG1</i> to switch open.		
	For systems with linear amplifiers, <i>RG1</i> for a decoupler pulse is important from the standpoint of amplifier stabilization under the following conditions: tn , dn equal { ³ H, ¹ H, ¹⁹ F} (high-band nuclei, ³ H does not apply to <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> systems), or tn , dn less than or equal to ³¹ P (low-band nuclei). For these conditions, the "decoupler" amplifier module is placed in <i>pulse</i> mode, in which it remains blanked as long as the receiver is on. In this mode, <i>RG1</i> must be sufficiently long to allow the amplifier to stabilize after blanking is removed: 5 to 10 μ s (2 μ s typical for <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i>) for high-band nuclei and 10 to 20 μ s (2 μ s typical for <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i>) for low-band nuclei. Solids require at least 1.5 μ s. On 500-MHz systems that use the ENI- 5100 class A amplifier for low-band nuclei on the observe channel, <i>RG1</i> should be 40–60 μ s.		
	If the tn nucleus and the dn nucleus are in different bands (e.g., tn is ¹ H and dn is ¹³ C), the "decoupler" amplifier module is placed in the <i>cw</i> mode, in which it is always unblanked regardless of the state of the receiver. In this mode <i>RG1</i> is unimportant with respect to amplifier stabilization prior to the decoupler pulse.		
Arguments:	· · ·		
	phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).		
	RG1 is the time, in seconds, before the start of the pulse that the amplifier is gated off.		
	RG2 is the time, in seconds, after the end of the pulse that the amplifier is gated on.		
Examples:	<pre>decrgpulse(pp,v3,rof1,rof2); decrgpulse(pp,zero,1.0e-6,0.2e-6);</pre>		
Related:	decpulsePulse first decoupler with amplifier gatingdec2rgpulsePulse second decoupler with amplifier gatingdec3rgpulsePulse third decoupler with amplifier gating		

	idecpulsePulse first decoupler transmitter with IPAidecrgpulsePulse first decoupler with amplifier gating and IPAirgpulsePulse observe transmitter with IPArgpulsePulse observe transmitter with amplifier gatingsimpulsePulse observe, decoupler channels simultaneouslysim3pulseSimultaneous pulse on 2 or 3 rf channels
dec2rgpulse	Pulse second decoupler with amplifier gating
Applicability:	Systems with a second decoupler.
Syntax:	<pre>dec2rgpulse(width,phase,RG1,RG2) double width; /* width of pulse in sec */ codeint phase; /* real-time variable for phase */ double RG1; /* gating delay before pulse in sec */ double RG2; /* gating delay after pulse in sec */</pre>
Description:	Performs an explicit amplifier-gated pulse on the second decoupler (DO2DEV).
Arguments:	width is the duration, in seconds, of the pulse.
	phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).
	RG1 is the delay, in seconds, between gating the amplifier on and gating the rf transmitter on (the phaseshift occurs at the beginning of this delay). RG1 is important for amplifier stabilization under the same conditions as described for decrgpulse.
	RG2 is the delay, in seconds, between gating the rf transmitter off and gating the amplifier off. homo has no effect on the gating on the second decoupler board. On UNITY <i>INOVA</i> and UNITY <i>plus</i> , homo 2 controls gating of second decoupler rf.
Examples:	<pre>dec2rgpulse(p1,v10,rof1,rof2);</pre>
Related:	decpulsePulse first decoupler with amplifier gatingdecrgpulsePulse first decoupler with amplifier gatingidecpulsePulse first decoupler with IPArgpulsePulse observe transmitter with amplifier gatingsimpulsePulse observe, decoupler channels simultaneouslysim3pulseSimultaneous pulse on 2 or 3 rf channels
dec3rgpulse	Pulse third decoupler with amplifier gating
Applicability:	UNITY INOVA and UNITY plus systems with a third decoupler.
Syntax:	<pre>dec3rgpulse(width,phase,RG1,RG2) double width; /* width of pulse in sec */ codeint phase; /* real-time variable for phase */ double RG1; /* gating delay before pulse in sec */ double RG2; /* gating delay after pulse in sec */</pre>
Description:	Performs an explicit amplifier-gated pulse on the third decoupler (DO3DEV).
Arguments:	width is the duration, in seconds, of the pulse.
	phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).
	RG1 is the delay, in seconds, between gating the amplifier on and gating the rf transmitter on (the phaseshift occurs at the beginning of this delay). RG1 is

transmitter on (the phaseshift occurs at the beginning of this delay). RG1 is important for amplifier stabilization under the same conditions as described for decrgpulse.

RG2 is the delay, in seconds, between gating the rf transmitter off and gating the amplifier off. homo has no effect on the gating on the third decoupler board. On UNITY *INOVA* and UNITY *plus*, homo 3 controls gating of third decoupler rf.

Examples:	<pre>dec3rgpulse(p1,v10,rof1,rof2);</pre>		
Related:	decpulse decrgpulse idecpulse rgpulse simpulse sim3pulse	Pulse first decoupler with amplifier gating Pulse first decoupler with amplifier gating Pulse first decoupler with IPA Pulse observe transmitter with amplifier gating Pulse observe, decoupler channels simultaneously Simultaneous pulse on 2 or 3 rf channels	
dec4rgpulse	Pulse fourth d	lecoupler with amplifier gating	
Applicability:	UNITY <i>INOVA</i> systems with a deuterium decoupler channel as the fourth decoupler.		
Syntax:	<pre>dec4rgpulse double width codeint phas double RG1; double RG2;</pre>	-	
Description:	Performs an explicit amplifier-gated pulse on the fourth decoupler (DO4DEV).		
Arguments:	width is the duration, in seconds, of the pulse.		
	phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).		
	 RG1 is the delay, in seconds, between gating the amplifier on and gating the rf transmitter on (the phaseshift occurs at the beginning of this delay). RG1 is important for amplifier stabilization under the same conditions as described for decrgpulse. RG2 is the delay, in seconds, between gating the rf transmitter off and gating the amplifier off. 		
Examples:	<pre>dec4rgpulse(p1,v10,rof1,rof2);</pre>		
Related:	decpulse decrgpulse idecpulse rgpulse simpulse sim3pulse	Pulse first decoupler with amplifier gating Pulse first decoupler with amplifier gating Pulse first decoupler with IPA Pulse observe transmitter with amplifier gating Pulse observe, decoupler channels simultaneously Simultaneous pulse on 2 or 3 rf channels	
decshaped_pul	se Perform	shaped pulse on first decoupler	

Applicability: UNITY *INOVA* and UNITY *plus* systems, or systems with waveform generator on rf channel for the first decoupler.

		-
Syntax:	decshaped_pulse()	pattern,width,phase,RG1,RG2)
	char *pattern;	/* name of .RF text file */
	double width;	/* width of pulse in sec */
	codeint phase;	/* real-time variable for phase */
	double RG1;	/* gating delay before pulse in sec */
	double RG2;	/* gating delay after pulse in sec */

Description: Performs a shaped pulse on the first decoupler. If a waveform generator is configured on the channel, it is used; otherwise, the linear attenuator and the

small-angle phase shifter are used to effectively perform an apshaped_decpulse statement.

When using the waveform generator, the shapes are downloaded into the waveshaper before the start of an experiment. When decshaped_pulse is called, the shape is addressed and started. The minimum pulse length is 0.2 µs. The overhead at the start and end of the shaped pulse varies:

- UNITY *INOVA*: 1 μ s (start), 0 (end)
- UNITYplus: 5.75 µs (start), 0 (end)
- System with Acquisition Controller board: 10.75 µs (start), 4.3 µs (end)
- System with Output board: 10.95 µs (start), 4.5 µs (end)

If the length is less than 0.2 $\mu s,$ the pulse is not executed and there is no overhead.

When using the linear attenuator and the small-angle phase shifter to generate a shaped pulse, the decshaped_pulse statement creates AP tables on the fly for amplitude and phase. *It also uses the real-time variables v12 and v13 to control the execution of the shape*. It does not use AP table variables. For timing and more information, see the description of apshaped_decpulse. Note that if using AP tables with shapes that have a large number of points, the FIFO can become overloaded with words generating the pulse shape and FIFO Underflow errors can result.

Arguments: pattern is the name of a text file in the shapelib directory that stores the rf pattern (leave off the .RF file extension).

width is the duration, in seconds, of the pulse.

phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.)

RG1 is the delay, in seconds, between gating the amplifier on and gating the first decoupler on (the phaseshift occurs at the beginning of this delay).

RG2 is the delay, in seconds, between gating the first decoupler off and gating the amplifier off.

Examples: decshaped_pulse("sinc",p1,v5,rof1,rof2);

Related:	apshaped_decpulse	First decoupler pulse shaping via AP bus
	dec2shaped_pulse	Perform shaped pulse on second decoupler
	dec3shaped_pulse	Perform shaped pulse on third decoupler
	shaped_pulse	Perform shaped pulse on observe transmitter
	simshaped_pulse	Simultaneous two-pulse shaped pulse
	<pre>sim3shaped_pulse</pre>	Simultaneous three-pulse shaped pulse

dec2shaped_pulse Perform shaped pulse on second decoupler

Applicability:	Systems with a wavefor	m g	enerator on rf channel for the second decoupler.
Syntax:	dec2shaped_pulse	e(pa	attern,width,phase,RG1,RG2)
	char *pattern;	/*	name of .RF text file */
	double width;	/*	width of pulse in sec */
	codeint phase;	/*	real-time variable for phase */
	double RG1;	/*	gating delay before pulse in sec */
	double RG2;	/*	gating delay after pulse in sec */
Description:	Performs a shaped pulse	e on	the second decoupler. If a waveform generator is

Description: Performs a shaped pulse on the second decoupler. If a waveform generator is configured on the channel, it is used; otherwise, the linear attenuator and the

small-angle phase shifter are used to effectively perform an apshaped_dec2pulse statement.

When using the waveform generator, the shapes are downloaded into the waveshaper before the start of an experiment. When dec2shaped_pulse is called, the shape is addressed and started. The minimum pulse length is $0.2 \,\mu$ s. The overhead at the start and end of the shaped pulse varies:

- UNITY *INOVA*: 1 μ s (start), 0 (end)
- UNITYplus: 5.75 µs (start), 0 (end)
- System with Acquisition Controller board: 10.75 µs (start), 4.3 µs (end)
- System with Output board: 10.95 µs (start), 4.5 µs (end)

If the length is less than 0.2 $\mu s,$ the pulse is not executed and there is no overhead.

When using the linear attenuator and the small-angle phase shifter to generate a shaped pulse, the dec2shaped_pulse statement creates AP tables on the fly for amplitude and phase. *It also uses the real-time variables v12 and v13 to control the execution of the shape*. It does not use AP table variables. For timing and more information, see the description of apshaped_dec2pulse. Note that if using AP tables with shapes that have a large number of points, the FIFO can become overloaded with words generating the pulse shape and FIFO Underflow errors can result.

Arguments: pattern is the name of a text file in the shapelib directory that stores the rf pattern (leave off the .RF file extension).

width is the duration, in seconds, of the pulse.

phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.)

RG1 is the delay, in seconds, between gating the amplifier on and gating the second decoupler on (the phaseshift occurs at the beginning of this delay).

RG2 is the delay, in seconds, between gating the second decoupler off and gating the amplifier off.

Examples: dec2shaped_pulse("gauss",p1,v9,rof1,rof2);

Related:apshaped_dec2pulseSecond decoupler pulse shaping via AP busdecshaped_pulsePerform shaped pulse on first decouplershaped_pulsePerform shaped pulse on observe transmittersim3shaped_pulseSimultaneous three-pulse shaped pulse

dec3shaped_pulse Perform shaped pulse on third decoupler

Applicability: UNITY INOVA and UNITY plus systems.

Syntax:	dec3shaped_puls	e(pattern,width,phase,RG1,RG2)
	char *pattern;	/* name of .RF text file */
	double width;	/* width of pulse in sec */
	codeint phase;	/* real-time variable for phase */
	double RG1;	/* gating delay before pulse in sec */
	double RG2;	/* gating delay after pulse in sec */

Description: Performs a shaped pulse on the third decoupler. If a waveform generator is configured on the channel, it is used; otherwise, the linear attenuator and the small-angle phase shifter are used to effectively perform an apshaped_dec3pulse statement.

When using the waveform generator, the shapes are downloaded into the waveshaper before the start of an experiment. When dec3shaped_pulse is called, the shape is addressed and started. The minimum pulse length is $0.2 \,\mu s$. The overhead at the start and end of the shaped pulse varies:

- UNITY INOVA: 1 µs (start), 0 (end)
- UNITYplus: 5.75 µs (start), 0 (end)
- System with Acquisition Controller board: 10.75 µs (start), 4.3 µs (end)
- System with Output board: 10.95 µs (start), 4.5 µs (end)

If the length is less than $0.2 \,\mu$ s, the pulse is not executed and there is no overhead.

When using the linear attenuator and the small-angle phase shifter to generate a shaped pulse, the dec3shaped_pulse statement creates AP tables on the fly for amplitude and phase. It also uses the real-time variables v12 and v13 to control the execution of the shape. It does not use AP table variables. For timing and more information, see the description of apshaped_dec3pulse. Note that if using AP tables with shapes that have a large number of points, the FIFO can become overloaded with words generating the pulse shape and FIFO Underflow errors can result.

Arguments: pattern is the name of a text file in the shapelib directory that stores the rf pattern (leave off the .RF file extension).

width is the duration, in seconds, of the pulse.

phase is the phase of the pulse. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).

RG1 is the delay, in seconds, between gating the amplifier on and gating the third decoupler on (the phaseshift occurs at the beginning of this delay).

RG2 is the delay, in seconds, between gating the third decoupler off and gating the amplifier off.

Examples: dec3shaped_pulse("gauss",p1,v9,rof1,rof2);

Related:	decshaped_pulse	Perform shaped pulse on first decoupler
	shaped_pulse	Perform shaped pulse on observe transmitter

decspinlock Set spin lock waveform control on first decoupler

Applicability: Systems with waveform generator on rf channel for the first decoupler.

Syntax:		pulselength,tipangle_resoln,
	phase,ncycles)	
	char *pattern;	/* name of .DEC text file */
	double 90_pulselength;	/* 90∞∞-deg pulse length in sec
	* /	
	double tipangle_resoln;	/* resolution of tip angle */
	codeint phase;	/* phase of spin lock */
	int ncylces;	/* number of cycles to execute */
scription:	Executes a waveform-generator-co	ontrolled spin lock on the first decoupler,

- Descri handling both rf gating and the mixing delay. Arguments can be variables (which require the appropriate getval and getstr statements) to permit changes via parameters (see the second example below).
- pattern is the name of the text file in the shapelib directory that stores the Arguments: decoupling pattern (leave off the .DEC file extension).
 - 90 pulselength is the pulse duration, in seconds, for a 90° tip angle.

tipangle_resoln is the resolution, in tip-angle degrees, to which the decoupling pattern is stored in the waveform generator.

phase is the phase of the spin lock. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).

ncycles is the number of times the spin-lock pattern is to be executed.

Examples:	<pre>decspinlock("mlev16",p190,dres,v1,30); decspinlock(spinlk,pp90,dres,v1,cycles);</pre>		
Related:	dec2spinlock dec3spinlock spinlock	Set spin lock waveform control on second decoupler Set spin lock waveform control on third decoupler Set spin lock waveform control on obs. transmitter	
dec2spinlock	Set spin lock waveform control on second decoupler		
Applicability:	Systems with a waveform generator on rf channel for the second decoupler.		
Syntax:	<pre>dec2spinlock(pattern,90_pulselength, tipangle resoln phase neveles)</pre>		

tipangle_resoin,pna	se,ncycles)	
char *pattern;	/* name of .DEC text file */	
double 90_pulselength;	<pre>/* 90-deg pulse length of channel */</pre>	
double tipangle_resoln;	<pre>/* resolution of tip angle */</pre>	
codeint phase;	/* phase of spin lock */	
int ncylces;	/* number of cycles to execute */	

- Description: Executes a waveform-generator-controlled spin lock on the second decoupler. Both the rf gating and the mixing delay are handled within this function. Arguments can be variables (which require the appropriate getval and getstr statements) to permit changes via parameters (see the second example below).
- Arguments: pattern is the name of the text file in the shapelib directory that stores the decoupling pattern (leave off the .DEC file extension).
 - 90_pulselength is the pulse duration, in seconds, for a 90° tip angle.

tipangle_resoln is the resolution, in tip-angle degrees, to which the decoupling pattern is stored in the waveform generator.

phase is the phase of the spin lock. It must be a real-time variable (v1 to v14, etc.) or a real-time constant (zero, one, etc.).

ncycles is the number of times that the spin-lock pattern is to be executed.

- Examples: (1) dec2spinlock("mlev16",p290,dres2,v1,42); (2) dec2spinlock(lock2,pwx2,dres2,v1,cycles);
 - Related:decspinlockSet spin lock waveform control on first decouplerspinlockSet spin lock waveform control on obs. transmitter

dec3spinlock Set spin lock waveform control on third decoupler

Applicability: UNITY *INOVA* and UNITY *plus* systems with a waveform generator on rf channel for the third decoupler.

Description:	Executes a waveform-generator-controlled spin lock on the third decoupler. Both the rf gating and the mixing delay are handled within this function. Arguments can be variables (which would need the appropriate getval and getstr statements) to permit changes via parameters (see the second example below).		
Arguments:	pattern is the name of the text file in the shapelib directory that stores the decoupling pattern (leave off the .DEC file extension).		
	90_pulselength	h is the pulse duration, in seconds, for a 90° tip angle.	
	tipangle_resoln is the resolution in tip-angle degrees to which the decoupling pattern is stored in the waveform generator.		
		of the spin lock. It must be a real-time variable (v1 to v14, constant (zero, one, etc.).	
	ncycles is the nur	mber of times that the spin-lock pattern is to be executed.	
Examples:	<pre>dec3spinlock("mlev16",p390,dres3,v1,42); dec3spinlock(lock2,pwx2,dres3,v1,cycles);</pre>		
Related:		Set spin lock waveform control on first decoupler Set spin lock waveform control on observe transmitter	
decstepsize	Set step size for fi	irst decoupler	
Applicability:	All systems except t	he <i>GEMINI 2000</i> .	
Syntax:	<pre>decstepsize(step_size) double step_size; /* phase step size of DODEV */</pre>		
Description:	Sets the step size of the first decoupler. It is functionally the same as <pre>stepsize(base,DODEV).</pre>		
Arguments:	step_size is the phase step size desired and is a real number or a variable.		
Examples:	<pre>decstepsize(30.0);</pre>		
Related:	dec2stepsize dec3stepsize obsstepsize stepsize	Set step size of second decoupler Set step size of third decoupler Set step size of observe transmitter Set small-angle phase step size, rf type C or D	
dec2stepsize	Set step size for s	econd decoupler	
Applicability:	Systems with a second decoupler.		
Syntax:	<pre>dec2stepsize(step_size) double step_size;</pre>		
Description:	Sets the step size of the first decoupler. This statement is functionally the same as <pre>stepsize(base,DO2DEV).</pre>		
Arguments:	step_size is the	phase step size desired and is a real number or a variable.	
Examples:	dec2stepsize(3	30.0);	
Related:	decstepsize dec3stepsize obsstepsize stepsize	Set step size of first decoupler Set step size of third decoupler Set step size of observe transmitter Set small-angle phase step size, rf type C or D	

dec3stepsize	Set step size for third decoupler		
Applicability:	UNITY INOVA and UNITY plus systems with a third decoupler.		
Syntax:	<pre>dec3stepsize(step_size) double step_size;</pre>		
Description:	Sets the step size as stepsize(b	of the third decoupler. This statement is functionally the same ase , $DO3DEV$).	
Arguments:	step_size is the	he phase step size desired and is a real number or a variable.	
Examples:	dec3stepsize	e(30.0);	
Related:	decstepsize dec2stepsize obsstepsize stepsize	Set step size of first decoupler Set step size of second decoupler Set step size of observe transmitter Set small-angle phase step size, rf type C or D	
decunblank	Unblank amplifi	er associated with first decoupler	
Applicability:	All systems except	ot MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	decunblank()		
Description:	Explicitly enables the amplifier for the first decoupler. This overwrites the implicit blanking and unblanking of the amplifier before and after pulses. decunblank is generally followed by a call to decblank.		
Related:	decblank obsblank obsunblank rcvroff rcvron	Blank amplifier associated with first decoupler Blank amplifier associated with observe transmitter Unblank amplifier associated with observe transmitter Turn off receiver Turn on receiver	
dec2unblank	Unblank amplifier associated with second decoupler		
Applicability:	-		
	dec2unblank()		
Description:			
Related:	dec2blank rcvroff rcvron	Blank amplifier associated with second decoupler Turn off receiver Turn on receiver	
dec3unblank	Unblank amplifi	er associated with third decoupler	
Applicability:	UNITY <i>INOVA</i> and UNITY <i>plus</i> systems with a third decoupler.		
Syntax:			
Description:	Explicitly enables the amplifier for the third decoupler. This overwrites the implicit blanking and unblanking of the amplifier before and after pulses. dec3unblank is generally followed by a call to dec3blank.		
Related:	rcvroff 7	Blank amplifier associated with third decoupler Furn off receiver Furn on receiver	

Chapter 3. Pulse Sequence Statement Reference -

delay	Delay for a specified time		
Syntax:	delay(time) double time;		
Description:	Sets a delay for a specified number of seconds.		
Arguments:	time specifies	the delay, in seconds.	
Examples:	delay(d1); delay(d2/2.	.0);	
Related:	dps_show hsdelay idelay incdelay initdelay vdelay	Draw delay or pulses in a sequence for graphical display Delay specified time with possible homospoil pulse Delay for a specified time with IPA Real time incremental delay Initialize incremental delay Delay with fixed timebase and real time count	
dhpflag	Switch decoup	pling from low-power to high-power	
Applicability:	On all systems	with class C amplifiers, except the GEMINI 2000.	
Syntax:	dhpflag		
Description:	•	Switches the system from low-power to high-power decoupling; e.g., dhpflag=TRUE (correct use of upper and lower case letters is necessary).	
Values:	TRUE; switche	s the system to high-power decoupling.	
	FALSE <i>i</i> switches the system to low-power decoupling.		
Related:	status	Draw delay or pulses in a sequence for graphical display	
divn	Divide integer	values	
divn Syntax:	Divide integer divn(vi,vj, codeint vi; codeint vj; codeint vk;	.vk) /* real-time variable for dividend */	
Syntax:	<pre>divn(vi,vj, codeint vi; codeint vj; codeint vk;</pre>	.vk) /* real-time variable for dividend */ /* real-time variable for divisor */	
Syntax:	<pre>divn(vi,vj, codeint vi; codeint vj; codeint vk; Sets the integer vi is the divide</pre>	.vk) /* real-time variable for dividend */ /* real-time variable for divisor */ /* real-time variable for quotient */	
Syntax: Description:	<pre>divn(vi,vj, codeint vi; codeint vj; codeint vk; Sets the integer vi is the divide</pre>	<pre>,vk)</pre>	

dps_off

Turn off graphical display of statements

Syntax: dps_off()

Examples: Turns off dps display of statements. Pulse statements following dps_off are not shown in the graphical display.

Related:	dps_on	Turn on graphical display of statements
	dps_show	Draw delay or pulses in a sequence for graphical display
	dps_skip	Skip graphical display of next statement

Turn on graphical display of statements dps_on Syntax: dps_on() Description: Turns on dps display of statements. Pulse statements following dps_on are shown in the graphical display. Related: dps_off Turn off graphical display of statements Draw delay or pulses in a sequence for graphical display dps_show dps skip Skip graphical display of next statement Draw delay or pulses in a sequence for graphical display dps_show Syntax: (1) dps_show("delay",time) double time; /* delay in sec */ Syntax: (2) dps_show("pulse", channel, label, width) char *channel; /* "obs", "dec", "dec2",or "dec3" */ char *label; /* text label selected by user */ double width; /* pulse length in sec */ Syntax: (3) dps_show("shape_pulse", channel, label, width) char *channel; /* "obs", "dec", "dec2", or "dec3" */ char *label; /* text label selected by user */ double width; /* pulse length in sec */ Syntax: (4) dps_show("simpulse", label_of_obs, width_of_obs, label of dec, width of dec) double width_of_obs; /* pulse length in sec */ double width_of_dec; /* pulse length in sec */ Syntax: (5) dps show("simshaped pulse", label of obs, width of obs, label of dec, width of dec) char *label_of_obs; /* text label selected by user */ char *label_of_dec; /* text label selected by user */ double width_of_dec; /* pulse length in sec */ Syntax: (6) dps show("sim3pulse", label of obs, width of obs, label_of_dec,width_of_dec,label_of_dec2, width of dec2) char *label_of_obs; /* text label selected by user */ double width_of_obs; /* pulse length in sec */ /* text label selected by user */ char *label_of_dec2; /* text label selected by user */ double width_of_dec2; /* pulse length in sec */ Syntax: (7) dps_show("sim3shaped_pulse", label_of_obs, width_of_obs,label_of_dec,width_of_dec, label_of_dec2,width_of_dec2) char *label_of_obs; /* text label selected by user */ double width_of_obs; /* pulse length in sec */

```
double width_of_dec; /* pulse length in sec */
             char *label_of_dec2; /* text label selected by user */
             double width_of_dec2; /* pulse length in sec */
    Syntax: (8) dps_show("zgradpulse", value, delay)
             double value; /* amplitude of gradient on z channel */
             double delay;
                                 /* length of gradient in sec */
    Syntax: (9) dps_show("rgradient", channel, value)
             char channel; /* 'X', 'x', 'Y', 'Y', 'Z', or 'z' */
             Syntax: (10) dps_show("vgradient", channel, intercept,
                 slope,mult)
             char channel; /* gradient channel 'x', 'y' or 'z' */
             int slope; /* gradient increment */
codeint mult; /* real-time variable */
    Syntax: (11) dps_show("shapedgradient", pattern, width, amp,
               channel,loops,wait)
             char *pattern; /* name of shape text file */
            double width; /* length of pulse */
double amp; /* amplitude of pulse */
char channel; /* gradient channel 'x', 'y', or 'z' */
int loops; /* number of loops */
int wait; /* WAIT or NOWAIT */
                                 /* WAIT or NOWAIT */
             int wait;
    Syntax: (12) dps_show("shaped2Dgradient", pattern, width, amp,
               channel,loops,wait,tag)
             char *pattern; /* name of shape text file */
            double width; /* length of pulse text file */
double width; /* length of pulse */
double amp; /* amplitude of pulses */
char channel; /* gradient channel 'x', 'y', or 'z' */
int loops; /* number of loops */
int wait; /* WAIT or NOWAIT */
int tag; /* unique number for gradient element */

                                  /* unique number for gradient element */
             int tag;
Description: Draws for dps graphical display the pulses, lines, and labels related to the
             statement (if it exists) given as the first argument.
               • Syntax 1 draws a line to represent a delay.
               • Syntax 2 draws a pulse picture and display a label underneath the picture.
               • Syntax 3 draws the picture of a shaped pulse and displays a label
                 underneath the picture.
               • Syntax 4 draws observe and decoupler pulses at the same time.
               • Syntax 5 draws a shaped pulse for observe and decoupler channels at the
                 same time.
               • Syntax 6 draws observe, decoupler, and second decoupler pulses at the
                 same time.
               • Syntax 7 draws a shaped pulse for observe, decoupler, and the second
                 decoupler channels at the same time.
               • Syntax 8 draws a pulse on the z channel.
               • Syntax 9 draws a pulse on the specified channel.
               • Syntax 10 draws a gradient picture.
               • Syntax 11 draws a shaped pulse on a specified channel.
```

• Syntax 12 draws a shaped pulse on a specified channel. For an explanation of the arguments (delay, shapedpulse, etc.), see the corresponding entry in this reference.

Examples:	dps_show("delay"	,d1);	
	dps_show("pulse","obs","obspulse",p1);		
	dps_show("pulse"	,"dec","pw",pw);	
	dps_show("shaped	_pulse","obs","shaped",p1*2);	
	dps_show("shaped	_pulse","dec2","gauss",pw);	
	dps_show("simpul	<pre>se","obs_pulse",p1,"dec_pulse",p2);</pre>	
	dps_show("simsha	<pre>ped_pulse","gauss",p1,"gauss",p2);</pre>	
	dps_show("sim3pu	lse","p1",p1,"p2",p2,"p1*2",p1*2);	
	dps_show("zgradp	ulse",123.0,d1);	
	dps_show("rgradi	ent",'x',1234.0);	
	dps_show("vgradi	ent",'x',0,2000,v10);	
	dps_show("shaped	gradient","sinc",1000.0,3000.0, \	
	'y',1,NOWAIT);		
	dps_show("shaped	2Dgradient","square",1000.0, \	
	3000.0,'y',0,N	OWAIT,1);	
Related:	delay	Delay for a specified time	
	dps_off	Turn off graphical display of statements	
	dps_on	Turn on graphical display of statements	
	dps_skip	Skip graphical display of next statement	
	pulse	Pulse observe transmitter with amplifier gating	
	rgradient	Set gradient to specified level	
	shaped_pulse	Perform shaped pulse on observe transmitter	
	shapedgradient	Generate shaped gradient pulse	
	shaped2Dgradient	Generate arrayed shaped gradient pulse	
	simpulse	Pulse observe and decouple channels simultaneously	
	sim3pulse	Pulse simultaneously on 2 or 3 rf channels	

	simshaped_puls sim3shaped_pul vgradient zgradpulse	
dps_skip	Skip graphical d	isplay of next statement
Syntax:	dps_skip()	
Description:	Skips dps display of the next statement. The statement following dps_skip is not shown in the graphical display.	
Related:	dps_on T	urn off graphical display of statements urn on graphical display of statements raw delay or pulses for graphical display of a sequence

Ε

elsenz	Execute succeeding statements if argument is nonzero

```
Syntax: (1) elsenz(vi)
            codeint vi; /* real-time variable tested as 0 or not */
```

Syntax:	(2)elsenz(n)		
,	int n; /* 1, 2, or 3: same as corresponding ifzero */		
Description:			
	Syntax 2 is used with GEMINI 2000 systems.		
Arguments:	vi is a real-time variable (v1 to v14, oph, etc.) tested for either being zero or non-zero.		
	n is the same value (1, 2, or 3) as used in the corresponding <i>ifzero</i> statement.		
Examples:	elsenz(v2); elsenz(1);		
Related:	endifEnd ifzero statementifzeroExecute succeeding statements if argument is zero		
endhardloop	End hardware loop		
Applicability:	All systems except the <i>GEMINI 2000</i> and any system equipped with the Output board, Part. No. 00-953520-0#, where # is from 0 to 4.		
Syntax:	endhardloop()		
Description:	Ends a hardware loop that was started by the starthardloop statement.		
Related:	acquireExplicitly acquire datastarthardloopStart hardware loop		
endif	End execution started by ifzero or elsenz		
Syntax:	-		
,	codeint vi; /* real-time variable to test if 0 or not */		
	<pre>(2) endif(n) int n;</pre>		
Description:	Ends conditional execution started by the <i>ifzero</i> and <i>elsenz</i> statements.		
	Syntax 1 is used with UNITYINOVA, MERCURY-VX, MERCURY, UNITYplus, UNITY, and VXR-S systems. Syntax 2 is used with GEMINI 2000 systems.		
Arguments:	vi is a real-time variable (v1 to v14, oph, etc.) that is tested for either being zero or non-zero.		
	n is the same value (1, 2, or 3) as used in the corresponding <i>ifzero</i> statement.		
Examples:	<pre>endif(v4); endif(2);</pre>		
Related:	elsenzExecute succeeding statements if argument is nonzeroifzeroExecute succeeding statements if argument is zero		

endloop End loop

	<pre>(2) endloop(n) int n;</pre>		
Description:	Ends a loop that was started by a loop statement.		
	Syntax 1 is used with UNITYINOVA, MERCURY-VX, MERCURY, UNITYplus, UNITY, and VXR-S systems. Syntax 2 is used with GEMINI 2000 systems.		
Arguments:	index is a real-time variable used as a temporary counter to keep track of the number of times through the loop. It must not be altered by any statements within the loop.		
	n is the same value (1, 2, or 3) as used in the corresponding loop statement.		
Examples:	<pre>endloop(v2); endloop(2);</pre>		
Related:	loop Start loop		
endmsloop	End multislice loop		
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.		
Syntax:	<pre>endmsloop(state,apv2) char state; /* compressed or standard */ codeint apv2; /* current counter value */</pre>		
Description:	Ends a loop that was started by a msloop statement.		
Arguments:	state is either 'c' to designate the compressed mode, or 's' to designate the standard arrayed mode. It should be the same value that was in the state argument in the msloop loop that it is ending.		
	apv2 is a real-time variable that holds the current counter value. This variable should be the same variable that was in the $apv2$ counter variable in the $msloop$ loop that it is ending.		
Examples:	endmsloop(seqcon[1],v12);		
Related:	msloopMultislice loopendloopEnd loopendpeloopEnd phase-encode loop		
endpeloop	End phase-encode loop		
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.		
Syntax:	<pre>endpeloop(state,apv2) char state;</pre>		
Description:	Ends a loop that was started by a peloop statement.		
Arguments:	state is either 'c' to designate the compressed mode, or 's' to designate the standard arrayed mode. It should be the same value that was in the state argument in the peloop loop that it is ending.		
	apv2 is a real-time variable that holds the current counter value. This variable should be the same variable that was in the $apv2$ counter variable in the peloop loop that it is ending.		
Examples:	endpeloop(seqcon[1],v12);		

Related: peloop Phase-encode loop

endloopEnd loopendmsloopEnd multi-slice loop

G

gate	Device gating (obsolete)	
Description:	<pre>gate(DECUPLR,TRUE) b gate(DECUPLR,FALSE) gate(DECUPLR2,TRUE)</pre>	y a decon() statement. by a decoff() statement. by a dec2on() statement.) by a dec2off() statement. rcvroff() statement. a rcvron() statement. xmtroff() statement.
getarray	Get arrayed parameter val	lues
Applicability:	Not applicable on MERCUR	Y-VX, MERCURY, and GEMINI 2000.
Syntax:	<pre>number=getarray(parr char *parname; double array[];</pre>	name,array) /* parameter name */ /* starting address of array */
Description:	Retrieves all values of an arrayed parameter from the parameter set. It performs a sizeof on the array address to check for the maximum number of statements that the array can hold. The number of statements in the arrayed parameter parname is determined and returned by getarray as an integer. This statement is very useful when reading in parameter values for a global list of PSG statements such as poffset_list and position_offset_list. When creating an acquisition parameter array that will be treated as lists, protection bit 8 (256) is set if the parameter is not to be treated as an arrayed acquisition parameter. An example of the pss parameter when compressing slice select portion of the acquisition is create(pss,real) setprotect(pss,on,256)	
Arguments:	parname.	argument that holds the number of values in
	_	neter, either arrayed or single value.
	array is the starting address	-
Examples:	<pre>double upss[256]; int uns; uns = getarray(upss, poffset_list(upss,gs)</pre>	<pre>/* declare array upss */ .upss); /* get values from upss */ ss,uns,v12);</pre>
Related:	<pre>create_delay_list create_freq_list create_offset_list poffset_list position_offset_list</pre>	Create table of delays Create table of frequencies Create table of offsets Set frequency from position list Set frequency from position list

getelem	Retrieve an element from an AP table	
Applicability:	All systems except the GEMINI 2000.	
Syntax:	codeint AP_index;	_index,AP_dest) /* table variable */ /* variable for index to element */ /* variable for destination */
Description:	Gets an element from an	AP table. The element is identified by an index.
Arguments:	table specifies the nar	ne of the table (t1 to t60).
	AP_index is an AP variable (v1 to v14, oph, ct, bsctr, or ssctr) that contains the index of the desired table element. Note that the first element of an AP table has an index of 0. For tables for which the autoincrement feature is set, the AP_index argument is ignored and can be set to any AP variable name; each element in such a table is by definition always accessed sequentially.	
	AP_dest is an AP varia element is placed.	ble (v1 to v14 and oph) into which the retrieved table
Examples:	getelem(t25,ct,v	1);
Related:	loadtable setautoincrement setdivnfactor setreceiver settable	Load AP table elements from table text file Set autoincrement attribute for an AP table Set divn-return attribute and divn-factor for AP table Associate the receiver phase cycle with an AP table Store an array of integers in a real-time AP table

getorientation Read image plane orientation

Applicability:	Systems with imaging or PFG modules. Not applicable to MERCURY-VX,
	MERCURY, and GEMINI 2000 systems.

Syntax:	<pre><error_return ==""> getorie</error_return></pre>	ntation(&char1,&char2, \
	<pre>&char3,search_string)</pre>	
	<pre>char *char1,*char2,*char3;</pre>	/* program variable pointers */
	char *search_string;	/* pointer to search string */

Description: Reads in and processes the value of a string parameter used typically for control of magnetic field gradients. The source of the string value is typically a usercreated parameter available in the current parameters of the experiment used to initiate acquisition.

Arguments: error_return can contain the following values:

- error_return is set to zero if getorientation was successful in finding the parameter given in search_string and reading in the value of that parameter.
- error_return is set to -1 if search_string was not empty but it did not contain the correct characters.
- error_return is set to a value greater than zero if the procedure failed or if the string value is made up of characters other than n, x, y, and z.

char1, char2, and char3 are user-created program variables of type char (single characters). The address operator (&) is used with these arguments to pass the address, rather than the values of these variables, to getorientation.

search_string is a literal string that getorientation will search for in the VNMR parameter set, i.e., the parameter name. For example, if search_string="orient", the value of parameter orient will be accessed. The value of the parameter should not exceed three characters and should only be made up of characters from the set n, x, y, and z.

The message can't find variable in tree aborts getorientation. This means there is no string associated with search_string or the parameter name cannot be found.

Examples: (1) pulsesequence()
{

```
. . .
         char phase, read, slice;
         . . .
         getorientation(&read,&phase,&slice,"orient");
         . . .
         }
         (2) pulsesequence()
         {
         . . .
         char rd, ph, sl;
         int error;
         error=getorientation(&rd,&ph,&sl,"ort");
         . . .
         }
Related:
        shapedvgradient
                              Dynamic variable shaped gradient function
        rgradient
                              Set gradient to specified level
                              Dynamic variable gradient function
         vgradient
```

getstr Look up value of string parameter

Syntax:	getstr(para char *parame char *intern	ter_name;	/*	name	of pa	aramet		name *	• /
Description:	Looks up the value of the string parameter parameter_name in the current experiment parameter list and introduces it into the pulse sequence in the variable internal_name. If parameter_name is not found in the current experiment parameter list, internal_name is set to the null string and PSG produces a warning message.				ent				
Arguments:	parameter_name is a string parameter.								
	internal_name is any legitimate C variable name defined at the beginning of the pulse sequence as an array of type char with dimension MAXSTR.				ing				
Examples:	getstr("xpol",xpol);								
Related:	getval Look up value of numeric parameter								

getval

Look up value of numeric parameter

Description: Looks up the value of the numeric parameter parameter_name in the current experiment parameter list and introduces it into the pulse sequence in the variable internal_name. If parameter_name is not found in the current experiment parameter list, internal_name is set to zero and PSG produces a warning message. Arguments: parameter_name is a numeric parameter. internal_name can be any legitimate C variable name that has been defined at the beginning of the pulse sequence as type double.

Examples: J=getval("J"); acqtime=getval("at"); delay(getval("mix"));

Related: getstr Look up value of string parameter

G_Delay Generic delay routine

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax: G_Delay(DELAY_TIME, d1, NULL, SLIDER_LABEL, SLIDER_SCALE, 1, SLIDER_MAX, 60, SLIDER_MIN, 0, SLIDER_UNITS, 1.0, 0);

Description: See the section "Generic Pulse Routine," page 121.

G Offset **Frequency offset routine**

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000. Syntax: G_Offset(OFFSET_DEVICE, TODEV,

```
OFFSET FREQ,
                tof,
                NULL,
SLIDER_LABEL,
SLIDER SCALE,
                   Ο,
SLIDER_MAX,
               1000,
SLIDER MIN,
               -1000,
SLIDER UNITS,
                   Ο,
0);
```

Description: See the section "Frequency Offset Subroutine," page 122.

G Power **Fine power routine**

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax: G Power(POWER VALUE, tpwrf, POWER DEVICE, TODEV, SLIDER_LABEL, NULL, SLIDER SCALE, 1, SLIDER_MAX, 4095, SLIDER MIN, 0, SLIDER UNITS, 1.0, 0);

Description: See the section "Fine Power Subroutine," page 125.

G Pulse **Generic pulse routine**

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax:	G_Pulse(PULSE_WIDTH,	pw,
	PULSE_PRE_ROFF,	rof1,
	PULSE_POST_ROFF,	rof2,
	PULSE_DEVICE,	TODEV,
	SLIDER_LABEL,	NULL,
	SLIDER_SCALE,	1,
	SLIDER_MAX,	1000,
	SLIDER_MIN,	Ο,
	SLIDER_UNITS,	1е-б,
	PULSE_PHASE,	oph,
	0);	

Description: See "Generic Pulse Routine," page 121.

Η

hdwshiminit	Initialize nevt	delay for hardware shimming		
Applicability:				
Syntax:	hdwshiminit()			
Description:	Enables hardware shimming during the following delay or during the following presaturation pulse, defined as a power level change followed by pulse. hdwshiminit is not necessary for the first delay or presaturation pulse in a pulse sequence, which is automatically enabled for hardware shimming.			
Examples:	hdwshiminit(); delay(d2); /*hardware shim during d2 if hdwshim='y'*/			
	hdwshiminit(); obspower(satpwr); rgpulse(satdly,v5, rof1, rof2); /*hardware shim during satdly if hdwshim='p'*/			
Related:	delay	Delay for a specified time		
hlv	Find half the v	alue of an integer		
Syntax:		/* real-time variable for starting value */ /* real-time variable for 1/2 starting value */		
Description:	Sets vj equal to	o the integer part of one-half of vi.		
Arguments:	: vi is the starting value, and vj is the integer part of one-half of the starting value. Both arguments much be real-time variables (v1 to v14, oph, etc.).			
Examples:	hlv(v2,v5);			
Related:	add assign dbl decr divn incr	Add integer values Assign integer values Double an integer value Decrement an integer value Divide integer values Increment an integer value		

mod2	Find integer value modulo 2
mod4	Find integer value modulo 4
modn	Find integer value modulo n
mult	Multiply integer values
sub	Subtract integer values

hsdelay	Delay specified time with possible homospoil pulse				
Syntax:	hsdelay(tin double time	•			
Description:	: Sets a delay for a specified number of seconds. If the homospoil parameter hs is set appropriately (see the definition of status), hsdelay inserts a homospoil pulse of length hst sec at the beginning of the delay.				
	Although the <i>GEMINI 2000</i> does not support homospoil, <i>GEMINI 2000</i> systems support hsdelay for compatibility with other systems.				
Arguments:	time specifies the length of the delay, in seconds.				
Examples:	hsdelay(d1); hsdelay(1.5e-3);				
Related:	Related:delayDelay for a specified timeidelayDelay for a specified time with IPAincdelayReal time incremental delayinitdelayInitialize incremental delayvdelayDelay with fixed timebase and real time count				

idecpulse	Pulse first decoupler transmitter with IPA				
Applicability:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.				
Syntax:	<pre>idecpulse(width,phase,label) double width; /* pulse width in sec */ codeint phase; /* real-time variable for phase */ char *label; /* slider label in acqi */</pre>				
Description:	Functions the same as the decpulse statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is typed. idecpulse is the same as decpulse if go is typed.				
Arguments:	width is the duration, in seconds, of the pulse.				
	phase is the phase of the pulse. It must be a real-time variable (v1 to v14, oph, etc.) or a real-time constant (zero, one, etc.).				
	label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).				
Examples:	idecpulse(pp,v1,"decpul"); idecpulse(pp,v2,"pp");				
Related:	decpulse Pulse the decoupler transmitter				

idecrgpulse Pulse first decoupler with amplifier gating and IPA

Idecigpuise	Tuise hist decoupler with ampliner gating and it A
Applicability:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.
Syntax:	<pre>idecrgpulse(width,phase,RG1,RG2,label) double width; /* pulse width in sec */ codeint phase; /* real-time variable for phase */ double RG1; /* gating delay before pulse in sec */ double RG2; /* gating delay after pulse in sec */ char *label; /* slider label in acqi */</pre>
Description:	Works similar to the decrgpulse statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is typed. idecrgpulse is the same as decrgpulse if go is typed.
Arguments:	width is the duration, in seconds, of the decoupler transmitter pulse.
	phase sets the decoupler transmitter phase. The value must be a real-time variable.
	RG1 is the time, in seconds, that the amplifier is gated on prior to the start of the pulse.
	RG2 is the time, in seconds, that the amplifier is gated off after the end of the pulse.
	label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).
Examples:	idecrgpulse(pp,v5,rof1,rof2,"decpul"); idecrgpulse(pp,v4,rof1,rof2,"pp");
Related:	decrgpulse Pulse decoupler transmitter with amplifier gating
idelay	Delay for a specified time with IPA
_	Delay for a specified time with IPA All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> .
_	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.
Applicability:	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> . idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */
Applicability: Syntax: Description:	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> . idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay
Applicability: Syntax: Description:	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> . idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay is the same as delay if go is entered.
Applicability: Syntax: Description:	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> . idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay is the same as delay if go is entered. time is the length of the delay, in seconds. label is the short character string to be given to the slider when displayed in
Applicability: Syntax: Description: Arguments:	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> . idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay is the same as delay if go is entered. time is the length of the delay, in seconds. label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program). idelay(d1, "delay");
Applicability: Syntax: Description: Arguments: Examples:	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> . idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay is the same as delay if go is entered. time is the length of the delay, in seconds. label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program). idelay(d1, "delay"); idelay(d1, "d1");
Applicability: Syntax: Description: Arguments: Examples: Related:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000. idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay is the same as delay if go is entered. time is the length of the delay, in seconds. label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program). idelay(dl, "delay"); idelay(dl, "dl"); delay Delay for a specified time Execute succeeding statements if argument is zero
Applicability: Syntax: Description: Arguments: Examples: Related: ifzero	All systems except MERCURY-VX, MERCURY, and GEMINI 2000. idelay(time,label) double time; /* delay in sec */ char *label; /* slider label in acqi */ Works similar to the delay statement but generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. idelay is the same as delay if go is entered. time is the length of the delay, in seconds. label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program). idelay(d1, "delay"); idelay(d1, "dl"); delay Delay for a specified time Execute succeeding statements if argument is zero (1) ifzero(vi)

elsenz statement. Conditional execution ends when the endif statement is reached. It is not necessary for any statements to appear between the ifzero and the elsenz or between the elsenz and the endif statements.

Syntax 1 is used with UNITY INOVA, MERCURY-VX, MERCURY, UNITY plus, UNITY, and VXR-S systems.

Syntax 2 is used with GEMINI 2000 systems.

Arguments: vi is a real-time variable (v1 to v14, oph, etc.) that is tested for being either zero or non-zero.

> n is the same value (1, 2, or 3) as used in the corresponding elsenz or endif statements.

Examples:	mod2(ct,v1);	/*	v1=010101 */
	ifzero(v1)	;	/*	test if v1 is zero */
	pulse(p	w,v2);	/*	execute if v1 is zero */
	delay(d	3);	/*	execute if v1 is zero */
	elsenz(v1)	;	/*	test if v1 is non-zero */
	pulse(2	.0*pw,v2);	/*	execute if v1 is non-zero */
	delay(d	3/2.0);	/*	execute if v1 is non-zero */
	endif(v1);		/*	end conditional execution $\ast/$
Related:	elsenz	Execute succee	ding	statements if argument is nonzero
	endif End ifzero state		emen	t
	initval	Initialize real-ti	ime v	variable to specified value

incdelay Set real-time incremental delay

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000. Syntax: incdelay(count, index) codeint count; /* real-time variable */

- /* time increment: DELAY1, DELAY2, etc. */ int index; Description: Enables real-time incremental delays. Before incdelay can be used to set a
 - delay, an associated **initdelay** statement must be executed to initialize the time increment and delay index.
- Arguments: count is a real-time variable (ct, v1 to v14, etc.) that multiplies the time increment (initialized by the initdelay statement) to set the delay time.

index is DELAY1, DELAY2, DELAY3, DELAY4, or DELAY5. It identifies which time increment is being multiplied by count to equal the delay.

Examples: incdelay(ct,DELAY1); incdelay(v3,DELAY2);

Related:	delay	Delay for a specified time
	hsdelay	Delay with possible homospoil pulse
	idelay	Delay for a specified time with IPA
	initdelay	Initialize incremental delay
	vdelay	Delay with fixed timebase and real time count

incgradient	Generate dynamic variable gradie	ent pulse
Applicability:	Not applicable on MERCURY-VX, MI	ERCURY, and GEMINI 2000.
Syntax:	<pre>incgradient(channel,base, mult2,mult3)</pre>	<pre>incl,inc2,inc3,mult1, \</pre>
	char channel;	/* gradient 'x', 'y', or 'z' */

int base;	/* base value */
<pre>int inc1,inc2,inc3;</pre>	/* increments */
<pre>codeint mult1,mult2,mult3;</pre>	/* multipliers */

Description: Provides a dynamic variable gradient pulse controlled using the AP math functions. It drives the chosen gradient to the level defined by the formula:

level=base+inc1*mult1+inc2*mult2+inc3*mult3

with increments incl, inc2, inc3 and multipliers mult1, mult2, mult3.

The range of the gradient level is -2047 to +2047 if the gradients are run through the DAC board, and -32767 to +32767 if the gradient waveform generator package is installed. If the requested level lies outside the legal range, it is clipped at the appropriate boundary value. Note that, while each variable in the level formula must fit in a 16-bit integer, partial sums and products in the calculation are done with double-precision 32-bit integers.

The action of the gradient after the use of the incgradient statement is controlled by the gradient power supply and optional gradient compensation boards. The gradient level is ramped at the maximum slew rate to the value requested by incgradient. This fact becomes a concern when using the incgradient statement in a loop with a delay statement to produce a modulated gradient. The delay statement should be sufficiently long so as to allow the gradient to reach the assigned value, that is,

 $delay \ge \frac{|new_level - old_level|}{full scale} \times risetime$

The following error messages are possible:

- Bad gradient specified: channel is caused by the channel character evaluating to other than 'x', 'y', or 'z'; or by being a string.
- mult[i] illegal RT variable: multiplier_i is caused by mult1, mult2, or mult3 having a value other than a AP math variable, v1 to v14.
- Arguments: channel is an expression that evaluates to the character 'x', 'y', or 'z'. (do not confuse characters 'x', 'y' and 'z' with strings "x", "y" and "z".)

base and inc1, inc2, inc3 are the base value and increments used in the formula for determining the gradient level.

mult1, mult2, mult3 are the multipliers used in the gradient level formula. These arguments should be AP math variables, v1 to v14. Note that AP tables (t1 to t60) are *not* allowed in this statement.

Examples: See the program inctst.c

Related:	getorientation	Read image plane orientation
	rgradient	Set gradient to specified level
	shapedgradient	Provide shaped gradient pulse to gradient channel
	shaped2Dgradient	Generate arrayed shaped gradient pulse
	shapedvgradient	Generate dynamic variable shaped gradient pulse
	vgradient	Generate dynamic variable gradient pulse

incr

Increment an integer value

Syntax: incr(vi)

	codeint vi;	/*	real-time	variable	to	increment	*/
Description:	Increments by 1 the	intege	er value given	by vi (i.e, v	vi=	vi+1).	

Arguments: vi is the integer to be incremented, It must be a real-time variable (v1 to v14, oph, etc.).

Examples: incr(v4);

Related:	add assign dbl decr divn hlv	Add integer values Assign integer values Double an integer value Decrement an integer value Divide integer values Half the value of an integer
	mod2 mod4 modn mult sub	Find integer value modulo 2 Find integer value modulo 4 Find integer value modulo n Multiply integer values Subtract integer values

indirect

Set indirect detection

Applicability: No longer useful to any system using VNMR 5.2 or later.

Syntax: indirect()

Description: Starting with VNMR 5.2, if tn is 'H1' and dn is not 'H1', the software automatically uses the decoupler as the observe channel and the broadband channel as the decoupler channel.

Create rf pattern file init_rfpattern

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000. Syntax: init rfpattern(pattern,rfpat struct,nsteps) /* name of .RF text file */ char *pattern; RFpattern *rfpat_struct; /* pointer to struct RFpattern */ /* number of steps in pattern */ int nsteps; typedef struct _RFpattern { double amp; /* amplitude of pattern step */
double time: /* length of pattern step in sec */ } RFpattern Description: Creates and defines rf patterns within a pulse sequence. The patterns can be created by any algorithm as long as each pattern step is correctly put into the rfpat_struct argument. The number of steps in the pattern also has to be furnished as an argument. init_rfpattern saves the created pattern as a pattern file (with the suffix .RF appended to the name) in the user's shapelib directory. This statement does not have any return value. Arguments: pattern is the name of the pattern file (without the .RF suffix). rfpat_struct is the rf structure that contains the pattern. nsteps is the number of steps in the pattern. Examples: #include "standard.h" pulsesequence()

```
{
int nsteps;
RFpattern pulse1[512], pulse2[512];
Gpattern gshape[512];
. . .
```

```
nsteps = 0;
        for (j=0; j<256; j++) {
            pulse1[j].phase = (double)j*0.5;
            pulse1[j].amp = (double)j*2;
            pulse1[j].time = 1.0;
            nsteps = nsteps +1;
        }
        init_rfpattern(plpat,pulse1,nsteps);
        nsteps = 512;
        for (j=0; j<nsteps; j++) {</pre>
            gshape[j].amp = 32767.0*sin((double)j/50.0);
            gshape[j].time = 1.0;
        }
        init_gradpattern("gpat",gshape,nsteps);
        . . .
        shaped_pulse(p1pat,p1,v1,rof1,rof1);
        . . .
        shapedgradient("gpat",.01, 16000.0, 'z', 1, WAIT);
        . . .
        }
Related:
                             Create gradient pattern file
        init_gradpattern
                             Pulse observe transmitter with amplifier gating
        pulse
        shaped_pulse
                             Perform shaped pulse on observe transmitter
        shapedgradient
                             Provide shaped gradient pulse to gradient channel
                             Pulse observe and decouple channels simultaneously
        simpulse
        simshaped_pulse
                             Perform simultaneous two-pulse shaped pulse
```

init_gradpattern Create gradient pattern file

Applicability: Not applicable on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

Syntax:	: init_gradpattern(pattern_name,gradpat_struct,		
	char *pattern;	/* name of .GID pattern file */	
	<pre>Gpattern *gradpat_struct;</pre>	/* pointer to struct Gpattern */	
	int nsteps;	/* number of steps in pattern */	
	typedef struct _Gpattern{		
	double amp;	<pre>/* amplitude of pattern step */</pre>	
	double time;	<pre>/* pattern step length in sec */</pre>	
	} Gpattern		

Description: Creates and defines gradient patterns within a pulse sequence. The patterns can be created by any algorithm as long as each pattern step is correctly put into the gradpat_struct argument. The number of steps in the pattern also has to be furnished as an argument. init_gradpattern saves the created pattern as a pattern file (with a .GRD suffix is appended to the name) in the user's shapelib directory. This statement has no return value.

```
Arguments: pattern is the name of the pattern file (without the .GRD suffix).
```

gradpat_struct is the gradient structure that contains the pattern.

nsteps is the number of steps in the pattern.

Examples: See the example for the init_rfpattern statement.

Related:	pulse	Pulse observe transmitter with amplifier gating
	shaped_pulse	Perform shaped pulse on observe transmitter
	simpulse	Pulse observe and decouple channels simultaneously
	simshaped_pulse	Perform simultaneous two-pulse shaped pulse

init_vscan	Initialize real-time variable for vscan statement	
Applicability:	Systems with imaging capability.	
Syntax:	<pre>init_vscan(vi,number_points) codeint vi;</pre>	
Description:	Initializes a real-time AP math variable for use with the vscan statement. init_vscan has no return value.	
Arguments:	vi is an AP math variable (v1 to v14). Its range is 1 to 32767.	
	number_points is the number of points to acquire in the scan. This is not limited to one acquisition but can be the sum of multiple acquires.	
Examples:	See the example used in the entry for vscan.	
Related:	vscan Dynamic variable scan function	
initdelay	Initialize incremental delay	
Applicability:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>initdelay(time_increment,index) double time_increment; /* time increment in sec */ int index; /* time increment: DELAY1, etc. */</pre>	
Description:	Initializes a time increment delay and its associated delay index. This statement must be executed before an incdelay statement can set an incremental delay. A maximum of five incremental delays (set by the index argument) can be defined in one pulse sequence.	
Arguments:	time_increment is the time increment, in seconds, that is multiplied by the count argument (set in the incdelay statement) for the delay time.	
	index is DELAY1, DELAY2, DELAY3, DELAY4, or DELAY5, and identifies which time increment is being initialized.	
Examples:	<pre>initdelay(1.0/sw,DELAY1); initdelay(1.0/sw1,DELAY2);</pre>	
Related:	delayDelay for a specified timehsdelayDelay with possible homospoil pulseidelayDelay for a specified time with IPAincdelayReal time incremental delayvdelayDelay with fixed timebase and real time count	
initparms_sis	Initialize parameters for spectroscopy imaging sequences	

- Applicability: Systems with imaging capability; however, this statement will be obsoleted in future versions of VNMR.
 - Syntax: void initparms_sis()
- Description: Sets the default state of the receiver to ON so that the receiver is enabled for explicit acquisitions. The original purpose of initparms_sis was to initialize the standard imaging parameters in imaging sequences, but starting with VNMR 5.3, initialization of these parameters has been folded into PSG.
- Examples: /* To upgrade older SIS sequences for Vnmr 5.1+: */
 /* insert initparms_sis() after the variable */
 /* declarations and update 'griserate' variable. */
 ...
 /* EXTERNAL TRIGGER */

```
double rcvry,hold;
initparms_sis();
griserate = trise/gradstepsz;
/**[3.2] PARAMETER READ IN FROM EXPERIMENT ******/
...
```

initval	Initialize a real-time variable to specified value		
Syntax:	<pre>initval(number,vi) double number; /* value to use for initialization */ codeint vi; /* variable to be initialized */</pre>		
Description:	Initializes a real- time variable with a real number. The real number input is rounded off and placed in the variable vi. Unlike add, sub, etc., initval is executed <i>once and only once</i> at the start of a non-arrayed 1D experiment or at the start of each increment in an <i>n</i> -dimensional or an arrayed experiment, not at the start of each transient; this must be taken into account in pulse sequence programming, as seen in the example below.		
Arguments:	number is the real number, from -32768.0 to 32767.0, to be placed in the real- time variable. Entering a value less than -32768.0 (after rounding off) results in using -32768, and entering a value greater than 32767.0 (after rounding off) results in using 32767.		
	vi is the real-time variable (v1 to v14, etc.).to be initialized		
Examples:	<pre>(1) initval(nt,v8);</pre>		
	<pre>(2) ifzero(ct); assign(v8,v7); elsenz(ct); decr(v7); endif(ct);</pre>		
Related:	elsenzExecute succeeding statements if argument is nonzeroifzeroExecute succeeding statements if argument is zeroloopStart loop		
iobspulse	Pulse observe transmitter with IPA		
Applicability:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.		
Syntax:	iobspulse(label) char *label; /* slider label in acqi */		
Description:	Functions the same as obspulse except iobspulse generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. If go is entered, iobspulse is the same as obspulse .		
Arguments:	label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).		
Examples:	iobspulse("pulse"); iobspulse("pw");		
Related:	obspulse Pulse observe transmitter with amplifier gating		
ioffeet	Change offset frequency with IPA		

ioffset Change offset frequency with IPA

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax: ioffset(frequency,device,label)

	<pre>double frequency; /* offset frequency */ int device; /* OBSch, DECch, DEC2ch, or DEC3ch */ char *label; /* slider label in acqi */</pre>
Description:	Functions the same as offset except that ioffset generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. If go is entered, ioffset is the same as offset .
Arguments:	frequency is the new offset frequency of the device specified.
	device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY <i>INOVA</i> and UNITY <i>plus</i> only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).
	label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).
Examples:	<pre>ioffset(tof,OBSch,"tof");</pre>
Related:	offset Change offset frequency of transmitter or decoupler
ipulse	Pulse observe transmitter with IPA
	All systems except <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> .
	ipulse(width,phase,label)
Synax.	<pre>double width; /* pulse length in sec */ codeint phase; /* real-time variable for phrase */ char *label; /* slider label in acqi */</pre>
Description:	Functions the same as pulse(width, phase) statement except that ipulse generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. If go is entered, ipulse is the same as pulse.
Arguments:	width specifies the duration, in seconds, of the pulse.
	phase sets the phase of the pulse. The value must be a real-time variable (v1 to v14, oph, etc.).
	label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).
Examples:	ipulse(pw,v4,"pulse"); ipulse(pw,v5,"pw");
Related:	pulse Pulse observe transmitter with amplifier gating
ipwrf	Change transmitter or decoupler fine power with IPA
Applicability:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.
Syntax:	<pre>ipwrf(power,device,label) double power; /* new fine power level */ int device; /* OBSch, DECch, DEC2ch, DEC3ch */ char *label; /* slider label in acqi */</pre>
Description:	Functions the same as rlpwrf statement except that ipwrf generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. If go is entered, ipwrf is ignored by the pulse sequence; use rlpwrf for this purpose. Do not execute rlpwrf and ipwrf together because they cancel each other's effect.
Arguments:	power is the new fine power level. It can range from 0.0 to 4095.0 (60 dB on UNITY <i>INOVA</i> and UNITY <i>plus</i> , about 6 dB on other systems).

device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).

ipwrm Change transmitter or decoupler lin. mod. power with IPA

Applicability: All systems except *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

Syntax:	ipwrm(value,devi	ce,label)
	double value;	<pre>/* new linear modulator power level */</pre>
	int device;	/* OBSch, DECch, DEC2ch, or DEC3ch */
	char *label;	/* slider label in acqi */

- Description: Functions the same as rlpwrm statement except that ipwrm generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. If go is entered, ipwrm is ignored by the pulse sequence; use rlpwrm for this purpose. Do not execute rlpwrm and ipwrm together as they cancel each other's effect.
- Arguments: value is the new linear modulator power level. It can range from 0.0 to 4095.0 (60 dB on UNITY*INOVA* and UNITY*plus*, about 6 dB on other systems).

device is OBSch (observe transmitter) or DECch (first decoupler). On the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).

Related: rlpwrm Set transmitter or decoupler linear modulator power

irgpulse Pulse observe transmitter with IPA

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000. Syntax: irgpulse(width,phase,RG1,RG2,label) double width; /* pulse length in sec */ codeint phase; /* real-time variable for phase */ double RG1; /* gating delay before pulse in sec */ double RG2; /* gating delay after pulse in sec */ char *label; /* slider label in acqi */ Description: Functions the same as the rgpulse statement except that irgpulse

- Description: Functions the same as the rgpulse statement except that irgpulse generates interactive parameter adjustment (IPA) information when gf or go('acqi') is entered. If go is entered, irgpulse is the same as rgpulse.
- Arguments: width specifies the duration, in seconds, of the observe transmitter pulse. phase sets the observe transmitter phase. It must be a real-time variable. RG1 is the time, in seconds, the amplifier is gated on prior to the start of the pulse.

Related: rlpwrf Set transmitter or decoupler fine power

RG2 is the time, in seconds, the amplifier is gated off after the end of the pulse.

label is the short character string to be given to the slider when displayed in the Acquisition window (acqi program).

Related: rgpulse Pulse observe transmitter with amplifier gating

	L	
lk_hold	Set lock correction circuitry to hold correction	
Applicability:	UNITY INOVA, MERCURY-VX, MERCURY, and UNITY plus systems only.	
Syntax:	lk_hold()	
Description:	Makes the lock correction circuitry hold the correction to the z0 constant, thereby ignoring any influence on the lock signal such as gradient or pulses at ² H frequency. The correction remains in effect until the statement lk_sample is called or until the end of an experiment. If an acquisition is aborted, the lock correction circuitry will be reset to sample the lock signal.	
Related:	lk_sample Set lock correction circuitry to sample lock signal	
lk_sample	Set lock correction circuitry to sample lock signal	
Applicability:	UNITY INOVA, MERCURY-VX, MERCURY, and UNITY plus systems only.	
Syntax:	lk_sample()	
Description:	Makes the lock correction circuitry continuously sample the lock signal and correct z0 with the time constant as set by the parameter lockacqtc. The correction remains in effect until the statement lk_hold is called.	
Related:	lk_hold Set lock correction circuitry to hold correction	
loadtable	Load AP table elements from table text file	
Applicability:	All systems except the GEMINI 2000.	
Syntax:	loadtable(file) char *file; /* name of table file */	
Description:	Loads AP table elements from a table file (a UNIX text file). It can be called multiple times within a pulse sequence but make sure that the same table name is not used more than once within all the table files accessed by the sequence. Table values can be greater than, equal to, or less than zero.	
Arguments:	file is the name of a table file in a user's private tablib or in the system tablib.	
Examples:	<pre>loadtable("tabletest");</pre>	
Related:	getelemRetrieve an element from an AP tablesetautoincrementSet autoincrement attribute for an AP tablesetdivnfactorSet divn-return attribute and divn-factor for AP tablesetreceiverAssociate the receiver phase cycle with an AP tablesettableStore an array of integers in a real-time AP table	

loop	Start loop		
Syntax:	<pre>(1) loop(count,index) codeint count /* number of times to loop */ codeint index /* real-time variable to use during loop */</pre>		
Syntax:	<pre>(2) loop(n,count,index) int n;</pre>		
Description:	Starts a loop to execute statements within the pulse sequence. The loop is ended by the endloop statement.		
	Syntax 1 is used with UNITYINOVA, MERCURY-VX, MERCURY, UNITYplus, UNITY, and VXR-S systems. Syntax 2 is used with GEMINI 2000 systems.		
Arguments:	count is a real-time variable used to specify the number of times through the loop. count can be any positive number, including zero.		
	index is a real-time variable used as a temporary counter to keep track of the number of times through the loop. The value must not be altered by any statements within the loop.		
	n is the same value (1, 2, or 3) as used in the corresponding endloop statement.		
Examples:	<pre>(1) initval(5.0,v1); /* set first loop count */ loop(v1,v10);</pre>		
	<pre>dbl(ct,v2);</pre>		
	(2) loop(2,5.0,v9);		
Related:	initvalInitialize real-time variable to specified valueendloopEnd loopmsloopMultislice loop		

Μ

magradient	Simultaneous gradient at the magic angle
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.
Syntax:	<pre>magradient(gradlvl) double gradlvl; /* gradient amplitude in G/cm */</pre>
Description:	Applies a simultaneous gradient on the x , y , and z axes at the magic angle to B ₀ . Information from a gradient table is used to scale and set values correctly. The gradients are left at the given levels until they are turned off. To turn off the gradients, add another magradient statement with gradlvl set to zero or insert the statement zero_all_gradients.
Arguments:	gradlvl is the gradient amplitude, in gauss/cm.

Examples:	<pre>magradient(3.0); pulse(pw,oph); delay(0.001 - pw); zero_all_gradients</pre>	();			
Related:	magradpulse mashapedgradient mashapedgradpulse vagradient vagradpulse vashapedgradient vashapedgradpulse zero_all_gradients	Simultaneous gradient pulse at the magic angle Simultaneous shaped gradient at the magic angle Simultaneous shaped gradient pulse at the magic angle Variable angle gradient Variable angle gradient pulse Variable angle shaped gradient Variable angle shaped gradient Zero all gradients			
magradpulse	Gradient pulse at the magic angle				
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.				
Syntax:	<pre>magradpulse(gradlv double gradlvl; double gradtime;</pre>	l,gradtime) /* gradient amplitude in G/cm */ /* gradient time in sec */			
Description:	Applies a simultaneous gradient pulse on the x , y , and z axes at the magic angle to B ₀ . Information from a gradient table is used to scale and set values correctly.				
	magradpulse differs from magradient in that the gradients are turned off after gradtime seconds. Use magradpulse if there are no other actions while the gradients are on. magradient is used if there are actions to be performed while the gradients are on.				
Arguments:	gradlvl is the gradient p	ulse amplitude, in gauss/cm.			
	gradtime is the time, in	seconds, to apply the gradient.			
Examples:					
Related:	magradient mashapedgradient mashapedgradpulse vagradient vagradpulse vashapedgradient vashapedgradpulse zero_all_gradients	Simultaneous gradient at the magic angle Simultaneous shaped gradient at the magic angle Simultaneous shaped gradient pulse at the magic angle Variable angle gradient Variable angle gradient pulse Variable angle shaped gradient Variable angle shaped gradient Zero all gradients			
mashapedgradient Simultaneous shaped gradient at the magic angle					
Applicability:	Not applicable on MERCU	RY-VX, MERCURY, and GEMINI 2000.			
Syntax:	<pre>loops,wait) char *pattern; double gradlvl; double gradtime; int loops; int wait;</pre>	<pre>attern,gradlvl,gradtime, \ /* name of gradient shape text file */ /* gradient amplitude in G/cm */ /* gradient time in seconds */ /* number of waveform loops */ /* WAIT or NOWAIT*/</pre>			
Description:	Applies a simultaneous gradient with shape pattern and amplitude				

gradlvl on the x, y, and z axes at the magic angle to B₀. Information is used from a gradient table to scale and set the values correctly.

mashapedgradient leaves the gradients at the given levels until they are

turned off. To turn off the gradients, add another mashapedgradient statement with gradlvl set to zero or include the zero_all_gradients statement.

mashapedgradpulse differs from mashapedgradient in that the gradients are turned off after gradtime seconds. mashapedgradient is used if there are actions to be performed while the gradients are on. mashapedgradpulse is best when there are no other actions required while the gradients are on.

Arguments: pattern is the name of a text file describing the shape of the gradient. The text file is located in \$vnmrsystem/shapelib or in the user directory \$vnmruser/shapelib.

gradlvl is the gradient amplitude, in gauss/cm.

gradtime is the gradient application time, in seconds.

loops is a value from 0 to 255 to loop the selected waveform. Gradient waveforms on UNITYINOVA systems do not use this field, and loops is set to 0 on UNITYINOVA systems.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient is completed before executing the next statement.

Examples: mashapedgradient("ramp_hold",3.0,trise,0,NOWAIT);
 pulse(pw,oph);
 delay(0.001-pw-2*trise);
 mashapedgradient("ramp_down",3.0,trise,0,NOWAIT);

Related:	magradient magradpulse mashapedgradpulse vagradient vagradpulse vashapedgradient vashapedgradpulse zero all gradients	Simultaneous gradient at the magic angle Simultaneous gradient pulse at the magic angle Simultaneous shaped gradient pulse at the magic angle Variable angle gradient Variable angle gradient pulse Variable angle shaped gradient Variable angle shaped gradient pulse Zero all gradients
	zero_arr_gradients	Zero an gradients

mashapedgradpulse Simultaneous shaped gradient pulse at the magic angle

Applicability: Not applicable on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

Syntax:	<pre>mashapedgradpulse(pattern,gradlvl,gradtime,theta,ph) char *pattern; /* name of gradient shape text file */ double gradlvl; /* gradient amplitude in G/cm */ double gradtime; /* gradient time in sec */</pre>		
Description:	Applies a simultaneous gradient with shape pattern and amplitude gradlvl on the x , y , and z axes at the magic angle to B_0 . mashapedgradpulse assumes that the gradient pattern zeroes the gradients at its end and so it does not explicitly zero the gradients. Information from a gradient table is used to scale and set values correctly.		
	mashapedgradpulse is used if there are no other actions required when the gradients are on. mashapedgradient is used if there are actions to be performed while the gradients are on.		
Arguments:	pattern is the name of a text file describing the shape of the gradient. The text file is located in <pre>\$vnmrsystem/shapelib</pre> or in the user directory <pre>\$vnmruser/shapelib</pre> .		

gradlvl is the gradient amplitude, in gauss/cm.

gradtime is the gradient application time, in seconds.

	graderine is the gradient approached time, in seconds.		
Examples:	<pre>mashapedgradpulse("hsine",3.0, 0.001);</pre>		
Related:	magradient magradpulse mashapedgradient vagradient vagradpulse vashapedgradient vashapedgradpuls zero_all_gradien	Variable angle gradient Variable angle gradient pulse Variable angle shaped gradient e Variable angle shaped gradient pulse	
mod2	Find integer value	modulo 2	
Syntax:	<pre>mod2(vi,vj) codeint vi; codeint vj;</pre>	/* variable for starting value */ /* variable for result */	
Description:	Sets the value of vj	equal to vi modulo 2.	
Arguments:	vi is the starting integer value and vj is the value of vi modulo 2 (the remainder after vi is divided by 2). Both arguments must be real-time variables (v1 to v14, etc.).		
Examples:	mod2(v3,v5);		
Related:	assignAssigndblDoubledecrDecreddivnDividehlvHalfincrIncredmod4FindmodnFindmultMulte	integer values gn integer values ole an integer value ement an integer value le integer values the value of an integer ment an integer value integer value modulo 4 integer value modulo n iply integer values ract integer values	
mod4	Find integer value modulo 4		
Syntax:	mod4(vi,vj) codeint vi; codeint vj;	/* variable for starting value */ /* variable for result */	
Description:	Sets the value of vj equal to vi modulo 4.		
Arguments:	vi is the starting integer value and vj is the value of vi modulo 4 (the remainder after vi is divided by 4). Both arguments must be real-time variables (v1 to v14, etc.).		
Examples:	mod4(v3,v5);		
Related:		integer value modulo 2 integer value modulo <i>n</i>	
modn	Find integer value modulo <i>n</i>		
Syntax:	modn(vi,vj,vk)	/* real-time variable for starting value */	

	adding with (t was bing waviable for module number t)		
	<pre>codeint vj; /* real-time variable for modulo number */ codeint vk; /* real-time variable for result */</pre>		
Description:	Sets the value of vk equal to vi modulo vj.		
Arguments:	vi is the starting integer value, vj is the modulo value, and vk is vi modulo vj (the remainder after vi is divided by vj). All arguments must be real-time variables (v1 to v14, etc.).		
Examples:	modn(v3,v5,v4);		
Related:	mod2Find integer value modulo 2mod4Find integer value modulo 4		
msloop	Multislice loop		
Applicability:	Not applicable on <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> .		
Syntax:			
Description:	Provides a sequence-switchable loop that can use real-time variables in what is known as a compressed loop or it can use the standard arrayed features of PSG. In imaging sequences, msloop uses the second character of the seqcon string parameter (seqcon[1]) for the state argument. msloop is used in conjunction with endmsloop.		
Arguments:	state is either 'c' to designate the compressed mode, or 's' to designate the standard arrayed mode.		
	\max_count initializes apv1. If state is 'c', this value should equal the number of slices. If state is 's', this value should be 1.0.		
	apv1 is real-time variable that holds the maximum count.		
	apv2 is a real-time variable that holds the current counter value. If state : 'c', apv2 counts from 0 to max_count-1. If state is 's', apv2 is so to zero.		
Examples:	<pre>msloop(seqcon[1],ns,v11,v12);</pre>		
	<pre> poffset_list(pss,gss,ns,v12); acquire(np,1.0/sw);</pre>		
	endmsloop(seqcon[1],v12);		
Related:	endmsloopEnd multislice looploopStart looppeloopPhase-encode loop		
mult	Multiply integer values		
	<pre>mult(vi,vj,vk) codeint vi; /* real-time variable for first factor */ codeint vj; /* real-time variable for second factor */ codeint vk; /* real-time variable for product */</pre>		

Description: Sets the value of vk equal to the product of the integer values vi and vj.

Arguments: vi is an integer value, vj is another integer value, and vk is the product of vi and vj. All arguments must be real-time variables (v1 to v14 etc.).

Examples: mult(v3,v5,v4);

Related:	add	Add integer values
	assign	Assign integer values
	dbl	Double an integer value
	decr	Decrement an integer value
	divn	Divide integer values
	hlv	Half the value of an integer
	incr	Increment an integer value
	mod2	Find integer value modulo 2
	mod4	Find integer value modulo 4
	modn	Find integer value modulo n
	sub	Subtract integer values

0

obl_gradient	Execute an oblique gradient	
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>obl_gradient(level1,level2,level3) double level1,level2,level3; /* gradient values in G/cm */</pre>	
Description:	Defines an oblique gradient with respect to the magnet reference frame. This statement is basically the same as the statement oblique_gradient except that obl_gradient uses the parameters psi, phi, and theta in the parameter set rather than setting them directly. It has no return value.	
	The pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.	
Arguments:	level1, level2, level3 are gradient values, in gauss/cm.	
Examples:	<pre>obl_gradient(0.0,0.0,gss); obl_gradient(gro,0.0,0.0);</pre>	
Related:	oblique_gradient Execute an oblique gradient	

oblique_gradientExecute an oblique gradient

Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>oblique_gradient(level1,level2,level3,psi,phi,theta) double level1,level2,level3; /* gradient values in G/cm */ double psi,phi,theta; /* Euler angles in degrees */</pre>	
Description:	Defines an oblique gradient with respect to the magnet reference frame. It has no return value. The gradient amplitudes (level1,level2,level3) are put through a coordinate transformation matrix using psi, phi, and theta to determine the actual <i>x</i> , <i>y</i> , and <i>z</i> gradient levels. These are then converted into DAC values and set with their corresponding gradient statements. For more coordinate system information, refer to the manual <i>User Guide: Imaging</i> .	
	The pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.	

Arguments:	level1, level2, level3 are gradient values, in gauss/cm.	
	psi is an Euler angle, in degrees, with a range of -90 to $+90$.	
	phi is an Euler angle, in degrees, with the range of -180 to $+180$.	
	theta is an Euler angle	e, in degrees, with the range -90 to $+90$.
Examples:	<pre>oblique_gradient(gvox1,0,0,vpsi,vphi,vtheta);</pre>	
Related:	obl gradient	Execute an oblique gradient

Execute a shaped oblique gradient obl_shapedgradient

	-	
Applicability:	Not applicable on MERCURY-VX	X, MERCURY, or GEMINI 2000.
Syntax:	<pre>obl_shapedgradient(pat1,pat2,pat3,width,lvl1, \</pre>	
	<pre>char *pat1,*pat2,*pat3; double width; double lvl1,lvl2,lvl3; int loops; int wait;</pre>	<pre>/* names of gradient shapes */ /* gradient length in sec */ /* gradient values in G/cm */ /* times to loop waveform */ /* WAIT or NOWAIT */</pre>
Description:	· · · ·	t with respect to the magnet reference frame.

Γ It is basically the same as the oblique_shapedgradient statement except that obl_shapedgradient uses the parameters psi, phi, and theta in the parameter set rather than setting them directly.

> The pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

pat1, pat2, pat3 are names of gradient shapes. (Note that the VNMR 5.1 Arguments: and 5.2 software releases used only one pattern in the argument list.)

width is the length of the gradient, in seconds.

level1, level2, level3 are gradient values, in gauss/cm.

loops is the number of times, from 1 to 255, to loop the waveform.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to stop until the gradient has completed before executing the next statement.

Examples: obl_shapedgradient("ramp_hold","","",trise,gro, \backslash 0.0,0.0,1,NOWAIT);

Related: Execute a shaped oblique gradient oblique_shapedgradient

Execute a shaped oblique gradient oblique_shapedgradient

Applicability:	Not applicable on MERCURY-VX, MERCURY, or GEMINI 2000.	
Suntary	obligue ghapedgradient(nat1 nat2 nat2 width	

Syntax:	oblique_shapedgradient(pat	tl,pat2,pat3,width, ∖
	lvl1,lvl2,lvl3,psi,p	bhi.	theta,loops,wait)
	<pre>char *pat1,*pat2,*pat3;</pre>	/*	names of gradient shapes */
	double width;	/*	gradient length in sec */
	double lvl1,lvl2,lvl3;	/*	gradient values in G/cm */
	double psi,phi,theta;	/*	Euler angles in degrees */
	int loops;	/*	times to loop waveform */
	int wait;	/*	WAIT or NOWAIT */

.....

Description: Defines a shaped oblique gradient with respect to the magnet reference frame. The gradient patterns (pat1, pat2, pat3) and the gradient amplitudes

(lvl1, lvl2, lvl3) are put through a coordinate transformation matrix using psi, phi, and theta to determine the actual *x*, *y*, and *z* gradient levels.

pat1 and lvl1 correspond to the logical read-out axis. pat2 and lvl2 correspond to the logical phase-encode axis. pat3 and lvl3 correspond to the logical slice-select axis.

Patterns are read in; scaled according to their respective amplitudes; rotated into *x*, *y*, and *z* patterns; rescaled; converted to DAC values; and written out to temporary files shapedgradient_x, shapedgradient_y, and shapedgradient_z in the user's shapelib directory; and set with their corresponding shapedgradient statements. If an axis does not have a pattern, use empty quotes ("") to indicate a null pattern. The patterns *must* have the same number of points, or an integral multiple number of points.

The pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: pat1, pat2, pat3 are names of gradient shapes. (Note that the VNMR 5.1 and 5.2 software releases used only one pattern in the argument list.)

width is the length of the gradient, in seconds.

lvl1, lvl2, lvl3 are gradient values, in gauss/cm.

psi is an Euler angle, in degrees, with a range of -90 to +90.

phi is an Euler angle, in degrees, with the range -180 to +180.

theta is an Euler angle, in degrees, with the range -90 to +90.

loops is the number of times, from 1 to 255, to loop the waveform.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to stop until the gradient has completed before executing the next statement.

WAIT or NOWAIT adds extra pulse sequence programming flexibility for imaging experiments. It allows performing other pulse sequence events during the gradient pulse. Because oblique_shapedgradient "talks" to the *x*, *y*, and *z* gradient axes, NOWAIT cannot be used to produce simultaneous oblique gradient pulses, even if they are orthogonal. In the following example,

oblique_shapedgradient(patx,tdelta,gdiff,0.0,0.0, \
 0.0,0.0,0.0, 1,NOWAIT);

oblique_shapedgradient(paty,tdelta 0.0,gdiff,0.0 \
 0.0,0.0,0.0, 1,NOWAIT);

oblique_shapedgradient(patz,tdelta,0.0,0.0,gdiff, \
 0.0,0.0,0.0, 1,WAIT);

the first two function calls set up all three gradients. In both cases, after a few microseconds, the gradient hardware is reset by the third function call, which is the only call fully executed. Even though the third call is executed, expect negative side-effects from the first two "suppressed" calls.

Examples: oblique_shapedgradient("ramp_hold","","",trise, \
 gvox1,0,0,vpsi,vphi,vtheta,1,NOWAIT);

Related: obl_shapedgradient Execute a shaped oblique gradient

obsblank Blank amplifier associated with observe transmitter

Syntax: obsblank()

Description:	Disables the amplifier for the observe transmitter. This statement is generally used after a call to obsunblank.	
Related:	decunblank obsunblank rcvroff rcvron	Unblank amplifier associated with first decoupler Unblank amplifier associated with observe transmitter Turn off receiver Turn on receiver
obsoffset	Change offset	frequency of observe transmitter
Syntax:	obsoffset(f double frequ	
Description:	Changes the offset frequency, in Hz, of the observe transmitter (parameter tof). It is functionally the same as offset (frequency, OBSch).	
	10 to 30 µs	s with rf types A or B, the frequency typically changes between , but 100 μ s is automatically inserted into the sequence by the atement so that the time duration of offset is constant and not dependent.
	synthesizer	s with rf type C, which necessarily have PTS frequency s, the frequency shift time is $15.05 \mu s$ for standard, non-latching s and $21.5 \mu s$ for the latching synthesizers with the overrange/ e option.
	μs (latching the sequenc automatical	s with rf type D (UNITY <i>plus</i>), the frequency shift time is 14.95 g with or without over-range). No 100- μ s delay is inserted into e by the offset statement. Offset frequencies are not returned ly to their "normal" values before acquisition; this must be done is in the example below.
	• For the UNITY <i>INOVA</i> , the frequency shift is $4 \mu s$.	
	 For the MERCURY-VX and MERCURY, this statement inserts a 86.4-μs delay, although the actual switching of the frequency takes 1 μs. 	
	• For the <i>GEMINI 2000</i> (rf types F or E): on broadband systems, only the decoupler can be shifted (8.6 μ s); on ¹ H/ ¹³ C systems, observe (6.48 μ s), decoupler (8.6 μ s), and homodecoupler (8.6 μ s) can be set.	
	statements	s with the Output board (and only those systems), all offset by default are preceded internally by a 0.2-µs delay (see the le statement for more details).
Arguments:	frequency is	the offset frequency desired for the observe channel.
Examples:	obsoffset(t	co);
Related:	decoffset dec2offset dec3offset offset	Change offset frequency of first decoupler Change offset frequency of second decoupler Change offset frequency of third decoupler Change offset frequency of transmitter or decoupler
obspower	Change obser	ve transmitter power level, lin. amp. systems
Applicability:	Systems with lin	near amplifiers.
Syntax:	obspower(po double power	
Description:	Changes observ rlpower(val	e transmitter power. This statement is functionally the same as .ue, OBSch).

Arguments: power sets the power level by assuming values from 0 (minimum power) to 63 (maximum power) on channels with a 63-dB attenuator or from -16 (minimum power) to 63 (maximum power) on channels with a 79-dB attenuator.

CAUTION: On systems with linear amplifiers, be careful when using values of obspower greater than 49 (about 2 watts). Performing continuous decoupling or long pulses at power levels greater than this can result in damage to the probe. Use config to set a safety maximum for the tpwr, dpwr, dpwr2, and dpwr3 parameters.

Related:	decpower	Change first decoupler power, linear amplifier systems
	dec2power	Change second decoupler power, linear amplifier systems
	dec3power	Change third decoupler power, linear amplifier systems
	rlpower	Change power level, linear amplifier systems

obsprgoff End programmable control of observe transmitter

Applicability: Systems with a waveform generator on the observe transmitter channel.

Syntax: obsprgoff()

- Description: Terminates any programmable phase and amplitude control on the observe transmitter started by the obsprgon statement under waveform generator control.
 - Related: obsprgon Start programmable control of observe transmitter

obsprgon

Applicability: Systems with a waveform generator on the observe transmitter channel.

Start programmable control of observe transmitter

Syntax: obsprgon(pattern,90 pulselength,tipangle resoln) /* name of .DEC text file */ char *pattern; double 90_pulselength; /* 90-deg pulse length, in sec */ double tipangle_resoln; /* tip-angle resolution */ Description: Executes programmable phase and amplitude control on the observe transmitter under waveform generator control. It returns the number of 50-ns ticks (as an integer value) in one cycle of the decoupling pattern. Explicit gating of the observe transmitter with xmtron and xmtroff is generally required. Arguments can be variables (which requires appropriate getval and getstr statements) to permit changes via parameters (see second example below). Arguments: pattern is the name of the text file (without the .DEC file suffix) in the shapelib directory that stores the decoupling pattern. 90 pulselength is the pulse duration, in seconds, for a 90° tip angle on the observe transmitter. tipangle_resoln is the resolution in tip-angle degrees to which the decoupling pattern is stored in the waveform generator. Examples: obsprgon("waltz16",pw90,90.0); obsprgon("modulation",pp90,dres); Related: decprgon Start programmable decoupling on first decoupler dec2prgon Start programmable decoupling on second decoupler End programmable control of observe transmitter obsprqoff

obspulse Pulse observe transmitter with amplifier gating

Syntax: obspulse()

Description:	A special case of the rgpulse (width, phase, RG1, RG2) statement, in which width is preset to pw and phase is preset to oph. Thus, obspulse is exactly equivalent to rgpulse (pw, oph, rof1, rof2). Note that obspulse has nothing whatsoever to do with data acquisition, despite its name. Except in special cases, data acquisition begins at the end of the pulse sequence.	
Related:	iobspulse ipulse irgpulse pulse rgpulse simpulse sim3pulse	Pulse observe transmitter with IPA Pulse observe transmitter with IPA Pulse observe transmitter with IPA Pulse observe transmitter with amplifier gating Pulse observe transmitter with amplifier gating Pulse observe, decoupler channels simultaneously Simultaneous pulse on 2 or 3 rf channels
obspwrf	Set observe tr	ansmitter fine power
Applicability:	Systems with fine power control. Not available on <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> systems.	
Syntax:	: obspwrf(power) double power; /* new fine power level for OBSch */	
Description:	: Changes observe transmitter fine power. This statement is functionally the same as rlpwrf (value, OBSch).	
Arguments:	value is the fi	ne power desired.
Examples:	obspwrf(4.0));
Related:	decpwrf dec2pwrf dec3pwrf rlpwrf	Set first decoupler fine power Set second decoupler fine power Set third decoupler fine power Set transmitter or decoupler fine power
obsstepsize	Set step size f	or observe transmitter
Applicability:	All systems except the <i>GEMINI 2000</i> .	
	<pre>obsstepsize(step_size) double step_size; /* small-angle phase step size */</pre>	
Description:	Sets the step size of the observe transmitter. This statement is functionally the same as <pre>stepsize(base,OBSch).</pre>	
Arguments:	step_size is	the phase step size desired and is a real number or a variable.
Examples:	obsstepsize	e(30.0);
Related:	decstepsize dec2stepsize dec3stepsize stepsize	· ·
obsunblank	Unblank amplifier associated with observe transmitter	
Syntax:	obsunblank	()
Description:		es the amplifier for the observe transmitter. obsunblank is ved by a call to obsblank.
Related:	decblank decunblank	Blank amplifier associated with first decoupler Unblank amplifier associated with first decoupler

obsblank	Blank amplifier associated with observe transmitter
rcvroff	Turn off receiver
rcvron	Turn on receiver

offset	Change offset frequency of transmitter or decoupler	
Applicability:	This statement will be eliminated in future versions of VNMR software. Although it is still functional, you should not write any new pulse sequences using it and should replace it in existing sequences with obsoffset, decoffset, dec2offset, or dec3offset, as appropriate.	
Syntax:	offset(frequency,device) double frequency; /* frequency offset */ int device; /* OBSch, DECch, DEC2ch, or DEC3ch */	
Description:	Changes the offset frequency of the observe transmitter (parameter tof), first decoupler (dof), second decoupler ($dof2$), or third decoupler ($dof3$).	
Arguments:	frequency is the offset frequency desired.	
	device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY <i>INOVA</i> and UNITY <i>plus</i> only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).	
Examples:	<pre>offset(do2,DECch); offset(to2,OBSch); delay(d2); offset(tof,OBSch);</pre>	
Related:	decoffsetChange offset frequency of first decouplerdec2offsetChange offset frequency of second decouplerdec3offsetChange offset frequency of third decouplerobsoffsetChange offset frequency of observe transmitterioffsetChange offset frequency with IPA	

Ρ

pe_gradient Applicability:	Oblique gradient with phase encode in one axis Not applicable on <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> .	
Syntax:	<pre>pe_gradient(stat1,stat2,stat3,step2,vmult2) double stat1,stat2,stat3; /* static gradient components */ double step2; /* variable gradient stepsize */ codeint vmult2; /* real-time math variable */</pre>	
Description:	Sets static oblique gradient levels plus one oblique phase encode gradient. The phase encode gradient is associated with the second axis of the logical frame. This corresponds to the convention read, phase, slice for the functions of the logical frame axes. This statement is the same as phase_encode_gradient except the Euler angles are read from the default set for imaging. lim2 is automatically set to half the nv (number of views) where nv is usually the number of phase encode steps.	
	Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.	

Arguments:	stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.			
	step2 is the value, in gauss/cm, of the component for the step size change in the variable portion of the gradient.			
	vmult2 is a real-time math variable (v1 to v14, ct, zero, one, two, three) or reference to AP tables (t1 to t60), whose associated values vary dynamically in a manner controlled by the user.			
Examples:	<pre>pe_gradient(0.0,-sgpe*nv/2.0,gss,sgpe,v6);</pre>			
Related:	phase_encode_gradient Oblique gradient with phase encode in 1 axis			
pe2_gradient	Oblique gradient with phase encode in two axes			
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.			
Syntax:	<pre>pe2_gradient(stat1,stat2,stat3,step2,step3, \ vmult2,vmult3)</pre>			
	<pre>double stat1,stat2,stat3; /* static gradient components */ double step2,step3; /* variable gradient stepsize */ codeint vmult2,vmult /* real-time math variables */</pre>			
Description:	Sets only two oblique phase encode gradients; otherwise, pe2_gradient is the same as pe3_gradient.			
	Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.			
Arguments:	stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.			
	step2, step3 are values, in gauss/cm, of the components for the step size change in the variable portion of the gradient.			
	vmult2, vmult3 are real-time math variables (v1 to v14, ct, zero, one, two, three) or references to AP tables (t1 to t60), whose associated values vary dynamically in a manner controlled by the user.			
Examples:	<pre>pe2_gradient(gro,sgpe*nv/2.0,sgpe2*nv2/2.0,sgpe, \ sgpe2,v6,v8);</pre>			
Related:	pe3_gradient Oblique gradient with phase encode in 3 axes			
pe3_gradient	Oblique gradient with phase encode in three axes			
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.			
Syntax:	<pre>pe3_gradient(stat1,stat2,stat3,step1,step2, \</pre>			
	<pre>step3,vmult1,vmult2,vmult3) double stat1,stat2,stat3; /* static gradient components */ double step1,step2,step3; /* gradient step sizes */ codeint vmult1,vmult2,vmult3; /* real-time variables */</pre>			
Description:	Sets three oblique phase encode gradients. This statement is the same as phase_encode3_gradient except the Euler angles are read from the default set for imaging. lim1, lim2, and lim3 are set to nv/2, nv2/2, and nv3/2, respectively.			

Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.

step1, step2, step3 are values, in gauss/cm, of the components for the step size change in the variable portion of the gradient.

vmult1, vmult2, vmult3 are real-time math variables (v1 to v14, ct, zero, one, two, three) or references to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user.

Related: phase_encode3_gradient Oblique gradient with phase encode in 3 axes

pe_shapedgradient Oblique shaped gradient with phase encode in one axis

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.

Description: Sets a static oblique shaped gradient plus one oblique phase encode shaped gradient. This is same as phase_encode_shapedgradient except in pe_shapedgradient the Euler angles are read from the default set for imaging. lim2 is automatically set to nv/2, where nv is usually the number of phase encode steps.

Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: pattern is the name of a gradient shape file.

width is the length, in seconds, of the gradient.

stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.

step2 is the value, in gauss/cm, of the component for the step size change in the variable portion of the gradient.

vmult2 is a real-time math variable (v1 to v14, ct, zero, one, two, three) or reference to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient has completed before executing the next statement.

tag is a unique integer that "tags" the gradient element from any other gradient elements used in the sequence. These tags are used for variable amplitude pulses.

Related: phase_encode_shapedgradient Oblique shaped gradient with PE on 1 axis

pe2_shapedgradient Oblique shaped gradient with phase encode in two axes

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax:	pe2_shapedgradient(patt	cern,width,stat1,stat2, \
	<pre>stat3,step2,step3,vmu</pre>	ult2,vmult3)
	char *pattern;	<pre>/* name of gradient shape file */</pre>
	double width;	/* length of gradient in sec */
	<pre>double stat1,stat2,stat3;</pre>	/* static gradient components */
	double step2,step3;	/* variable gradient step size */
	<pre>codeint vmult2,vmult3;</pre>	/* real-time math variables */

Description: Sets two oblique phase encode shaped gradients; otherwise, this statement is the same as pe3_shapedgradient.

Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: pattern is the name of a gradient shape file.

width is the length, in seconds, of the gradient.

stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.

step2, step3 are values, in gauss/cm, of the components for the step size change in the variable portion of the gradient.

vmult2, vmult3 are real-time math variables (v1 to v14, ct, zero, one, two, three) or references to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user.

Related: pe3_shapedgradient Oblique shaped gradient with phase encode in 3 axes

pe3_shapedgradient Oblique shaped gradient with phase encode in three axes

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax: pe3_shapedgradient(pattern,width,stat1,stat2, \
 stat3,step1,step2,step3,vmult1,vmult2,vmult3)
 char *pattern; /* name of gradient shape file */
 double width; /* width of gradient in sec */
 double stat1,stat2,stat3; /* static gradient components */
 double step1,step2,step3; /* var. gradient components */
 codeint vmult1,vmult2,vmult3; /* real-time variables */

Description: Sets three oblique phase encode shaped gradients. This statement is the same as the statement phase_encode3_shapedgradient except the Euler angles are read from the default set for imaging. The lim1, lim2, and lim3 arguments in phase_encode3_shapedgradient are set to nv/2, nv2/2, and nv3/2, respectively.

Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: pattern is the name of a gradient shape file.

width is the length, in seconds, of the gradient.

stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.

step1, step2, step3 are values, in gauss/cm, of the components for the step size change in the variable portion of the gradient.

vmult1, vmult2, vmult3 are real-time math variables (v1 to v14, ct, zero, one, two, three) or references to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user.

Related: phase_encode3_shapedgradient Oblique sh. gradient with PE on 3 axes

peloop	Phase-encode loop	
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>peloop(state,max_count,apvl,apv2) char state;</pre>	
Description:	Provides a sequence-switchable loop that can use real-time variables in what is known as a compressed loop, or it can use the standard arrayed features of PSG. In the imaging sequences it uses the third character of the seqcon string parameter seqcon[2] for the state argument. The statement is used in conjunction with the endpeloop statement.	
	peloop differs from msloop in how it sets the apv2 variable in standard arrayed mode (state is 's'). In standard arrayed mode, apv2 is set to nth2D-1 if max_count is greater than zero. nth2D is a PSG internal counting variable for the second dimension. When in the compressed mode, apv2 counts from zero to max_count-1.	
Arguments:	state is either 'c' to designate the compressed mode, or 's' to designate the standard arrayed mode.	
	apv1 is a real-time variable that holds the maximum count.	
	apv2 is a real-time variable that holds the current counter value. If state is 's' and max_count is greater than zero, apv2 is set to nth2D-1; otherwise, it is set to zero.	
Examples:	<pre>: peloop(seqcon[2],nv,v5,v6); msloop(seqcon[1],nv,v11,v12);</pre>	
	<pre> poffset_list(pss,gss,ns,v12):</pre>	
	<pre> pe_gradient(gror,-0.5*sgpe*nv,gssr,sgpe,v6);</pre>	
	acquire(np,1.0/sw);	
	<pre>endmsloop(seqcon[1],v12); endpeloop(seqcon{2},v6;</pre>	
Related:	endpeloopEnd phase-encode looploopStart loopmsloopMultislice loop	
phase_encode_	gradient Oblique gradient with phase encode in one axis	
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>phase_encode_gradient(stat1,stat2,stat3,step2, \ vmult2,lim2,ang1, ang2, ang3) double stat1,stat2,stat3; /* static gradient components */ double step2; /* variable gradient stepsize */ codeint vmult2; /* real-time math variable */ double lim2; /* max. gradient value step */ double ang1,ang2,ang3; /* Euler angles in degrees */ Sate static shlippe and ient levels also are ablieve sheep area do and ient The</pre>	

Description: Sets static oblique gradient levels plus one oblique phase encode gradient. The phase encode gradient is associated with the second axis of the logical frame.

This corresponds to the convention: read, phase, slice for the functions of the logical frame axes. It has no return value.

Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.

step2 is the value, in gauss/cm, of the component for the step size change in the variable portion of the gradient.

vmult2 is a real-time math variable (v1-v14, ct, zero, one, two, three) or reference to AP tables (t1 to t60), whose associated values vary dynamically in a manner controlled by the user.

lim2 is a value representing the dynamic step that will generate the maximum gradient value for each component. This provides error checking in pulse sequence generation and is normally nv/2.

angl is Euler angle psi, in degrees, with the range -90 to +90.

ang 2 is Euler angle phi, in degrees, with the range -180 to +180.

ang 3 is Euler angle theta, in degrees, with the range -90 to +90.

Related:	oblique_gradient	Execute an oblique gradient
	oblique_shapedgradient	Execute a shaped oblique gradient
	pe_gradient	Oblique gradient with PE on 1 axis
	phase_encode_shapedgradient	Oblique sh. gradient with PE on 1 axis
	phase_encode3_gradient	Oblique gradient with PE on 3 axes
	phase_encode3_shapedgradient	Oblique sh. gradient with PE on 3 axes
	phase_encode_shapedgradient phase_encode3_gradient	Oblique sh. gradient with PE on 1 axis Oblique gradient with PE on 3 axes

phase_encode3_gradient Oblique gradient with phase encode in three axes

Applicability: Not applicable on MERCURY, MERCURY-VX, and GEMINI 2000.

Syntax:	phase_encode3_gradient(s	stat1,stat2,stat3, \
	<pre>step1,step2,step3,vmul</pre>	t1,vmult2,vmult3, \
	lim1,lim2,lim3,ang1,an	ng2,ang3)
	<pre>double stat1,stat2,stat3;</pre>	<pre>/* static gradient components */</pre>
	<pre>double step1,step2,step3;</pre>	/* var. gradient stepsize */
	codeint vmult1,vmult2,vmult	t3; /* real-time variables */
	<pre>double lim1,lim2,lim3;</pre>	/* max. gradient value steps */
	<pre>double ang1,ang2,ang3;</pre>	/* Euler angles in degrees */

Description: Sets three oblique phase encode gradients. It has no return value.

Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved.

Arguments: stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame.

step1, step2, step3 are values, in gauss/cm, of the components for the step size change in the variable portion of the gradient.

vmult1, vmult2, vmult3 are real-time math variables (v1 to v14, ct, zero, one, two, three) or references to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user.

lim1, lim2, lim3 are values representing the dynamic step that will generate the maximum gradient value for each component. This provides error checking in pulse sequence generation and is normally nv/2.

ang1 is Euler angle psi, in degrees, with the range -90 to +90. ang2 is Euler angle phi, in degrees, with the range -180 to +180. ang3 is Euler angle theta, in degrees, with the range -90 to +90. Examples: phase_encode3_gradient(0,0,0,0,0,2.0*gcrush/ne, \ zero,zero,v12,0,0,0,psi,phi,theta); Related: pe3_gradient Oblique gradient with PE in 3 axes phase_encode_shapedgradient Oblique sh. gradient with PE on 1 axis phase_encode3_shapedgradient Oblique sh. gradient with PE on 3 axes

phase_encode_shapedgradient Oblique shaped gradient with PE in one axis

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000. Syntax: phase_encode_shapedgradient(pattern,width, \ stat1,stat2,stat3,step2,vmult2,lim2, ang1,ang2,ang3,vloops,wait,tag) /* name of gradient shape file */ char *pattern; double width; /* width of gradient in sec */ double stat1,stat2,stat3; /* static gradient components */ double step2; /* var. gradient step size */ /* real-time math variable */ codeint vmult2; double lim2; /* max. gradient value steps */ double ang1,ang2,ang3; /* Euler angles in degrees */ /* number of loops */ codeint vloops; /* WAIT or NOWAIT */ int wait; int tag; /* tag to a gradient element */ Description: Sets static oblique shaped gradients plus one oblique phase encode shaped gradient. The phase encode gradient is associated with the second axis of the logical frame. This corresponds to the convention: read, phase, slice for the functions of the logical frame axes. One gradient shape is used for all three axes. It has no return value. Pulse sequence generation aborts if the DACs on a particular gradient are overrun after the angles and amplitude have been resolved. Arguments: pattern is the name of a gradient shape file. width is the length, in seconds, of the gradient. stat1, stat2, stat3 are values, in gauss/cm, of the components for the static portion of the gradient in the logical reference frame. step2 is the value, in gauss/cm, of the component for the step size change in the variable portion of the gradient. vmult2 is a real-time math variable (v1 to v14, ct, zero, one, two, three) or reference to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user. lim2 is the value representing the dynamic step that will generate the maximum gradient value for the component. This provides error checking in pulse sequence generation and is normally nv/2. angl is the Euler angle psi, in degrees, with the range of -90 to +90. ang 2 is the Euler angle phi, in degrees, with the range of -180 to +180. ang 3 is the Euler angle theta, in degrees, with the range of -90 to +90.

vloops is a real-time math variable (vl to vl4, ct, zero, one, two, three) or references to AP tables (tl to t60) that dynamically sets the number of times to loop the waveform.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient has completed before executing the next statement.

tag is a unique integer that "tags" the gradient element from any other gradient elements used in the sequence. These tags are used for variable amplitude pulses.

Related:	oblique_gradient	Execute an oblique gradient
	oblique_shapedgradient	Execute a shaped oblique gradient
	pe_shapedgradient	Oblique sh. gradient with PE in 1 axis
	phase_encode3_shapedgradient	Oblique sh. gradient with PE on 3 axes

phase_encode3_shapedgradient Oblique shaped gradient with PE in three axes

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.

```
Syntax: phase_encode3_shapedgradient(pattern,width,
                                                                    \backslash
              stat1,stat2,stat3,step1,step2,step3,
              vmult1,vmult2,vmult3,lim1,lim2,lim3,
                                                              \backslash
              ang1,ang2,ang3,loops,wait)
                                /* name of gradient shape file */
/* ...
            char *pattern;
            double width;
                                         /* width of gradient in sec */
           double stat1,stat2,stat3; /* static gradient components */
double step1,step2,step3; /* var. gradient step sizes */
            codeint vmult1,vmult2,vmult3; /* real-time variables */
           /* Euler angles in degrees */
           double ang1,ang2,ang3;
                                         /* number of times to loop */
            int loops;
            int wait;
                                         /* WAIT or NOWAIT */
Description: Sets three oblique phase encode shaped gradient. Note that this statement has a
            loops argument that is an integer, as opposed to the vloops argument in
           phase_encode_shapedgradient. It has no return value.
            Pulse sequence generation aborts if the DACs on a particular gradient are
            overrun after the angles and amplitude have been resolved.
Arguments: pattern is the name of the gradient shape file.
            width is the length, in seconds, of the gradient.
            stat1, stat2, stat3 are values, in gauss/cm, of the components for the
            static portion of the gradient in the logical reference frame.
```

step1, step2, step3 are values, in gauss/cm, of the components for the step size change in the variable portion of the gradient.

vmult1, vmult2, vmult3 are real-time math variables (v1 to v14, ct, zero, one, two, three) or references to AP tables (t1 to t60) whose associated values vary dynamically in a manner controlled by the user.

lim1, lim2, lim3 are values representing the dynamic step that will generate the maximum gradient value for each component. This provides error checking in pulse sequence generation and is normally nv/2.

angl is the Euler angle psi, in degrees, with the range of -90 to +90.

ang 2 is the Euler angle phi, in degrees, with the range of -180 to +180.

ang 3 is the Euler angle theta, in degrees, with the range of -90 to +90.

loops is non-real-time integer value, from 1 to 255, that sets the number of times to loop the waveform.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient has completed before executing the next statement.

Related:	pe3_shapedgradient	Oblique sh. gradient with PE in 3 axes
	phase_encode_shapedgradient	Oblique sh. gradient with PE on 1 axis
	phase_encode3_gradient	Oblique gradient with PE in 3 axes

phaseshift Set phase-pulse technique, rf type A or B

Applicability: Systems with rf type A or B (MERCURY-VX, MERCURY, and GEMINI 2000 systems are rf type E or F).

Syntax:	phaseshift(base,mult	ipl	ier,device)
	double base;	/*	<pre>base small-angle phase shift */</pre>
	codeint multiplier;	/*	real-time variable */
	int device;	/*	channel, TODEV or DODEV */
anintian	Implements the "phase pulse"	taal	hnique

- Description: Implements the "phase-pulse" technique.
- Arguments: base is a real number, expression, or variable representing the base phase shift in degrees. Any value is acceptable.

multiplier is a real-time variable (v1 to v14, ct, etc.). The value must be positive. The actual phase shift is ((base*multiplier)mod360).

device is TODEV (observe transmitter) or DODEV (first decoupler).

Examples: phaseshift(60.0,ct,TODEV); phaseshift(-30.0,v1,DODEV);

poffset

Set frequency based on position

Applicability:	Not applicable on <i>MERCURY</i>	-VX, MERCURY, and GEMINI 2000.
Syntax:	<pre>poffset(position,lev</pre>	rel)
	double position;	/* slice position in cm */
	double level;	/* gradient level in G/cm */
Description:	Sets the rf frequency from pos	ition and conjugate gradient values. poffs

set is functionally the same as position_offset except that poffset takes the value of resfrq from the resto parameter and always assumes the device is the observe transmitter device TODEV.

Arguments: position is the slice position, in cm.

level is the gradient level, in gauss/cm, used in the slice selection process.

Examples: poffset(pss[0],gss);

Related: position_offset Set frequency based on position

poffset list Set frequency from position list

Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax: poffset_list(posarray,grad,nslices,apv1) double position_array[]; /* position values in cm */ double level; /* gradient level in G/cm */ /* number of slices */ double nslices;

Chapter 3. Pulse Sequence Statement Reference -

	codeint vi;	<pre>/* variable or AP table */</pre>
Description:	Sets the rf frequency from a position list, conjugate gradient value, and dynamic math selector. poffset_list is functionally the same as position_offset_list except that poffset_list takes the value of resfrq from the resto parameter, assumes the device is the observe transmitter device OBSch, and assumes that the list number is zero.	
Arguments: position_array is a list of position values, in cm.		of position values, in cm.
	level is the gradient level,	in gauss/cm, used in the slice selection process.
	nslices is the number of s	lices or position values.
	vi is a dynamic real-time va	riable (v1 to v14) or AP table (t1 to t60).
Examples:	<pre>poffset_list(pss,gss,ns,v8);</pre>	
Related:	getarray position_offset_list	Retrieves all values of an arrayed parameter Set frequency from position list

position_offset Set frequency based on position

Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>position_offset(pos,grad,resfrq,device) double pos;</pre>	
Description:	Sets the rf frequency from position and conjugate gradient values. It has no return value.	
Arguments:	pos is the slice position, in cm.	
	grad is the gradient level, in gauss/cm, used in the slice selection process.	
	resfrq is the resonance offset value, in Hz, for the nucleus of interest.	
	device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY <i>INOVA</i> and UNITY <i>plus</i> only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).	
Examples:	<pre>position_offset(posl,gvox1,resto,OBSch);</pre>	
Related:	poffsetSet frequency based on positionposition_offset_listSet frequency from position list	

position_offset_listSet frequency from position list

Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.								
Syntax:	$position_offset_list(posarray,grad,nslices, \setminus$								
	resfrq,device,list	resfrq,device,list_number,apv1)							
	double posarray[];	/* position values in cm */							
	double level; /* gradient level in G/cm */								
	double nslices; /* number of slices */								
	double resfrq; /* resonance offset in Hz */								
	int device;	int device; /* OBSch, DECch, DEC2ch, or DEC3ch */							
	<pre>int list_number; /* number for global list */</pre>								
	codeint vi; /* real-time variable or AP table *								
Description:	Sets the rf frequency from a po	sition list, conjugate gradient value, and dynamic							

Description: Sets the rf frequency from a position list, conjugate gradient value, and dynamic math selector. The dynamic math selector (apv1) holds the index for required slice offset value as stored in the array. The arrays provided to this statement

must count zero up; that is, array[0] must have the first slice position and array[ns-1] the last. It has no return value.

Arguments: position_array is a list of position values, in cm.

level is the gradient level, in gauss/cm, used in the slice selection process.

nslices is the number of slices or position values.

resfrq is the resonance offset, in Hz, for the nucleus of interest.

device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

list_number is a value for identifying a global list. The first global list must begin at zero and each created list must be incremented by one.

vi is a dynamic real-time variable (v1 to v14) or AP table (t1 to t60).

Related:	getarray	Retrieves all values of an arrayed parameter
	<pre>poffset_list</pre>	Set frequency from position list
	position_offset	Set frequency based on position

Change power level, linear amplifier systems

- Applicability: Systems with linear amplifiers. Not available on *GEMINI 2000* systems. Use of statements obspower, decpower, dec2power, or dec3power, as appropriate, is preferred.
- Description: Changes transmitter or decoupler power by assuming values of 0 (minimum power) to 63 (maximum power) on channels with a 63-dB attenuator or -16 (minimum power) to 63 (maximum power) on channels with a 79-dB attenuator. On systems with an Output board, by default, power statements are preceded internally by a 0.2-µs delay (see the apovrride statement for more details).
- Arguments: power is the power desired. It must be stored in a real-time variable (v1-v14, etc.), which means it cannot be placed directly in the power statement. This allows the power to be changed in real-time or from pulse to pulse. Setting the power argument is most commonly done using initval (see example below). To avoid consuming a real-time variable, use the rlpower statement instead of the power statement.

device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

CAUTION: On systems with linear amplifiers, be careful when using values of power greater than 49 (about 2 watts). Performing continuous decoupling or long pulses at power levels greater than this can result in damage to the probe. Use config to set a safety maximum for the tpwr, dpwr, dpwr2, and dpwr3 parameters.

Examples: pulsesequence()
 {
 double newpwr;
 newpwr=getval("newpwr");
 initval(newpwr,v2);

power

	power(v2,OE	3Sch);
	···· }	
Related:	} decpower dec2power initval obspower pwrf rlpower rlpwrf	Change first decoupler power, linear amplifier systems Change second decoupler power, linear amplifier systems Change third decoupler power, linear amplifier systems Initialize a real-time variable to a specified value Change observe transmitter power, linear amplifier systems Change transmitter or decoupler fine power Change transmitter or decoupler power, linear amplifier Set transmitter or decoupler fine power
pulse	Pulse observe	transmitter with amplifier gating
Syntax:		n,phase) ; /* pulse length in sec */
Description:	statement, but w respectively. Th	e the same as the rgpulse(width, phase, RG1, RG2) with RG1 and RG2 set to the parameters rof1 and rof2, us, pulse is a special case of rgpulse where the "hidden" 1 and rof2 remain "hidden."
Arguments:	width specifie	s the width of the observe transmitter pulse.
	phase sets the	phase and must be a real-time variable.
Examples:	pulse(pw,v2	2);
Related:	dps_show obspulse ipulse irgpulse obspulse rgpulse simpulse sim3pulse	Draw delay or pulses in a sequence for graphical display Pulse observe transmitter with IPA Pulse observe transmitter with IPA Pulse observe transmitter with IPA Pulse observe transmitter with amplifier gating Pulse observe transmitter with amplifier gating Pulse observe, decoupler channels simultaneously Simultaneous pulse on 2 or 3 rf channels
pwrf	Change transr	nitter or decoupler fine power
Applicability:	-	ne attenuators. Not available on MERCURY-VX, MERCURY,
Syntax:	<pre>pwrf(power, int power; int device;</pre>	<pre>device) /* new value for fine power control */ /* OBSch, DECch, DEC2ch, or DEC3ch */</pre>
Description:	-	e power of the device specified by adjusting the optional fine not execute pwrf and ipwrf together because they will cancel act.
Arguments:	etc.), which mea	ne power desired. It must be a real-time variable (v1 to v14, ans it cannot be placed directly in the pwrf statement. It can 4095 (60 dB on UNITY <i>INOVA</i> and UNITY <i>plus</i> , about 6 dB on
	UNITY INOVA and	Sch (observe transmitter) or DECch (first decoupler). On the UNITY <i>plus</i> only, device can also be DEC2ch (second EC3ch (third decoupler).

Examples: pwrf(v1,OBSch);

Related:	ipwrf	Change transmitter or decoupler fine power
	power	Change transmitter or decoupler power, linear amp. system
	rlpwrf	Set transmitter or decoupler fine power

pwrm	Change transmitter or decoupler linear modulator power						
Applicability:	UNITY INOVA and UNITY plus systems only. Use of statements obspwrf, decpwrf, dec2pwrf, or dec3pwrf, as appropriate, is preferred.						
Syntax:	<pre>pwrm(power,device) int power;</pre>						
Description:	optional fine atte	Changes the linear modulator power of the device specified by adjusting the optional fine attenuators. Do not execute pwrm and <u>ipwrm</u> together because they will cancel each other's effect.					
Arguments:	power is the linear modulator power desired. It must be a real-time variable (v1 to v14, etc.), which means the power level as an integer cannot be placed directly in the pwrm statement. power can range from 0 to 4095 (60 dB on UNITY <i>INOVA</i> and UNITY <i>plus</i> , about 6 dB on UNITY systems).						
	device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY <i>INOVA</i> and UNITY <i>plus</i> only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).						
Examples:	pwrm(v1,OBS	Sch);					
Related:	decpwrf dec2pwrf dec3pwrf ipwrf ipwrm obspwrf rlpwrm	Set first decoupler fine power Set second decoupler fine power Set third decoupler fine power Change transmitter or decoupler fine power with IPA Change transmitter or decoupler linear modulator power Set observe transmitter fine power Set transmitter or decoupler linear modulator power					

R

rcvroff Turn off receiver gate and amplifier blanking gate

Syntax: rcvroff()

Description: On UNITY INOVA and GEMINI 2000 systems, the receiver is normally off during the pulse sequence and iis turned on only during acquisition. On other systems, rcvroff provides explicit receiver gating in the pulse sequence. The rcvroff statement also unblanks, or enables, the observe transmitter.

Receiver gating is normally controlled automatically by decpulse, decrgpulse, dec2rgpulse, dec3rgpulse, obspulse, pulse, and rgpulse. At the end of each of these statements, the receiver is automatically turned back on *if and only if the receiver has not been previously turned off* *explicitly by a* rcvroff *statement*. In all cases, the receiver is implicitly turned back on immediately prior to data acquisition.

Related:	rcvron	Turn on receiver gate and amplifier blanking gate
	recoff	Turn off receiver only
	recon	Turn on receiver only

 rcvron
 Turn on receiver gate and amplifier blanking gate

 Syntax:
 rcvron()

Description: On UNITY INOVA and GEMINI 2000 systems, the receiver is normally off during the pulse sequence. It is turned on only during acquisition. On other systems, rcvron provides explicit receiver gating in the pulse sequence. The rcvron statement also blanks, or disables, the observe transmitter

> Receiver gating is normally controlled automatically by obspulse, pulse, and rgpulse on UNITYplus, and UNITY systems, and by decpulse, decrgpulse, dec2rgpulse, and dec3rgpulse on UNITY systems. At the end of each of these statements, the receiver is automatically turned back on *if and only if the receiver has not been previously turned off explicitly by a* rcvroff *statement*. In all cases, the receiver is implicitly turned back on immediately prior to data acquisition.

Related:	rcvroff	Turn off receiver gate and amplifier blanking gate
	recoff	Turn off receiver gate only
	recon	Turn on receiver gate only

readuserap

Read input from user AP register

Applicability: UNITY INOVA systems.

Description: Reads input from user AP bus register 3 to a real-time variable. The user can then act on this information using real-time math and real time control statements while the pulse sequence is running. Register 3 is lines 1 to 8 of the USER AP connector J8212 on the Breakout panel on the rear of the left console cabinet. This register interfaces to a bidirectional TTL-compatible 8-bit buffer, which has a 100-ohm series resistor for circuit protection.

readuserap stops parsing acodes (acquisition codes) until the lines in the buffer have been read and the value placed in to the specified real-time variable. In order for the parser to parse and stuff more words into the FIFO before underflowing, the readuserap statement puts in a 500 μ s delay after reading the input. However, depending on what is to be done after reading the lines, a longer delay may be needed to avoid FIFO underflow.

If an error occurs in reading, a warning message is sent to the host and a value of -1 is returned to the real-time variable.

Arguments: vi is a real-time variable (v1 to v14, etc.) that indexes a signed or unsigned number read from user AP register 3.

Examples: /* Check a value read in from input register and */
 /* execute a pulse if it is the expected value. */
 double testval;
 testval=getval(testval) /* set value to check */
 initval(testval,v2);
 loop(two,v1); /* reset below makes loop go */

```
readuserap(v1); /* until expected value reads in */
                       delay(d2);
                       sub(v1,v2,v3);
                       ifzero(v3);
                           pulse(pw,oph);
                           assign(one,v1);
                       elsenz(v3)
                                                            /*reset counter*/
                           assign(zero,v1);
                       endif(v3);
                   endloop(v1);
         Related:
                   setuserap
                                   Set user AP register
                   vsetuserap
                                   Set user AP register using real-time variable
recoff
                   Turn off receiver gate only
    Applicability: UNITY INOVA systems.
         Syntax: recoff()
     Description: On UNITY INOVA systems, receiver gating has been decoupled from amplifier
                   blanking. The recoff statement is similar to the rcvroff statement in that
                   it defaults the receiver off throughout the pulse sequence; however, unlike
                   rcvroff, the recoff statement only affects the receiver gate and does not
                   affect the amplifier blanking gate. In all cases, the receiver is turned off when
                   applying pulses and turned on during acquisition. The default state of the
                   receiver is off for UNITY INOVA systems (except for whole body systems and for
                   imaging pulses sequences that have the initparms sis statement at the
                   beginning).
                   initparms_sis
                                       Initialize parameters for spectroscopy imaging sequences
         Related:
                   rcvroff
                                       Turn off receiver gate and amplifier blanking gate
                   rcvron
                                       Turn on receiver gate and amplifier blanking gate
                                       Turn on receiver gate only
                   recon
                   Turn on receiver gate only
recon
                  UNITY INOVA systems.
    Applicability:
         Syntax: recon()
     Description: On UNITY INOVA systems, receiver gating has been decoupled from amplifier
                   blanking. The recoff statement is similar to the revron statement in that it
                   defaults the receiver on throughout the pulse sequence; however, unlike
                   rcvron, the recon statement only affects the receiver gate and does not affect
                   the amplifier blanking gate. In all cases, the receiver is turned off when applying
                   pulses and turned on during acquisition. The default state of the receiver is off
                   for UNITY INOVA systems (except for whole body systems and for imaging pulses
                   sequences that have the initparms_sis statement at the beginning).
         Related:
                   initparms_sis
                                       Initialize parameters for spectroscopy imaging sequences
                                       Turn off receiver gate and amplifier blanking gate
                   rcvroff
                                       Turn on receiver gate and amplifier blanking gate
                   rcvron
                   recoff
                                       Turn off receiver gate only
rgpulse
                   Pulse observe transmitter with amplifier gating
```

codeint phase;	/* real-time variable for phase */
double RG1;	/* gate delay before pulse in sec */
double RG2;	<pre>/* gate delay after pulse in sec */</pre>

Description: Pulses the observe transmitter with amplifier gating. The amplifier is gated on prior to the start of the pulse by RG1 sec and gated off RG2 sec after the end of the pulse. The total length of this event is therefore not simply width, but width+RG1+RG2.

The amplifier gating times RG1 and RG2 may be specified explicitly. The parameters rof1 and rof2 are often used for these times. These parameters are normally "hidden" parameters, not displayed on the screen and entered by the user. Their values can be interrogated by entering the name of the parameter followed by a question mark (e.g., rof1?).

Arguments: width specifies the duration, in seconds, of the observe transmitter pulse.

phase sets the observe transmitter phase and must be a real-time variable.

RG1 is the time, in seconds, the amplifier is gated on prior to the start of the pulse (typically 10 μ s for ¹H/¹⁹F, 40 μ s for other nuclei, and 2 μ s for the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*).

RG2 is the time, in seconds, before the amplifier is gated off after the end of the pulse (typically 10 μ s on the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*, and about 10 to 20 μ s on other systems).

Examples: rgpulse(pw,v1,rof1,rof2); rgpulse(2.0*pw,v2,1.0e-6,0.2e-6);

Related:	iobspulse	Pulse observe transmitter with IPA
	ipulse	Pulse observe transmitter with IPA
	irgpulse	Pulse observe transmitter with IPA
	obspulse	Pulse observe transmitter with amplifier gating
	pulse	Pulse observe transmitter with amplifier gating
	simpulse	Pulse observe, decoupler channels simultaneously
	sim3pulse	Simultaneous pulse on 2 or 3 rf channels

rgradient Set gradient to specified level

Applicability:	Systems with imaging or PFG modules.					
Syntax:	<pre>rgradient(channel) char channel; double value;</pre>	/* gradient 'x', 'y', or 'z' */				
Description:	U	the gradient current amplifier to specified value. In imaging, rgradient a gradient to a specified level in DAC units.				
Arguments:	channel specifies the gradient to set. It uses one of the characters 'X', 'x', 'Y', 'y', 'Z' or 'z'. In imaging, channel can be 'gread', 'gphase', or 'gslice'.					
	value specifies the gradient level by a real number (a DAC setting in im from -4096.0 to 4095.0 for the Performa I PFG module, and from -327 32767.0 for the Performa II PFG module.					
Examples:	rgradient('z',1327.0);					
Related:	dps_show getorientation shapedgradient	Draw delay or pulses in a sequence for graphical display Read image plane orientation Generate shaped gradient				

vgradient	Set gradient to a level determined by real-time math
zgradpulse	Create a gradient pulse on the z channel

rlpower Change power level, linear amplifier systems

Applicability: Systems with linear amplifiers. This statement is due to be eliminated in future versions of VNMR software. Although it is still functional, you should not write pulse sequences using it and should replace it in existing sequences with obspower, decpower, dec2power, or dec3power, as appropriate.

Syntax:	rlpower(power,device)									
	double power;	/*	new	lev	rel	for	coarse	powe	er */	
	int device;	/*	OBSc	h,	DEC	Cch,	DEC2ch,	or	DEC3ch	*/

- Description: Changes transmitter or decoupler power the same as the power statement but avoids consuming a real-time variable for the value. On systems with the Output board (and only on these systems), by default, rlpower statements are preceded internally by a 0.2-µs delay (see the apovrride statement for more details).
- Arguments: power sets the power level by assuming values of 0 (minimum power) to 63 (maximum power) on channels with a 63-dB attenuator or -16 (minimum power) to 63 (maximum power) on channels with a 79-dB attenuator.

device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY *INOVA* and UNITY *plus* only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler).

CAUTION: On systems with linear amplifiers, be careful when using values of rlpower greater than 49 (about 2 watts). Performing continuous decoupling or long pulses at power levels greater than this can result in damage to the probe. Use config to set a safety maximum for the tpwr, dpwr, dpwr2, and dpwr3 parameters.

Examples:	 pulsesequence() 	
	{	
	double satpwr;	
	<pre>satpwr=getval("satpwr");</pre>	
	•••	
	rlpower(satpwr,OBSch);	
	• • •	
	}	

(2) rlpower(63.0,OBSch);

decpower	Change first decoupler power, linear amplifier systems	
dec2power	Change second decoupler power, linear amplifier systems	
dec3power	Change third decoupler power, linear amplifier systems	
obspower	Change observe transmitter power, linear amplifier systems	
power	Change transmitter or decoupler power, linear amp. sys.	
rlpwrf	Set transmitter or decoupler fine power	
	dec2power dec3power obspower power	

rlpwrf

Set transmitter or decoupler fine power

Applicability: Systems with fine power control. Not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems. This statement is due to be eliminated in future versions of VNMR software. Although it is still functional, you should not write any new pulse sequences using it and should replace it in existing sequences with obspwrf, decpwrf, dec2pwrf, or dec3pwrf, as appropriate.

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Syntax:	<pre>rlpwrf(pow double powe: int device;</pre>	r; /* new level for fine power */	
Description:	except rlpwr	nitter or decoupler fine power the same as the pwrf statement, E uses a real-number variable for the power level desired instead real-time variable for the level.	
Arguments:	power is the fi	ine power desired.	
	UNITY INOVA and	Sch (observe transmitter) or DECch (first decoupler). For the d UNITY <i>plus</i> only, device can also be DEC2ch (second DEC3ch (third decoupler).	
Examples:	rlpwrf(4.0	,OBSch);	
Related:	decpwrf dec2pwrf dec3pwrf ipwrf obspwrf power pwrf rlpwrf	Set first decoupler fine power Set second decoupler fine power Set third decoupler fine power Change transmitter or decoupler fine power with IPA Set observe transmitter fine power Change transmitter or decoupler power, lin. amp. sys. Change transmitter or decoupler fine power Set transmitter or decoupler fine power	
rlpwrm	Set transmitte	er or decoupler linear modulator power	
Applicability:	UNITY INOVA and	l UNITY <i>plus</i> systems.	
Syntax:	rlpwrm(pow double powe: int device;		
Description:	Changes transmitter or decoupler linear modulator power the same as the pwrm statement, but to avoid using real-time variables, rlpwrm uses a C variable of type double as the argument for the amount of change.		
Arguments:	power is the linear modulation (fine) power desired.		
	device is OBSch (observe transmitter), DECch (first decoupler), DEC2ch (second decoupler), or DEC3ch (third decoupler).		
Examples:	rlpwrm(4.0	,OBSch);	
Related:	ipwrm pwrm	Change transmitter or decoupler lin. mod. power with IPA Change transmitter or decoupler linear modulator power	
rotorperiod	Obtain rotor p	period of MAS rotor	
Applicability:	Systems with N	AAS (magic-angle spinning) rotor synchronization hardware.	
Syntax:	rotorperio codeint per:	-	
Description:	Obtains the rote	or period.	
Arguments:	integer in units	eal-time variable into which is placed the rotor period as an of 100 ns. For example, for rotorperiod(v4), if v4 lue 1700, the rotor period is 170 μ s and the rotor speed is 1E+7 Hz.	
Examples:	rotorperio	d(v4);	
Related:	rotorsync xgate	Gated pulse sequence delay from MAS rotor position Gate pulse sequence from an external event	

rotorsync	Gated pulse sequence delay from MAS rotor position		
Applicability:	Systems with MAS (magic-angle spinning) rotor synchronization hardware.		
Syntax:	<pre>rotorsync(rotations) codeint rotations;</pre>		
Description:	Inserts a variable-length delay that allows synchronizing the execution of the pulse sequence with a particular orientation of the sample rotor. When the rotorsync statement is encountered, the pulse sequence is stopped until the number of rotor rotations has occurred.		
Arguments:	rotations is a real-time variable that specifies the number of rotor rotations to occur before restarting the pulse sequence.		
Examples:	rotorsync(v6);		
Related:	rotorperiodObtain rotor period of MAS rotorxgateGate pulse sequence from an external event		

S

setautoincrement Set autoincrement attribute for an AP table

Applicability:	All systems except the GEMINI 2000.		
Syntax:	<pre>setautoincreme codeint table;</pre>		
Description:	0 at the start of an FII	nt attribute in an AP table. The index into the table is set to D acquisition and is incremented after each access into the autoincrement feature cannot be accessed within a	
Arguments:	table is the name of the table (t1 to t60).		
Examples:	<pre>setautoincrement(t9);</pre>		
Related:	getelem loadtable setdivnfactor setreceiver settable	Retrieve an element from an AP table Load AP table elements from table text file Set divn-return attribute and divn-factor for AP table Associate the receiver phase cycle with an AP table Store an array of integers in a real-time AP table	

setdivnfactor Set divn-return attribute and divn-factor for AP table

Applicability:	All systems except the GEMINI 2000.		
Syntax:	<pre>setdivnfactor(table,divn_factor) codeint table;</pre>		
Description:	Sets the divn-return attribute and divn-factor for an AP table. The actual index into the table is now set to (index/divn-factor). {01}2 is therefore translated by the <i>acquisition processor</i> , not by PSG (pulse sequence generation), into 0011. The divn-return attribute results in a divn-factor-fold compression of the AP table at the level of the acquisition processor.		
Arguments:	table specifies the name of the table (t1 to t60).		
	divn_factor specifies the divn-factor for the table.		

Examples: setdivnfactor(t7,4);

getelem loadtable	Retrieve an element from an AP table Load AP table elements from table text file
setautoincrement	Set autoincrement attribute for an AP table
setreceiver	Associate the receiver phase cycle with an AP table
settable	Store an array of integers in a real-time AP table
	loadtable setautoincrement setreceiver

setreceiverAssociate the receiver phase cycle with an AP tableApplicability:All systems except the GEMINI 2000.

Syntax:	setrece	eiver(table)				
	codeint	table	; /*	real-time	table	variable	*/

Description: Assigns the ctth element of a table to the receiver variable oph. If multiple setreceiver statements are used in a pulse sequence, or if the value of oph is changed by real-time math statements such as assign, add, etc., the last value of oph prior to the acquisition of data determines the value of the receiver phase.

- Arguments: table specifies the name of the table (t1 to t60).
- Examples: setreceiver(t18);

Related:	getelem	Retrieve an element from an AP table
	loadtable	Load AP table elements from table text file
	setautoincrement	Set autoincrement attribute for an AP table
	setdivnfactor	Set divn-return attribute and divn-factor for AP table
	settable	Store an array of integers in a real-time AP table

setstatus S

Set status of observe transmitter or decoupler transmitter

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000.

Syntax:	<pre>setstatus(channel,on,mode,sync,mod_freq)</pre>		
	int channel;	<pre>/* OBSch, DECch, DEC2ch, or DEC3ch */</pre>	
	int on;	/* TRUE (=on) or FALSE (=off) */	
	char mode;	/* 'c', 'w', 'g', etc. */	
	int sync;	/* TRUE (=synchronous) or FALSE */	
	<pre>double mod_freq;</pre>	<pre>/* modulation frequency */</pre>	

Description: Sets the status of a transmitter independent of the status statement, thus overriding decoupler parameters such as dm and dmm. Since the setstatus statement is part of the pulse sequence, it has no effect when only an su command is executed. It is the only way the observe transmitter can be modulated on UNITY *INOVA* and UNITY *plus* systems.

Arguments: channel is OBSch (observe transmitter), DECch (first decoupler), DEC2ch (second decoupler), or DEC3ch (third decoupler).

on is TRUE (turn on decoupler) or FALSE (turn off decoupler).

mode is one of the following values for a decoupler mode (for further information on decoupler modes, refer to the description of the dmm parameter in the manual *VNMR Command and Parameter Reference*):

- 'c' sets continuous wave (CW) modulation.
- 'f' sets fm-fm modulation (swept-square wave).
- 'g' sets GARP modulation.
- 'm' sets MLEV-16 modulation.

	• 'n' sets noise mo	dulation.		
	• 'p' sets programm	nable pulse modulation (i.e., waveform generation).		
	• 'r' sets square wave modulation.			
	• 'u' sets user-supplied modulation from external hardware.			
	• 'w' sets WALTZ-	16 modulation.		
	• 'x' sets XY32 mc	dulation.		
		On the UNITY <i>INOVA</i> and UNITY <i>plus</i> , 'c', 'f', 'g', 'm', 'p', 'r', 'u', 'w', and 'x' are available. On the UNITY and VXR-S, 'c', 'f', 'n', 'p'		
		ler is synchronous, on UNITY <i>INOVA</i> and UNITY <i>plus</i> E (decoupler is asynchronous).		
	mod_freq is the mode	ulation frequency.		
Examples:		TRUE,'w',FALSE,dmf); ,FALSE,'c',FALSE,dmf2);		
Related:	status Change	status of decoupler and homospoil		
settable	Store an array of inte	gers in a real-time AP table		
Applicability:	All systems except the	GEMINI 2000.		
Syntax:		<pre>ime,numelements,intarray) /* real-time table variable */ /* number in array */ /* pointer to array of elements */</pre>		
Description:	attributes can be subseq	n a real-time AP table. The autoincrement or divn-return uently associated with a table defined by settable by ement and setdivnfactor.		
Arguments:	table is the name of t	he table (t1 to t60).		
	number_elements	s the size of the table.		
	-32768 to 32767. Befor	that contains the table elements, which can range from e calling settable, this array must be predefined and pulse sequence using C statements.		
Examples:	<pre>settable(t1,10,i</pre>	nt_array);		
Related:	getelem loadtable setautoincrement setdivnfactor setreceiver	Retrieve an element from an AP table Load AP table elements from table text file Set autoincrement attribute for an AP table Set divn-return attribute and divn-factor for AP table Associate the receiver phase cycle with an AP table		
setuserap	Set user AP register			
Applicability:	UNITY INOVA systems.			
Syntax:	<pre>setuserap(value, real value; int register;</pre>	register) /* value sent to user AP register */ /* AP bus register number: 0, 1, 2, or 3 */		
Description:	interface to user device connectors J8212 and J	the four 8-bit AP bus registers that provide an output s. The outputs of these registers go to the USER AP 8213, located on the back of the left console cabinet. 00-ohm series resistor for circuit protection.		

Chapter 3. Pulse Sequence Statement Reference -

Arguments: value is a signed or unsigned number (real or integer) to output to the specified user AP register. The number is truncated to an 8-bit byte.

register is the AP register number, mapped to output lines as follows:

- Register 0 is J8213, lines 9 to 16.
- Register 1 is J8213, lines 1 to 8.
- Register 2 is J8212, lines 9 to 16.
- Register 3 is J8212, lines 1 to 8.

Examples: setuserap(127.0,0);

Related: readuserap Read input from user AP register vsetuserap Set user AP register using real-time variable

shapedpulse Perform shaped pulse on observe transmitter

Applicability: This statement is due to be eliminated in future versions of VNMR software. Although it is still functional, you should not write any new pulse sequences using it and should replace it in existing sequences with shaped_pulse, which functions exactly the same as shapedpulse.

shaped_pulse Perform shaped pulse on observe transmitter

- Applicability: UNITY *INOVA* and UNITY *plus* systems, or systems with a waveform generator on the observe transmitter channel.
 - Syntax: shaped_pulse(pattern,width,phase,RG1,RG2)

char *pattern;	/*	name of .RF text file */
double width;	/*	width of pulse in sec */
codeint phase;	/*	real-time variable for phase */
double RG1;	/*	gating delay before pulse in sec */
double RG2;	/*	gating delay after pulse in sec */

Description: Performs a shaped pulse on the observe transmitter. If a waveform generator is configured on the channel, it is used; otherwise, the linear attenuator and the small-angle phase shifter are used to effectively perform an apshaped_pulse statement.

When using the waveform generator, the shapes are downloaded into the waveshaper before the start of an experiment. When $shaped_pulse$ is called, the shape is addressed and started. The minimum pulse length is 0.2 μ s. The overhead at the start and end of the shaped pulse varies with the system:

- UNITY INOVA: 1 μ s (start), 0 (end)
- UNITYplus: 5.75 µs (start), 0 (end)
- System with Acquisition Controller board: 10.75 µs (start), 4.3 µs (end)
- System with Output board: 10.95 µs (start), 4.5 µs (end)

If the length is less than $0.2 \,\mu s$, the pulse is not executed and there is no overhead.

When using the linear attenuator and the small-angle phase shifter to generate a shaped pulse, the shaped_pulse statement creates AP tables on the fly for amplitude and phase. It also uses the real-time variables v12 and v13 to control the execution of the shape. It does not use AP table variables. For timing and more information, see the description of apshaped_pulse. Note that if using AP tables with shapes that have a large number of points, the FIFO

can become overloaded with words generating the pulse shape and FIFO Underflow errors can result.

Arguments: file is the name of a text file in the shapelib directory that stores the rf pattern (leave off the .RF file extension).

width is the duration, in seconds, of the pulse on the observe transmitter

phase is the phase of the pulse and must be a real-time variable.

RG1 is the delay, in seconds, between gating the amplifier on and gating the observe transmitter on (the phase shift occurs at the beginning of this delay).

RG2 is the delay, in seconds, between gating the observe transmitter off and gating the amplifier off.

Examples: shaped_pulse("gauss",pw,vl,rof1,rof2); Related: apshaped_pulse Observe transmitter pulse shaping via AP bus decshaped_pulse Shaped pulse on first decoupler dec2shaped_pulse Shaped pulse on second decouple r simshaped_pulse Simultaneous two-pulse shaped pulse sim3shaped_pulse Simultaneous three-pulse shaped pulse

shapedgradient Generate shaped gradient pulse

- -

. .

Applicability: Systems with waveform generation on imaging or PFG module.

Syntax:	<pre>shapedgradient(pattern,width,amp,channel,loops,wait)</pre>		
	char *pattern;	/* name of shape text file */	
	double width;	/* length of pulse */	
	double amp;	/* amplitude of pulse */	
	char channel;	/* gradient channel 'x', 'y', or 'z' */	/
	int loops;	/* number of loops */	
	int wait;	/* WAIT or NOWAIT */	

. . .

.

Description: Operates the selected gradient channel to provide a gradient pulse to the selected set of gradient coils. The pulse is created using a gradient waveform generator and has a pulse shape determined by the arguments name, width, amp, and loops. Unlike the shaped rf pulses, the shaped gradient leaves the gradients at the last value in the gradient pattern when the pulse completes.

Arguments: pattern is the name of a text file without a .GRD extension to describe the shape of the pulse. The text file with a .GRD extension should be located in \$vnmrsystem/shapelib or in the users directory \$vnmruser/shapelib.

width is the requested length of the pulse in seconds. The pulse length is affected by two factors: (1) the minimum time of every element in the shape file must be at least 10 μ s long, and (2) the time for every element must be a multiple of 50 ns. If the width of the pulse is less than 10 μ s times the number of steps in the shape, a warning message is generated. The shaped gradient software rounds each element to a multiple of 50 ns. If the requested width differs from the actual width by more than 2%, a warning message is displayed.

amp is a value that scales the amplitude of the pulse. Only the integer portion of the value is used and it ranges from 32767 to -32767; where 32767 is full scale and -32767 is negative full scale.

channel selects the gradient coil channel desired and should evaluate to the characters 'x', 'y', or 'z'. (Be sure not to confuse the characters 'x', 'y', or 'z' with the strings "x", "y", or "z".)

loops is a value, from 1 to 255, that allows the user to loop the selected waveform. Note that the given value is the number of loops to be executed and that the values 0 and 1 cause the pattern to execute once.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient is completed before executing the next statement. The total time it will wait is width*loops. If loops is supplied as 0, it will be counted as 1 when determining its total time.

```
Examples: shapedgradient("hsine",0.02,32767,'y',1,NOWAIT);
```

```
#include "standard.h"
        #define POVR 1.2e-5 /* shaped pulse overhead=12 us */
        pulsesequence()
        {
        for (i=-32000; i<=32000; i+16000)
        {
        shapedgradient("hsine",pw+d3+rx1+rx2,i,'x', \
            1,NOWAIT);
        shapedpulse("sinc",pw,oph,rx1,rx2);
        delay(d3);
        }
        /* This step sets a square gradient from a low value */
        /* to a high value while executing a shaped pulse */
        /* and a delay during each gradient value. */
        . . .
        }
Related:
        dps_show
                            Draw delay or pulses in a sequence for graphical display
                            Set gradient to a specified level
        rgradient
        shapedgradient
                            Provide shaped gradient pulse to gradient channel
                            Arrayed shaped gradient function
        shaped2Dgradient
                            Set gradient to a level determined by real-time math
        vgradient
```

shaped2Dgradient Generate arrayed shaped gradient pulse

```
Applicability: Systems with WFG on imaging or PFG module.
     Syntax: shaped2Dgradient(pattern,width,amp,channel, \
                loops,wait,tag)
             char *pattern; /* name of pulse shape text file */
             double width;
                                   /* length of pulse */
                                   /* amplitude of pulse */
             double amp;
             char channel;
                                    /* gradient channel 'x', 'y', or 'z' */
             int loops;
                                   /* number of loops */
             int wait;
                                   /* WAIT or NOWAIT */
             int tag;
                                    /* unique number for gradient element */
 Description: Operates the selected gradient channel to provide a gradient pulse to the
             selected set of gradient coils. This statement is basically the same as the
             shapedgradient statement except that shaped2Dgradient is tailored
             to be used in pulse sequences where the amplitude is arrayed (imaging
             sequences). For sequences that array the amplitude, it does not use the amount
             of waveform generator memory that the shapedgradient statement uses,
             but there is a penalty in the amount of overhead time used in setting it up. The
             pulse is created using a gradient waveform generator and has a pulse shape
             determined by the name, width, amp, and loops arguments.
```

Arguments:	pattern is the name of a text file without a .GRD extension that describes the
	shape of the pulse. The text file with a .GRD extension should be located in
	<pre>\$vnmrsystem/shapelib or in the users directory \$vnmruser/</pre>
	shapelib.

width is the requested length of the pulse in seconds. The width of the pulse is affected by two factors: (1) the minimum time of every element in the shape file must be at least 200 ns long, and (2) the time for every element must be a multiple of 50 ns. If the width of the pulse is less than 10 µs times the number of steps in the shape, a warning message is generated. The shaped gradient software will round each element to a multiple of 50 ns. If the requested width differs from the actual width by more than 2%, a warning message is displayed.

amp is a value that scales the amplitude of the pulse. Only the integer portion of the value is used and it ranges from 32767 to -32767; where 32767 is full scale and -32767 is negative full scale.

channel selects the gradient coil channel desired and should evaluate to the characters 'x', 'y', or 'z'. (Be sure not to confuse the characters 'x', 'y', or 'z' with the strings "x", "y", or "z".)

loops is a value, from 1 to 255, that allows the user to loop the selected waveform. Note that the given value is the number of loops to be executed and that the values 0 and 1 cause the pattern to execute once. Due to a digital hardware bug affecting looping, patterns must be carefully constructed to achieve the desired results.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient is completed before executing the next element. The total time it will wait is width*loops.

tag is a unique integer that "tags" the gradient element from any other gradient elements used in the sequence.

Examples: #include "standard.h" pulsesequence() { shaped2Dgradient("hsine",d3,0.0-gpe,'x',0,NOWAIT,1); delay(d3); shaped2Dgradient("hsine",d4,gpe,'y',0,NOWAIT,2); . . . } Related: dps_show Draw delay or pulses in a sequence for graphical display Set gradient to a specified level rgradient Provide shaped gradient pulse to gradient channel shapedgradient Set gradient to a level determined by real-time math vgradient

shapedincgradient Generate dynamic variable gradient pulse

int	loops;	/*	number of loops */
int	wait;	/*	WAIT or NOWAIT */

Description: Provides a dynamic, variable shaped gradient pulse controlled using the AP math functions. The statement drives the chosen gradient with the specified pattern, scaled to the level defined by the formula:

level = a0 + a1*x1 + a2*x2 + a3*x3

The pulse is created using a gradient waveform generator and has a pulse shape determined by the pattern, width, and loops arguments, as well as the calculation of level.

Unlike the shaped rf pulses, the shapedincgradient will leave the gradients at the last value in the gradient pattern when the pulse completes. The range of the gradient level is -32767 to +32767. If the requested level lies outside the legal range, it is clipped at the appropriate boundary value. Note that, while each variable in the calculation of level must fit in a 16-bit integer, intermediate sums and products in the calculation are done with double precision, 32-bit integers.

The following error messages are possible:

- Machine configuration doesn't allow gradient patterns is displayed if this statement is used on a system without gradient waveshaping hardware.
- shapedincgradient: x[i] illegal RT variable: xi or shapedincgradient: no match! is displayed if the requested shape cannot be found or if a width of zero is specified.
- Arguments: channel selects the gradient coil channel desired and should evaluate to the characters 'x', 'y', or 'z'. (Be careful not to confuse the characters 'x', 'y', or 'z' with the strings "x", "y", or "z".)

pattern is the name of a text file without a .GRD extension to describe the shape of the pulse. The text file with a .GRD extension should be located in \$vnmrsystem/shapelib or in the users directory \$vnmruser/ shapelib.

width is the requested length of the pulse in seconds. The width of the pulse is affected by two factors: (1) the minimum time of every element in the shape file must be at least $10 \,\mu$ s, and (2) the time for every element must be a multiple of 50 ns. If the width of the pulse is less than $10 \,\mu$ s times the number of steps in the shape), a warning message is generated. The shapedincgradient software will round each element to a multiple of 50 ns. If the requested width differs from the actual width by more than 2%, a warning message is displayed.

a0, a1, a2, a3, x1, x2, x3 are values used in the calculation of "level."

loops is a value, from 1 to 255, that allows the user to loop the selected waveform. Note that the given value is the number of loops to be executed and that the values 0 and 1 cause the pattern to execute once. Due to a digital hardware bug affecting looping, patterns must be carefully constructed to achieve the desired results.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient is completed before executing the next element. The total time it will wait is width*loops. If loops is supplied as 0, it will be counted as 1 when determining its total time.

Related:

Read image plane orientation Set gradient to a specified level

getorientation

rgradient

shapedgradient	Provide shaped gradient pulse to gradient channel
shaped2Dgradient	Generate arrayed shaped gradient pulse
vgradient	Set gradient to a level determined by real-time math

Generate dynamic variable shaped gradient pulse shapedvgradient

Applicability: Systems with WFG on imaging or PFG module.

Syntax:	$shapedvgradient(pattern,width,amp_const, \setminus$		
	<pre>amp_incr,amp_vmult,channel,vloops,wait,tag)</pre>		
	char *pattern; /* name of pulse shape text file */		
	double width; /* length of pulse */		
	double amp_const; /* sets amplitude of pulse */		
	<pre>double amp_incr; /* sets amplitude of pulse */</pre>		
	codeint amp_vmult; /* sets amplitude of pulse */		
	char channel; /* gradient channel 'x', 'y', or 'z' */		
	codeint vloops; /* variable for number of loops */		
	int wait; /* WAIT or NOWAIT */		
	int tag; /* unique number for gradient element */		

Description: Operates the selected gradient channel to provide a shaped gradient pulse to the selected set of gradient coils. This statement is tailored to provide a dynamic variable shaped gradient level controlled using the system AP math functions and real-time looping. The statement drives the chosen gradient shape to the level defined by the formula:

amplitude = amp const + amp incr*amp vmult

The range of the gradient amplitude is-32767 to +32767, where 32767 is full scale and -32767 is negative full scale.

If the requested level lies outside this range, it is truncated to the appropriate boundary value. Note that the vloops argument is also controlled by a realtime AP math variable. Unlike the shaped rf pulses, the shaped gradient leaves the gradients at the last value in the gradient pattern when the pulse completes.

Arguments: name is the name of a text file without a .GRD extension to describe the shape of the pulse. The text file with a .GRD extension should be located in \$vnmrsystem/shapelib or in the user's directory \$vnmruser/ shapelib.

> width is the requested length of the pulse in seconds. The width of the pulse is affected by two factors: (1) the minimum time of every element in the shape file must be at least $10 \,\mu$ s, and (2) the time for every element must be a multiple of 50 ns. If width is less than 10 µs times the number of steps in the shape, a warning message is generated. The shaped gradient software will round each element to a multiple of 50 ns. If the requested width differs from the actual width by more than 2%, a warning message is displayed.

> amp_const, amp_incr, and amp_vmult scale the amplitude of the pulse according to the formula above. amp const and amp incr can be values of type double or integer. amp_vmult must be a real-time AP math variable (v1 to v14) or a table pointer (t1 to t60). The amplitude ranges are also given above.

> channel selects the gradient coil channel desired and should evaluate to the characters 'x', 'y', or 'z'. (Be careful not to confuse the characters 'x', 'y', or 'z' with the strings "x", "y", or "z".)

> vloops allows the user to loop the selected waveform. Values range from 1 to 255. This also must be a real-time AP math variable (v1 to v14) or a table

pointer (t1 to t60). Do not use 0 for vloops, because this may cause inconsistencies when WAIT is selected for the wait_4_me argument. Due to a digital hardware bug affecting looping, patterns must be carefully constructed to achieve the desired results.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient is completed before executing the next element. The total time it will wait is width*vloops. It uses the incdelay statement when waiting for the gradient pulse to complete.

tag is a unique integer that "tags" this gradient statement from any other gradient statement used in the sequence.

```
Examples: #include "standard.h"
                 pulsesequence()
                 {
                 . . .
                 char gphase, gread, gslice;
                 . . .
                 amplitude=(int)(0.5*ni*gpe);
                 stat=getorientation(&gread,&gphase,&gslice,"orient")
                 ;
                 initval(1.0,v1);
                 initval(nf,v9);
                 loop(v9,v5);
                 . . .
                 shapedvgradient("hsine",d3,amplitude,igpe, \
                         v5,gphase,v1,NOWAIT,1);
                 endloop(v5);
                 . . .
                 }
        Related:
                incdelay
                                     Set real-time incremental delay
                                     Set gradient to specified level
                 rgradient
                 shapedgradient
                                     Generate shaped gradient pulse
                 shaped2Dgradient Generate arrayed shaped gradient pulse
                                     Generate dynamic variable gradient pulse
                 vgradient
                 Pulse observe and decouple channels simultaneously
simpulse
        Syntax: simpulse(obswidth,decwidth,obsphase,decphase,
                    RG1,RG2)
                 double obswidth, decwidth; /* pulse lengths in sec */
                 codeint obsphase,decphase; /* variables for phase */
                 double RG1;
                                                 /* gating delay before pulse */
                 double RG2;
                                                 /* gating delay after pulse */
    Description: Gates the observe and decoupler channels. The shorter of the two pulses is
                 centered on the longer pulse, while the amplifier gating occurs before the start
                 of the longer pulse (even if it is the decoupler pulse) and after the end of the
                 longer pulse.
                 For UNITY INOVA, the absolute difference in the two pulse widths must be greater
                 than or equal to 0.2 \,\mus; otherwise, a timed event of less than the minimum value
                 (0.1 \ \mu s) would be produced:
```

• if the difference is less than 0.1 μ s, the pulses are made equally long.

- If the difference is from 0.1 to 0.2 μ s, the difference is made 0.2 μ s.
- If the difference is larger than $0.2 \,\mu s$, the difference is made as close as the timing resolution allows (0.0125 μs).

For systems other than UNITY *INOVA*, the minimum time is $0.2 \,\mu$ s; thus, the times are doubled (the difference must be 0.4 μ s, resolution is 0.025 μ s).

Arguments: obswidth and decwidth are the duration, in sec, of the pulse on the observe transmitter and first decoupler, respectively.

obsphase and decphase are the phase of the pulse on the observe transmitter and the first decoupler, respectively. Each must be a real-time variable.

RG1 is the delay, in seconds, between gating the amplifier on and gating the first rf transmitter on (all phase shifts occur at the beginning of this delay).

RG2 is the delay, in seconds, between gating the final rf transmitter off and gating the amplifier off.

Examples: simpulse(pw,pp,v1,v2,0.0,rof2);

Related:	decpulse	Pulse the decoupler transmitter	
	decrgpulse	Pulse decoupler transmitter with amplifier gating	
	dps_show	Draw delay or pulses in a sequence for graphical display	
	rgpulse	Pulse observe transmitter with amplifier gating	
	sim3pulse	Simultaneous pulse on 2 or 3 rf channels	
	sim4pulse	Simultaneous pulse on four channels	

sim3pulse Pulse simultaneously on 2 or 3 rf channels

Applicability: UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S systems with two or more independent rf channels.

- Description: Performs a simultaneous, three-pulse pulse on three independent rf channels. A simultaneous, two-pulse pulse on the observe transmitter and second decoupler can also be performed by setting the pulse length for the first decoupler to 0.0 (see the second example below for how this is done).

Timing limitations connected with the difference in pulse widths are covered in the description of simpulse.

Arguments: pw1, pw2, and pw3 are the pulse length, in seconds, of channels OBSch, DECch, and DEC2ch, respectively.

phase1, phase2, and phase3 are the phases of the corresponding pulses. These must be real-time variables (v1 to v14, oph, etc.).

RG1 is the delay, in seconds, between gating the amplifier on and gating the first rf transmitter on (all phase shifts occur at the beginning of this delay).

RG2 is the delay, in seconds, between gating the final rf transmitter off and gating the amplifier off.

Examples:	<pre>sim3pulse(pw,p1,p2,oph,v10,v1,rof1,rof2); sim3pulse(pw,0.0,p2,oph,v10,v1,rof1,rof2);</pre>		
Related:	decpulse decrgpulse dps_show rgpulse simpulse sim4pulse	Pulse the decoupler transmitter Pulse decoupler transmitter with amplifier gating Draw delay or pulses in a sequence for graphical display Pulse observe transmitter with amplifier gating Pulse observe, decoupler channels simultaneously Simultaneous pulse on four channels	
sim4pulse	Simultaneous pulse on four channels		
Applicability:	UNITY <i>INOVA</i> , UNITY <i>plus</i> , and UNITY systems with two or more independent rf channels.		
Syntax:	<pre>sim4pulse(pw1,pw2,pw3,pw4,phase1,phase2, \ phase3,phase4,RG1,RG2) double pw1,pw2,pw3,pw4; /* pulse length in sec */ codeint phase1,phase2; /* variables for phase */ codeint phase3,phase4; /* variables for phase */ double RG1; /* gating delay before pulse */ double RG2; /* gating delay after pulse */</pre>		
Description:	pulses are set to 0.0, no pulse is executed on that channel.		
	Timing limitations connected with the difference in pulse widths is covered in the description of simpulse.		
Arguments:	S: pw1, pw2, pw3, and pw4 are the pulse length, in seconds, of channels OBSch, DECch, DEC2ch, and DEC3ch, respectively.		
	phase1, phase2, phase3, and phase4 are the phases of the corresponding pulses. Each must be real-time variable (v1-v14, oph, etc.)		
	RG1 is the delay, in seconds, between gating on the amplifier and turning on the first transmitter (all phases set at beginning of RG1, even if pwn is 0.0).		
RG2 is the delay, in seconds, between the f amplifier off.		n seconds, between the final transmitter off and gating the	
Examples:	sim4pulse(pw,2*pw,p1,2*p1,oph,v3,ZERO,TWO,RG1,RG2); sim4pulse(pw,0.0,0.0,2*p1,oph,ZERO,ZERO,TWO,RG1,RG2);		
Related:	simpulse P	ulse observe channel with amplifier gating ulse observe and decoupler channel simultaneously ulse simultaneously on 2 or 3 channel s	

simshaped_pulse Perform simultaneous two-pulse shaped pulse

Applicability:	Systems with a waveform generator on two or more rf channels.		
Syntax:	<pre>simshaped_pulse(obsshape,decshape,obswidth, \ decwidth,obsphase,decphase,RG1,RG2)</pre>		
	<pre>char *obsshape,*decshape; double obswidth, decwidth; codeint obsphase,decphase;</pre>		
	double RG1; double RG2;	<pre>/* gating delay before pulse */ /* gating delay after pulse */</pre>	
Description:	Performs a simultaneous, two-pulse shaped pulse on the observe transmitter and		

Description: Performs a simultaneous, two-pulse shaped pulse on the observe transmitter and the first decoupler under waveform generator control. The overhead at the start and end of the two-pulse shaped pulse varies with the system:

- UNITY *INOVA*: 1.45 μs (start), 0 (end).
- UNITY*plus*: 11.5 µs, 0.
- Systems with an Acquisition Controller board: 21.5 µs, 8.6 µs.
- Systems with an Output board: 21.7 µs, 8.8 µs.

These values hold regardless of the values for the arguments obswidth and decwidth.

If either obswidth or decwidth is 0.0, no pulse occurs on the corresponding channel. If both obswidth and decwidth are non-zero and either obsshape or decshape is set to the null string (''), then a hard pulse occurs on the channel with the null shape name. If either the pulse width is zero or the shape name is the null string, then a waveform generator is not required on that channel.

Arguments: obsshape is the name of the text file in the shapelib directory that contains the rf pattern to be executed on the observe transmitter.

decshape is the name of the text file in the shapelib directory that contains the rf pattern to be executed on the first decoupler.

obswidth is the length of the pulse, in seconds, on the observe transmitter.

decwidth is the length of the pulse, in seconds, on the first decoupler.

obsphase is the phase of the pulse on the observe transmitter. The value must be a real-time variable (v1 to v14, oph, etc.).

decphase is the phase of the pulse on the first decoupler. The value must be a real-time variable (v1 to v14, oph, etc.).

RG1 is the delay, in seconds, between gating the amplifier on and gating the first rf transmitter on (all phase shifts occur at the beginning of this delay).

RG2 is the delay, in seconds, between gating the final rf transmitter off and gating the amplifier off.

Related:	decshaped_pulse	Shaped pulse on first decoupler	
	dec2shaped_pulse	Shaped pulse on second decoupler	
	shaped_pulse	Shaped pulse on observe transmitter	
	sim3shaped_pulse	Simultaneous three-pulse shaped pulse	

sim3shaped_pulse Perform a simultaneous three-pulse shaped pulse

Applicability: Systems with a waveform generator on three or more rf channels.

Syntax: sim3shaped_pulse(obsshape,decshape,dec2shape, \
 obswidth,decwidth,dec2width,obsphase, \
 decphase,dec2phase,RG1,RG2)
 char *obsshape; /* name of obs .RF file */
 char *decshape; /* name of dec .RF file */
 char *dec2shape; /* name of dec2 .RF file */
 double obswidth; /* obs pulse length in sec */
 double decwidth; /* dec pulse length in sec */
 double dec2width; /* dec2 pulse length in sec */
 codeint obsphase; /* obs real-time var. for phase */
 codeint dec2phase; /* dec2 real-time var for phase */
 double RG1; /* gating delay before pulse in sec */

	double RG2;	/* gating delay after pulse in sec */	
Description: Performs a simultaneous, three-pulse shaped pu		three-pulse shaped pulse under waveform generator ent rf channels. The overhead at the start and end of	
	• ^{UNITY} <i>INOVA</i> : 1.95 μs ((start), 0 (end).	
	• UNITY <i>plus</i> : 17.25 µs, 0.		
	· ·	uisition Controller board: 32.25 µs, 12.9 µs.	
	 Systems with an Output board: 32.45 µs, 13.1 µs. 		
	These values hold regardless of the values of the arguments obswidth, decwidth, and dec2width.		
	shaped pulse on any comb	an also be used to perform a simultaneous two-pulse bination of three rf channels. This can be achieved by ngths to the value 0.0 (see the second example below this is done).	
	on the channel with the nu	are set to the null string (''), then a hard pulse occurs Ill shape name. If either the pulse width is zero or the ng, then a waveform generator is not required on that	
Arguments:	-	the text file in the shapelib directory that contains ed on the observe transmitter.	
	decshape is the name of the text file in the shapelib directory that contains the rf pattern to be executed on the first decoupler.		
		of the text file in the shapelib directory that be executed on the second decoupler.	
	of the pulse, in seconds, on the observe transmitter.		
decwidth is the length of the pulse, in seconds, on the first		of the pulse, in seconds, on the first decoupler.	
dec2width is the length of the pulse, in seconds, on the second		of the pulse, in seconds, on the second decoupler.	
	obsphase is the phase of be a real-time variable (v.	f the pulse on the observe transmitter. The value must 1 to v14, oph, etc.).	
	decphase is the phase of a real-time variable (v1 to	f the pulse on the first decoupler. The value must be ov14, oph, etc.).	
	dec2phase is the phase of the pulse on the second decoupler. The value must be a real-time variable (v1 to v14, oph, etc.).		
	RG1 is the delay, in seconds, between gating the amplifier on and g rf transmitter on (all phase shifts occur at the beginning of this de		
	RG2 is the delay, in secon gating the amplifier off.	ds, between gating the final rf transmitter off and	
Examples:		"gauss","hrm180","sinc",pw,p1,p2, \	
	v2,v5,v6,rof1,ro sim3shaped_pulse(v2,v5,v6,rof1,ro	"dumy","hrm180","sinc",0.0,p1,p2, \	
Related:	decshaped_pulse	Shaped pulse on first decoupler	
	dec2shaped_pulse	Shaped pulse on second decoupler	
	shaped_pulse simshaped_pulse	Shaped pulse on observe transmitter Simultaneous two-pulse shaped pulse	

sli Set SLI lines

Applicability: Systems with imaging capability and the Synchronous Line Interface (SLI) board, an option that provides an interface to custom user equipment.

Syntax:	<pre>sli(address,mode,value)</pre>			
	int address;	/* SLI board address */		
	int mode;	/* SLI_SET, SLI_OR, SLI_AND, SLI_XOR */		
	unsigned value;	/* bit pattern */		

Description: Sets lines on the SLI board. It has no return value. The board contains 32 TTLcompatible logic signals that can be set by these functions. Each line has an LED indicator and a 100-ohm series resistor for circuit protection. The lines are accessible through the 50-pin ribbon connector J4 on the front edge of the SLI board. The pin assignments are as follows:

- Pins 1 and 49 are a +5 V supply through 100-ohm series resistor (enabled by installing jumper J3L)
- Pins 3 to 10 control bits 0 to 7
- Pins 12 to 19 control bits 8 to 15
- Pins 21 to 28 control bits 16 to 23
- Pins 41 to 48 control bits 24 to 31
- Pins 2, 11, 20, 29, 40, and 50 are ground

sli has a pre-execution delay of 10.950 μ s but no post-execution delay. The delay is composed of a 200-ns startup delay with 5 AP bus cycles (1 AP bus cycle = 2.150 μ s).

The logic levels on the SLI lines are not all set simultaneously. The four bytes of the 32 bit word are set consecutively, the low-order byte first. The delay between setting of consecutive bytes is 1 AP bus cycle ± 100 ns. (This 100-ns timing jitter is non-cumulative.)

The error message Illegal mode: n is caused by the mode argument not being one of SLI_SET, SLI_OR, SLI_XOR, or SLI_AND.

- Arguments: address is the address of the SLI board in the system. It must match the address specified by jumper J7R on the board. Note that the jumpers 19-20 through -2 specify bits 2 through 11, respectively. Bits 0 and 1 are always zero. An installed jumper signifies a "one" bit, and a missing jumper a "zero". The standard addresses for the SLI in the VME card cage:
 - Digital (left) side is C90 (hex) = 3216
 - Analog (right) side is 990 (hex) = 2448

mode determines how to combine the specified value with the current output of the SLI to produce the new output. The four possible modes:

- SLI_SET is to load the new value directly into the SLI
- SLI_OR is to logically OR the new value with the old
- SLI_AND is to logically AND the new value with the old
- SLI_XOR is to logically XOR the new value with the old

value (as modified by the mode argument) specifies the bit pattern to be set in the SLI board. This should be a non-negative number, between 0 (all lines low) and 2^{32} -1 (all lines high).

Examples: pulsesequence()

```
. . .
```

Note that sli and address are not standard parameters, but need to be created by the user if they are mentioned in a user pulse sequence (for details, see the description of the create command).

Related:	sp#on	Turn on specified spare line	
	sp#off	Turn off specified spare line	
	vsli	Set SLI lines from real-time variable	

sp#off	Turn off specified spare line		
Applicability:	Not available on MERCURY-VX and MERCURY systems.		
Syntax:	(UNITYINOVA) sploff() to sp5off()		
	(UNITYplus, UNITY, or VXR-S) sploff(), sp2off() (GEMINI 2000) sploff()		
Description:	Turns off the specified user-dedicated spare line connector (sploff for SPARE 1, sp2off for SPARE 2, etc.) for high-speed device control.		
	• UNITY <i>INOVA</i> has five spare lines available from the Breakout panel on the back of the left console cabinet.		
	• UNITY <i>plus</i> has two spare lines located on the front panel of the Pulse Sequence Controller board in the digital cardcage.		
	• UNITY and VXR-S have two spare lines on the Interface board.		
	• <i>GEMINI 2000</i> has one spare line.		
Examples:	<pre>sploff(); sp4off();</pre>		
Related:	sp#onTurn on specified spare line		
sp#on	Turn on specified spare line		
- Applicability:			
Syntax:	(UNITY INOVA) splon() to splon()		
	(UNITYplus, UNITY, or VXR-S) splon(), sp2on() (GEMINI 2000) splon()		
Description:	Turns on the specified user-dedicated spare line connector (splon for SPARE 1, sp2on for SPARE 2, etc.) for high-speed device control. On the UNITY INOVA each spare line changes from low to high when turned on.		
	• UNITY <i>INOVA</i> has five spare lines available from the Breakout panel on the back of the left console cabinet.		
	• UNITY <i>plus</i> has two spare lines located on the front panel of the Pulse Sequence Controller board in the digital cardcage.		
	• UNITY and VXR-S have two spare lines on the Interface board.		

/

	• GEMINI 2000 has one spare line.	
Examples:	<pre>splon(); sp5on();</pre>	
Related:	<pre>sp#off Turn off specified spare line</pre>	
spinlock	Control spin lock on observe transmitter	
Applicability:	Systems with a waveform generator on the observe transmitter channel.	
Syntax:	<pre>spinlock(pattern,90_pulselength,tipangle_resoln, \ phase,ncycles) char *pattern;</pre>	
Description:	Executes a waveform-generator-controlled spin lock on the observe transmitter. Both the rf gating and the mixing delay are handled within this function.	

- Description: Executes a waveform-generator-controlled spin lock on the observe transmitter. Both the rf gating and the mixing delay are handled within this function. Arguments can be variables (which require the appropriate getval and getstr statements) to permit changes via parameters (see the second example below).
- Arguments: pattern is the name of the text file in the shapelib directory that stores the decoupling pattern (leave off the .DEC file extension).
 90_pulselength is the pulse duration for a 90° tip angle on the observe

yo_pulselength is the pulse duration for a 90° tip angle on the observe transmitter.

tipangle_resoln is the resolution in tip-angle degrees to which the decoupling pattern is stored in the waveform generator.

phase is the phase angle of the spin lock. It must be a real-time variable (v1 to v14, oph, etc.).

ncycles is the number of times that the spin-lock pattern is to be executed.

```
Examples: spinlock("mlev16", pw90, 90.0, v1, 50);
spinlock(locktype, pw, resol, v1, cycles);
Related: decspinlock First decoupler spinlock waveform control
```

Related:	decspinlock	First decoupler spin lock waveform control
	dec2spinlock	Second decoupler spin lock waveform control
	dec3spinlock	Third decoupler spin lock waveform control

starthardloop Start hardware loop

Applicability:	All systems except the <i>GEMINI 2000</i> and any system equipped with an Output board, Part. No. 00-953520-0#, where # is from 0 to 4.	
Syntax:	<pre>starthardloop(vloop) codeint vloop; /* real-time variable for loop count */</pre>	
Description:		
	Only instructions that require no further intervention by the acquisition computer (pulses, delays, acquires, and other scattered instructions) are allowed	

computer (pulses, delays, acquires, and other scattered instructions) are allowed in a hard loop. Most notably, no real-time math statements are allowed, thereby precluding any phase cycle calculations. The number of events included in the hard loop, including the total number of data points if acquisition is performed, is subject to the following limitations:

- 2048 or less for the Data Acquisition Controller board, Pulse Sequence Controller board, or *MERCURY-VX* and *MERCURY* STM/Output board.
- 1024 or less for the Acquisition Controller board.
- 63 or less for the Output board (see the description section of the acquire statement for further information about these boards).

In all cases, the number of events must be greater than one. No nesting of hard loops is allowed.

For the Output board, a hardware loop must be preceded by some timed event other than an explicit acquisition or another hardware loop. If two hardware loops must follow one another, it will therefore be necessary to insert a statement like delay(0.2e-6) between the first endhardloop and the second starthardloop. With only a single hardware loop, there is no timing limitation on the length of a single cycle of the loop. With two hardware loops (such as a loop of pulses and delays followed by an implicit acquisition), the first hardware loop must have a minimum cycle length of approximately 80 µs. With three or more hardware loops, loops that are not the first or last must have a minimum cycle length of about 100 µs.

For the Data Acquisition Controller, Pulse Sequence Controller, Acquisition Controller, and *MERCURY-VX* and *MERCURY* STM/Output boards, there are no timing restrictions between multiple, back-to-back hard loops. There is one subtle restriction placed on the actual duration of a hard loop if back-to-back hard loops are encountered: the duration of the *i*th hard loop must be $N(i+1) * 0.4 \mu$ s, where N(i+1) is the number of events occurring in the (i+1)th hard loop.

- Arguments: vloop is the number of hardware loop repetitions. It must be a real-time variable (v1 to v14, ct, etc.) and *not* an integer, a real number, or a regular variable.
- Examples: starthardloop(v2);

Related: acquire		Explicitly acquire data	
	endhardloop	End hardware loop	

status

Change status of decoupler and homospoil

Syntax: status(state)

int state; /* index: A, B, C, ..., Z */

Description: Controls decoupler and homospoil gating (homospoil not available on the *GEMINI 2000*). Parameters controlled by status are dm (first decoupler mode), dmm (first decoupler modulation mode), and hs (homospoil). For systems with a third rf channel, dm2 (second decoupler mode), dm3 (third decoupler mode), dmm2 (second decoupler modulation mode), and dmm3 (third decoupler modulation mode) are also controlled.

Each of these parameters can have multiple states: status(A) sets each parameter to the state described by the first letter of its value, status(B) uses the second letter, etc. If a pulse sequence has more status statements than there are status modes for a particular parameter, control reverts to the last letter of the parameter value. Thus if dm = 'ny', status(C) will look for the third letter, find none, and then use the second letter (y) and turn the decoupler on (actually, leave the decoupler on). The states do not have to increase monotonically during a pulse sequence. It is perfectly possible to write a pulse sequence that starts with status(A), goes later to status(B), then goes back to status(A), then to status(C), etc.

Homospoil is treated slightly differently than the decoupler. If a particular homospoil code letter is 'y', delays coded as hsdelay that occur during the time the status corresponds to that code letter will begin with a homospoil pulse, the duration of which is determined by the parameter hst. Thus if hs='ny', all hsdelay delays that occur during status(B) will begin with a homospoil pulse. The final status always occurs during acquisition, at which time a homospoil pulse is not permitted. Thus, if a particular pulse sequence uses status(A), status(B), and status(C), dm and other decoupler parameters can have up to three letters, but hs has only two, because having hs='y' during status(C) is meaningless and is consequently ignored.

On all systems with class C amplifiers, except the *GEMINI 2000*, to switch from low-power to high-power decoupling, insert dhpflag=TRUE; or dhpflag=FALSE; in a pulse sequence just before a status statement.

Arguments: state sets the status mode to A, B, C, ..., or Z.

Examples: status(A);

dhpflag	Switch decoupling from low-power to high-power
hsdelay	Delay specified time with possible homospoil pulse
setstatus	Set status of observe transmitter or a decoupler transmitter
statusdelay	Execute the status statement with a given delay time

statusdelay Execute the status statement with a given delay time

Applicability:

Related:

UNITY INOVA, UNITY plus, UNITY, VXR-S

Syntax: statusdelay(state,time)
 int state; /* index: A, B, C, ..., Z */
 double time; /* delay time, in sec. */

Description: Executes the status statement and delays for the time provided as an argument.

The current status statement takes a variable amount of time to execute, which depends on the number of rf channels configured in the system, the previous status state of each decoupler channel, and the new status state of each decoupler channel. This time is small (on the order of a few microseconds without programmable decoupling to tens of microseconds with programmable decoupling) but can be significant in certain experiments. statusdelay allows the user to specify a defined period of time for the status statement to execute.

If the amount of time given as an argument is not long enough to account for the overhead delays of status; the pulse sequence will still run, but a warning message will be generated to let the user know of the discrepancy.

The following table lists the maximum amount of time per channel for the status statement to execute.

System	Without programmable decoupling (µs)	With programmable decoupling (µs)
UNITYINOVA	2.5	2.5
UNITY <i>plus</i>	5.75	10.35

	System	Without programmable decoupling (µs)	With programmable decoupling (µs)
	UNITY	2.15	12.9
	VXR-S	0	10.75
Arguments:	state specifies the s	tatus mode as A,B,C,,Z.	
	time specifies the del	ay time, in seconds.	
Examples:	statusdelay(A,d statusdelay(B,0		
Related:	status Chang	e status of decoupler and home	ospoil
stepsize	Set small-angle pha	se step size, rf type C or	D
Applicability:	Systems with rf type C or D, and <i>MERCURY-VX</i> and <i>MERCURY</i> . This statement is due to be eliminated in future versions of VNMR software. Although it is still functional, you should not write any pulse sequences using it and should replace it in existing sequences with obsstepsize, decstepsize, dec2stepsize, or dec3stepsize, as appropriate.		
Syntax:	<pre>stepsize(step_size,device) double step_size; /* step size of phase shifter */ int device;</pre>		-
Description:	Sets the step size of the small-angle phase increment for a particular device. The phase information into statements decpulse, decrgpulse, dec2rgpulse, dec3rgpulse, pulse, rgpulse, and simpulse is still expressed in units of 90°.		
Arguments:	step_size is a real number or a variable for the phase step size desired.		
	device is OBSch (observe transmitter) or DECch (first decoupler). For the UNITY <i>INOVA</i> and UNITY <i>plus</i> only, device can also be DEC2ch (second decoupler) or DEC3ch (third decoupler). The step_size phase shift selected is active only for the xmtrphase statement if device is OBSch, only for the dcplrphase statement if device is DECch, only for the dcplr2phase statement if device is DEC2ch, or only for the dcplr3phase statement if the device is DEC3ch.		
Examples:	stepsize(30.0,0 stepsize(step,D		
Related:	dcplrphase dcplr2phase dcplr3phase decstepsize dec2stepsize dec3stepsize obsstepsize xmtrphase	Set small-angle phase of first Set small-angle phase of seco Set small-angle phase of third Set step size of first decouple Set step size of second decoup Set step size of third decouple Set step size of observe transport Set small-angle phase of observe	nd decoupler, rf type C or D l decoupler, rf type C or D r pler er mitter
sub	Subtract integer val	ues	
Syntax:	_		
	codeint vi; /*	real-time variable real-time variable	

codeint vj; /* real-time variable for subtrahend */
codeint vk; /* real-time variable for difference */

Description: Sets the value of vk equal to vi-vj.

Arguments: vi is the integer value of the minuend, vj is the integer value of the subtrahend, and vk is the difference of vi and vj. Each argument must be a real-time variable (v1 to v14, oph, etc.).

Examples: sub(v2, v5, v6);

Related:	add	Add integer values
	assign	Assign integer values
	dbl	Double an integer value
	decr	Decrement an integer value
	divn	Divide integer values
	hlv	Half the value of an integer
	incr	Increment an integer value
	mod2	Find integer value modulo 2
	mod4	Find integer value modulo 4
	modn	Find integer value modulo n
	mult	Multiply integer values

Т

tsadd	Add an integer to AP table elements		
Applicability:	All systems except the GEMINI 2000.		
Syntax:	<pre>tsadd(table,scalarval,moduloval) codeint table; /* real-time table variable */ int scalarval; /* integer added */ int moduloval; /* modulo value of result */</pre>		
Description:	A run-time scalar operation that adds an integer to elements of an AP table.		
Arguments:	table specifies the name of the table (t1 to t60).		
	scalarval is an integer to be added to each element of the table.		
	moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0.		
Examples:	tsadd(t31,4,4);		
Related:	tsdivDivide an integer into AP table elementstsmultMultiply an integer with AP table elementstssubSubtract an integer from AP table elements		
tsdiv	Divide an integer into AP table elements		
Applicability:	All systems except the GEMINI 2000.		
Syntax:	<pre>tsdiv(table,scalarval,moduloval) codeint table; /* real-time table variable */ int scalarval; /* integer divisor */ int moduloval; /* modulo value of result */</pre>		
Description:	A run-time scalar operation that divides an integer into the elements of an AP table.		
Arguments:	table specifies the name of the table (t1 to t60).		

scalarval is an integer to be divided into each element of the table. scalarval must not equal 0; otherwise, an error is displayed and PSG aborts. moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0. Examples: tsdiv(t31,4,4); Related: tsadd Add an integer to AP table elements tsmult Multiply an integer with AP table elements tssub Subtract an integer from AP table elements tsmult Multiply an integer with AP table elements Applicability: All systems except the GEMINI 2000. Syntax: tsmult(table,scalarval,moduloval) codeint table; /* real-time table variable */ int scalarval; /* integer multiplier */ /* modulo value of result */ int moduloval; Description: A run-time scalar operation that multiplies an integer with the elements of an AP table. Arguments: table specifies the name of the table (t1 to t60). scalarval is an integer to be multiplied with each element of the table. moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0. Examples: tsmult(t31,4,4); Add an integer to AP table elements Related: tsadd tsdiv Divide an integer into AP table elements tssub Subtract an integer from AP table elements Subtract an integer from AP table elements tssub Applicability: All systems except the GEMINI 2000. Syntax: tssub(table,scalarval,moduloval) codeint table; /* real-time table variable */ int scalarval; /* integer subtracted */ /* modulo value of result */ int moduloval; Description: A run-time scalar operation that subtracts an integer from the elements of an AP table. Arguments: table specifies the name of the table (t1 to t60). scalarval is an integer to be subtracted from each element of the table. moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0. Examples: tssub(t31,4,4); Related: tsadd Add an integer to AP table elements tsdiv Divide an integer into AP table elements Multiply an integer with AP table elements tsmult

ttadd Add an AP table to a second table

Applicability: All systems except the GEMINI 2000.

Syntax:	<pre>ttadd(table_dest,table_mod,moduloval) codeint table_dest; /* real-time table variable */ codeint table_mod; /* real-time table variable */ int moduloval; /* modulo value of result */</pre>		
Description:	A run-time vector operation that adds one AP table to a second table.		
Arguments:	tablenamedest is the name of the destination table (t1 to t60).		
	table_mod is the name of the table (t1 to t60) that modifies table_dest. Each element in table_dest is modified by the corresponding element in table_mod and the result is stored in table_dest. The number of elements in table_dest must be greater than or equal to the number of elements in table_mod.		
	moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0.		
Examples:	ttadd(t28,t42,6);		
Related:	ttdiv Divide an AP table into a second table		
	ttmult Multiply an AP table by a second table		
	ttsub Subtract an AP table from a second table		
ttdiv	Divide an AP table into a second table		
Applicability:	All systems except the GEMINI 2000.		
Syntax:	<pre>ttdiv(table_dest,table_mod,moduloval) codeint table_dest; /* real-time table variable */ codeint table_mod; /* real-time table variable */ int moduloval; /* modulo value of result */</pre>		
Description:	A run-time vector operation that divides one AP table into a second table.		
Arguments:	table_dest is the name of the destination table (t1 to t60).		
	table_mod is the name of the table (t1 to t60) that modifies table_dest. Each element in table_dest is modified by the corresponding element in table_mod and the result is stored in table_dest. The number of elements in table_dest must be greater than or equal to the number of elements in table_mod. No element in table_mod can equal 0.		
	moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0.		
Examples:	ttdiv(t28,t42,6);		
Related:	ttaddAdd an AP table to a second tablettmultMultiply an AP table by a second tablettsubSubtract an AP table from a second table		
ttmult	Multiply an AP table by a second table		
Applicability:			
Syntax:	<pre>ttmult(table_dest,table_mod,moduloval) codeint table_dest; /* real-time table variable */ codeint table_mod; /* real-time table variable */ int moduloval; /* modulo value of result */</pre>		
Description:	A run-time vector operation that multiplies one AP table by a second table.		
Arguments:			

table_mod is the name of the table (t1 to t60) that modifies table_dest. Each element in table_dest is modified by the corresponding element in table_mod and the result is stored in table_dest. The number of elements in table_dest must be greater than or equal to the number of elements in table_mod.

moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0.

Examples: ttmult(t28,t42,6);

Related:	ttadd	Add an AP table to a second table
	ttdiv	Divide an AP table into a second table
	ttsub	Subtract an AP table from a second table

ttsub Subtract an AP table from a second table

Applicability: All systems except the GEMINI 2000.

Description: A run-time vector operation that subtracts one AP table from a second table.

Arguments: table_dest is the name of the destination table (t1 to t60).

table_mod is the name of the table (t1 to t60) that modifies table_dest. Each element in table_dest is modified by the corresponding element in table_mod and the result is stored in table_dest. The number of elements in table_dest must be greater than or equal to the number of elements in table_mod.

moduloval is the modulo value taken on the result of the operation if moduloval is greater than 0.

Examples: ttsub(t28,t42,6);

Related:	ttadd	Add an AP table to a second table
	ttdiv	Divide an AP table into a second table
	ttmult	Multiply an AP table by a second table

Set quadrature phase of observe transmitter txphase Syntax: txphase(phase) codeint phase; /* variable for quadrature phase */ Description: Sets the observe transmitter quadrature phase to the value referenced by the real-time variable so that the transmitter phase is changed independently from a pulse. This may be useful to "preset" the transmitter phase at the beginning of a delay that precedes a particular pulse. For example, in the sequence txphase(v2); delay(d2); pulse(pw, v2);, the transmitter phase is changed at the start of the d2 delay. In a "normal" sequence, an rof1 time precedes the pulse to change the transmitter phase. phase is the quadrature phase for the observe transmitter. It must be a real-time Arguments: variable (v1 to v14, oph, ct, etc.). Examples: txphase(v3); Related: decphase Set quadrature phase of first decoupler

dec2phaseSet quadrature phase of second decouplerdec3phaseSet quadrature phase of third decoupler

V

vagradient	Variable angle gradient		
Syntax:	<pre>vagradient(gradlvl, double gradlvl; double theta; double phi;</pre>	<pre>theta,phi) /* gradient amplitude in G/cm */ /* angle from z axis in degrees */ /* angle of rotation in degrees */</pre>	
Description:	Applies a gradient of amplitude gradlvl at an angle theta from the <i>z</i> axis and rotated about the <i>xy</i> plane at an angle phi. Information from a gradient table is used to scale and set the values correctly. The values applied to each gradient axis are as follows:		
	<pre>x = gradlvl * (sin(y = gradlvl * (cos(z = gradlvl * (cos(</pre>	phi)*sin(theta))	
	To turn off the gradients, add	adients at the given levels until they are turned off. a vagradient statement with gradlvl set to ll_gradients statement.	
		re are actions to be performed while the gradients mpler to use if there are no other actions performed	
Arguments:	gradlvl is the gradient amplitude, in gauss/cm.		
	theta defines the angle, in	degrees, from the z axis.	
	phi defines the angle of rot	ation, in degrees, about the xy plane.	
Examples:	<pre>vagradient(3.0, 54.7, 0.0); pulse(pw,oph); delay(0.001 - pw); zero_all_gradients();</pre>		
Related:	magradpulse mashapedgradient mashapedgradpulse vagradpulse vashapedgradient vashapedgradpulse	Simultaneous gradient at the magic angle Simultaneous gradient pulse at the magic angle Simultaneous shaped gradient at the magic angle Simultaneous shaped gradient pulse at the magic angle Variable angle gradient pulse Variable angle shaped gradient Variable angle shaped gradient Zero all gradients	
vagradpulse	Variable angle gradient p	ulse	
Applicability:	Not applicable on MERCUR	PY-VX, MERCURY, and GEMINI 2000.	
Syntax:	<pre>vagradpulse(gradlvl double gradlvl; double gradtime; double theta; double phi;</pre>	,gradtime,theta,phi) /* gradient amplitude in G/cm */ /* gradient time in sec */ /* angle from z axis in degrees */ /* angle of rotation in degrees */	

Description: Applies a gradient pulse of amplitude gradlvl at an angle theta from the z axis and rotated about the xy plane at an angle phi. Information from a gradient table is used to scale and set the values correctly. The values applied to each gradient axis are as follows:

```
x = gradlvl * (sin(phi)*sin(theta))
y = gradlvl * (cos(phi)*sin(theta))
z = gradlvl * (cos(theta))
```

The gradients are turned off after gradtime seconds.

vagradpulse is simpler to use if there are no other actions while the gradients are on. vagradient is used if there are actions to be performed while the gradients are on.

Arguments: gradlvl is the gradient amplitude, in gauss/cm.

gradtime is the time, in seconds, to apply the gradient.

theta is the angle, in degrees, from the z axis

phi is the angle of rotation, in degrees, about the *xy* plane.

Examples: vagradpulse(3.0,0.001,54.7,0.0);

magradient	Simultaneous gradient at the magic angle
magradpulse	Simultaneous gradient pulse at the magic angle
mashapedgradient	Simultaneous shaped gradient at the magic angle
mashapedgradpulse	Simultaneous shaped gradient pulse at the magic angle
vagradient	Variable angle gradient
vashapedgradient	Variable angle shaped gradient
vashapedgradpulse	Variable angle gradient pulse
zero_all_gradients	Zero all gradients
	magradpulse mashapedgradient mashapedgradpulse vagradient vashapedgradient vashapedgradpulse

vashapedgradientVariable angle shaped gradient

Applicability:	Not applicable on MERCUR	Y-V	X, MERCURY, and GEMINI 2000.
Syntax:	<pre>vashapedgradient(pa phi,loops,wait)</pre>	tte	$rn, gradlvl, gradtime, theta, \setminus$
	char* pattern;	/*	<pre>name of gradient shape text file */</pre>
	double gradlvl;	/*	gradient amplitude in G/cm */
	double gradtime;	/*	time to apply gradient in sec */
	double theta;	/*	angle from z axis in degrees */
	double phi;	/*	angle of rotation in degrees */
	int loops;	/*	number of waveform loops */
	int wait;	/*	WAIT or NOWAIT */
Descriptions	A multice a supplicant allows and		we with an amplitude areadler, at an angle

Description: Applies a gradient shape pattern with an amplitude gradlvl at an angle theta from the z axis and rotated about the xy plane at an angle phi. Information from a gradient table is used to scale and set the values correctly. The amplitudes applied to each gradient axis are as follows:

```
x = gradlvl * (sin(phi)*sin(theta))
y = gradlvl * (cos(phi)*sin(theta))
z = gradlvl * (cos(theta))
```

vashapedgradient leaves the gradients at the given levels until they are turned off. To turn off the gradients, add another vashapedgradient statement with gradlvl set to zero or insert a zero_all_gradients statement. Note that vashapedgradient assumes the gradient pattern zeroes the gradients at its end, and it does not explicitly zero the gradients. vashapedgradient is used if there are actions to be performed while the gradients are on,

Arguments: pattern is a text file that describes the shape of the gradient. The text file is located in \$vnmrsystem/shapelib or in the users directory \$vnmruser/shapelib.

gradlvl is the gradient amplitude, in gauss/cm.

gradtime is the time, in seconds, to apply the gradient.

theta is the angle, in degrees, from the z axis.

phi is the angle of rotation, in degrees, about the *xy* plane.

loops is a value from 0 to 255 to loop the selected waveform. Gradient waveforms on the UNITY *INOVA* do not use this field and it should be set to 0.

wait is a keyword, either WAIT or NOWAIT, that selects whether or not a delay is inserted to wait until the gradient is completed before executing the next statement.

```
Examples: vashapedgradient("ramp_hold",3.0,trise,54.7, \
        0.0,0,NOWAIT);
    pulse(pw,oph);
    delay(0.001-pw-2*trise);
    vashapedgradient("ramp_down",3.0,trise,54.7, \
        0.0,0,NOWAIT);
```

Related:	magradient	Simultaneous gradient at the magic angle
	magradpulse	Simultaneous gradient pulse at the magic angle
	mashapedgradient	Simultaneous shaped gradient at the magic angle
	mashapedgradpulse	Simultaneous shaped gradient pulse at the magic angle
	vagradient	Variable angle gradient
	vagradpulse	Variable angle gradient pulse
	vashapedgradpulse	Variable angle shaped gradient pulse
	zero_all_gradients	Zero all gradients

vashapedgradpulse Variable angle shaped gradient pulse

Applicability:	Not applicable on MERCURY	VX, MERCURY, and GEMINI 2000.
Syntax:	<pre>vashapedgradpulse(pa theta,phi)</pre>	ttern, gradlvl, gradtime, \setminus
	char *pattern;	/* gradient shape text file */
	double gradlvl;	/* gradient amplitude in G/cm */
	double gradtime;	/* gradient time in seconds */
	double theta;	<pre>/* angle from z axis in degrees */</pre>
	double phi;	<pre>/* angle of rotation in degrees */</pre>
Description:	theta from the z axis and ro	tern with an amplitude gradlvl at an angle tated about the <i>xy</i> plane at an angle phi. ble is used to scale and set the values correctly.

```
x = gradlvl * (sin(phi)*sin(theta))
y = gradlvl * (cos(phi)*sin(theta))
z = gradlvl * (cos(theta))
```

The amplitudes applied to each gradient axis are as follows:

The gradient are turned off after gradtime seconds. Note that vashapedgradpulse assumes that the gradient pattern zeroes the gradients at its end and does not explicitly zero the gradients.

vashapedgradpulse is simpler to use then the vashapedgradient statement if there are no other actions while the gradients are on. vashapedgradient is used when there are actions to be performed while the gradients are on.

Arguments: pattern is a text file that describes the shape of the gradient. The text file is located in \$vnmrsystem/shapelib or in the user directory \$vnmruser/ shapelib.

gradlvl is the gradient amplitude, in gauss/cm.

gradtime is the time, in seconds, to apply the gradient.

theta is the angle, in degrees, from the z axis.

phi is the angle of rotation, in degrees, about the xy plane.

Examples: vashapedgradpulse("hsine",3.0,0.001,54.7,0.0);

Related:	magradient	Simultaneous gradient at the magic angle
	magradpulse	Simultaneous gradient pulse at the magic angle
	mashapedgradient	Simultaneous shaped gradient at the magic angle
	mashapedgradpulse	Simultaneous shaped gradient pulse at the magic angle
	vagradient	Variable angle gradient
	vagradpulse	Variable angle gradient pulse
	vashapedgradient	Variable angle shaped gradient
	zero_all_gradients	Zero all gradients

Set delay with fixed timebase and real-time count vdelay

Applicability: All systems except MERCURY-VX, MERCURY, and GEMINI 2000. Syntax: vdelay(timebase, count) int timebase: /* NGEC HORA MORA on CEC */

	int timebase;	/ ^	NSEC, USEC, MSEC, or SEC */	
	codeint count;	/*	real-time variable for count */	
ription:	Sets a delay for a time perio	od e	qual to the product of the specified timebase	

- Descrip periou equal to the ay e pi ۶P and the count.
- Arguments: timebase is one of the four defined time bases: NSEC (see note below), USEC (microseconds), MSEC (milliseconds), or SEC (seconds).

count is a real-time variable (v1 to v14). For predictable acquisition, the realtime variable should have a value of 2 or more.

If timebase is set to NSEC, the delay depends on which acquisition controller board is used on the system (see the description section of the acquire statement for further information about these boards.):

- On systems with a Data Acquisition Controller board, the minimum delay is a count of 0 (100 ns), and a count of *n* corresponds to a delay of (100 +(12.5*n)) ns. For example, vdelay(NSEC, v1), when v1=4, gives a delay of (100 + (12.5*4)) ns or 150 ns.
- On systems with a Pulse Sequence Controller board or an Acquisition Controller board, the minimum delay is a count of 2 (200 ns). A count greater than 2 is the minimum delay plus the resolution (25 ns) of the board. For example, vdelay(NSEC, v1), when v1=4, gives a delay of (200 +25) ns or 225 ns.
- On systems with Output boards, the minimum delay is a count of 2 (200 ns). A count greater than 2 is the minimum delay plus the resolution (100 ns) of the board. For example, vdelay (NSEC, v1), when v1=4, gives a delay of (200 + 100) ns or 300 ns.

```
Examples: vdelay(USEC,v3);
```

Related:	create_delay_list	Create table of delays
	delay	Delay for a specified time
	hsdelay	Delay specified time with possible homospoil pulse
	idelay	Delay for a specified time with IPA
	incdelay	Real time incremental delay
	initdelay	Initialize incremental delay
	vfreq	Select frequency from table
	voffset	Select frequency offset from table
	vdelay_list	Get delay value from delay list with real-time index

```
vdelay_list Get delay value from delay list with real-time index
   Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.
        Syntax: vdelay_list(list_number,vindex)
                /* real time variable */
                codeint vindex;
    Description: Provides a means of indexing into previously created delay lists using a real-
                time variable or an AP table. The indexing into the list is from 0 to N-1, where
                N is the number of items in the list. The delay table has to have been created
                with the create_delay_list statement. It has no return value.
     Arguments: tlist number is the number between 0 and 255 for each list. This number
                must match the list_number used when creating the table.
                vindex is a real-time variable (v1 to v14) or an AP table (t1 to t60).
     Examples: pulsesequence()
                {
                . . .
                int noffset, ndelay, listnum;
                double offsets1[256],offsets2[256],delay[256];
                . . .
                /* initialize offset and delay lists */
                create_offset_list(offsets1,noffset,OBSch,0);
                create_delay_list(delay,ndelay,1);
                create_offset_list(offsets2,noffset,DECch,2);
                voffset(0,v4); /* get v4 from observe offset list */
                vdelay_list(1,v5); /* get v5 from delay list */
                voffset(2,v4); /* get v4 from decouple offset list */
                . . .
                }
       Related:
                                       Create table of delays
                create_delay_list
                delay
                                       Delay for a specified time
                                       Delay specified time with possible homospoil pulse
                hsdelay
                                       Delay for a specified time with IPA
                idelay
                incdelay
                                       Real time incremental delay
                                       Initialize incremental delay
                initdelay
                                       Select frequency from table
                vfreq
                voffset
                                       Select frequency offset from table
                                       Set delay with fixed timebase and real-time count
                vdelay
```

vfreq	Select frequency from table		
Applicability:	Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.		
Syntax:	<pre>vfreq(list_number,vindex) int list_number; /* same index as for create_freq_list */ codeint vindex; /* real-time variable */</pre>		
Description:	Provides a means of indexing into previously created frequency lists using a real-time variable or an AP table. The indexing into the list is from 0 to $N-1$, where N is the number of items in the list. The frequency table must have been created with the create_freq_list statement. It has no return value.		
Arguments:	<pre>list_number is the number between 0 and 255 for each list. This number must match the list_number used when creating the table.</pre>		
	vindex is a real-time variable (v1 to v14) or an AP table (t1 to t60).		
Examples:	See the example for the vdelay statement.		
Related:	create_freq_listCreate table of frequenciesvdelaySelect delay from tablevoffsetSelect frequency offset from table		
vgradient	Set gradient to a level determined by real-time math		
Applicability:	Systems with imaging or PFG modules. Not applicable to <i>MERCURY-VX</i> , <i>MERCURY</i> , and <i>GEMINI 2000</i> systems.		
Syntax:	<pre>vgradient(channel,intercept,slope,mult) char channel; /* gradient channel 'x', 'y' or 'z' */ int intercept; /* initial gradient level */ int slope; /* gradient increment */ codeint mult; /* real-time variable */</pre>		
Description:	Provides a dynamic variable gradient controlled using the AP real-time math functions. It has no return value. The statement drives the chosen gradient to the level defined by the formula:		
	level = intercept + slope*mult.		
	The gradient level ranges from -2047 to $+2047$ for systems with 12-bit DACs, or from -32767 to $+32767$ for gradients using the waveform generators, which have 16- bit DACs. If the requested level lies outside this range, it is rounded to the appropriate boundary value.		
	After vgradient, the action of the gradient is controlled by the gradient power supply. The gradient level is ramped at the preset slew rate (2047 DAC units per millisecond) to the value requested by vgradient. This fact becomes a concern when using vgradient in a loop with a delay element, in order to produce a modulated gradient. The delay element should be sufficiently long so as to allow the gradient to reach the assigned value: $delay \ge \frac{ new_level - old_level }{2047} \times risetime$		
Arguments:	channel specifies the gradient to be set and is one of the characters 'X', 'x', 'Y', 'Y', 'Z', or 'z'. In imaging, channel can also be 'gread', 'gphase', or 'gslice'.		
	intercept and slope are integers. In imaging, intercept is the initial gradient DAC setting and slope is the gradient DAC increment.		
	mult is a real-time variable (v1 to v14, etc.). In imaging, mult is set so that intercept+slope*mult is the output.		

```
Examples: (1) mod2(ct,v10);
                                            /* v10 is 0,1,0,1,0,1,... */
                vgradient('z',0,2000,v10);
                                  /* z gradient is 0,2000,0,2000,... */
                delay(d2);
                                              /* delay for duration d2 */
                rgradient('z',0.0);
                                             /* gradient turned off */
                 (2) mod4(ct,v10);
                                   /* v10 is 0,1,2,3,4,0,1,2,3,4,... */
                vgradient('z',-5000.0,2500.0,v10);
                                        /* z is -5000,-2500,0,2500 */
                (3) pulsesequence()
                 {
                 . . .
                char gphase, gread, gslice;
                 int amplitude, igpe, stat;
                double gpe;
                 . . .
                gpe = getval("gpe");
                amplitude = (int)(0.5*ni*gpe);
                igpe = (int)gpe;
                stat =
                getorientation(&gread,&gphase,&gslice,"orient");
                 . . .
                 initval(nf,v9);
                loop(v9,v5);
                    . . .
                    vgradient(gphase,amplitude,igpe,v5);
                    . . .
                 endloop(v5);
                 . . .
                 }
       Related:
                                       Draw delay or pulses in a sequence for graphical display
                dps_show
                                       Read image plane orientation
                getorientation
                rgradient
                                       Set gradient to specified level
                shapedgradient
                                       Provide shaped gradient pulse to gradient channel
                                       Generate arrayed shaped gradient pulse
                shaped2Dgradient
                shapedvgradient
                                       Generate dynamic variable shaped gradient pulse
                 zgradpulse
                                       Create a gradient pulse on the z channel
voffset
                Select frequency offset from table
   Applicability: Not applicable on MERCURY-VX, MERCURY, and GEMINI 2000.
        Syntax: voffset(list_number,vindex)
                 int list_number;
                                      /* number of list */
                                       /* real-time or AP table variable */
                codeint vindex;
    Description: Provides a means of indexing into previously created frequency offset lists
                using a real-time variable or an AP table. The indexing into the list is from 0 to
                N-1, where N is the number of items in the list. The offset table has to have been
                created with the create offset list statement. It has no return value.
     Arguments: list_number is the number between 0 and 255 for each list. This number
```

must match the list_number used when creating the table. vindex is a real-time variable (v1 to v14) or an AP table (t1 to t60).

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Examples: See the example for the vdelay statement. Related: create_offset_list Create table of frequency offsets Select delay from table vdelay vfreq Select frequency from table Provide dynamic variable scan vscan Applicability: Systems with imaging capability. Syntax: vscan(rtvar) codeint rtval; /* AP math variable */ Description: Provides a dynamic scan capability for compressed-compressed image sequences. It uses an AP real-time variable as a counter. This real-time variable must be supplied by the user, but need not be initialized since the init_vscan statement provides the initialization. vscan uses the standard nt parameter to determine the number of scans it performs. Since it is a realtime variable, it is limited to 32K scans. When vscan is used, system-supplied scan functionality is disabled, similar to the use of the acquire statement. vscan has no return value. Arguments: rtvar is an AP math variable (v1 to v14). Its range is 1 to 32767. Examples: pulsesequence() ł . . . char gphase, gread, gslice; int amplitude, igpe, stat; double gpe; . . . initval(nv,v10); initval(nf,v9); loop(v10,v6); init_vscan(v11,np*nf); loop(v9,v5);. . . acquire(np,1/sw); . . . endloop(v5);vscan(v11); endloop(v6); . . . } Related: Explicitly acquire data acquire init_vscan Initialize real-time variable for vscan statement Set user AP register using real-time variable vsetuserap Applicability: UNITY INOVA systems. Syntax: vsetuserap(vi,register) codeint vi; /* variable output to AP bus register */ /* AP bus register: 0, 1, 2, or 3 */ int register; Description: Sets one of the four 8-bit AP bus registers that provide an output interface to custom user equipment. The outputs of these registers go the USER AP

connectors J8212 and J8213, located on the back of the left console cabinet. The outputs have a 100-ohm series resistor for circuit protection.

Arguments: vi is an index to a real-time variable that contains a signed or unsigned real number or integer to output to the specified user AP register.

register is the AP register number, mapped to output lines as follows:

- Register 0 is J8213, lines 9 to 16.
- Register 1 is J8213, lines 1 to 8.
- Register 2 is J8212, lines 9 to 16.
- Register 3 is J8212, lines 1 to 8.

Examples: vsetuserap(v1,1);

Related:	readuserap	Read input from user AP register
	setuserap	Set user AP register

vsli Set SLI lines from real-time variable

Applicability: Systems with imaging capability and the Synchronous Line Interface (SLI) board, an option that provides an interface to custom user equipment.

lress,mode,var)		
ess; /* SLI	I board address */	
; /* SLI	I_SET, SLI_OR, SLI_AND, SLI_XOR	*/
var; /* rea	al-time variables for SLI lines	*/
ę	; /* SLI	ess; /* SLI board address */ ; /* SLI_SET, SLI_OR, SLI_AND, SLI_XOR

Description: Sets lines from real-time variables on the SLI board. It has no return value.

vsli has a pre-execution delay of 10.950 μ s but no post-execution delay. The delay is composed of a 200-ns startup delay with 5 AP bus cycles (1 AP bus cycle = 2.150 μ s).

The logic levels on the SLI lines are not all set simultaneously. The four bytes of the 32 bit word are set consecutively, the low-order byte first. The delay between setting of consecutive bytes is 1 AP bus cycle ± 100 ns. (This 100-ns timing jitter is non-cumulative.)

The following error messages are possible:

- Illegal mode: n is caused by the mode argument *not* being one of SLI_SET, SLI_OR, SLI_XOR, or SLI_AND.
- Illegal real-time variable: n is caused by the var argument being outside the range v1 to v13.
- Arguments: address is the address of the SLI board in the system. It must match the address specified by jumper J7R on the board. Note that the jumpers 19-20 through -2 specify bits 2 through 11, respectively. Bits 0 and 1 are always zero. An installed jumper signifies a "one" bit, and a missing jumper a "zero". The standard addresses for the SLI in the VME card cage:
 - Digital (left) side is C90 (hex) = 3216
 - Analog (right) side is 990 (hex) = 2448

mode determines how to combine the specified value with the current output of the SLI to produce the new output. The four possible modes:

- SLI_SET is to load the new value directly into the SLI
- SLI_OR is to logically OR the new value with the old
- SLI_AND is to logically AND the new value with the old

• SLI_XOR is to logically XOR the new value with the old

var specifies the real-time variables to use to set the SLI lines. Because the SLI has 32 bits and the real-time variables have only 16 bits, two real time variables are used for each call. The one specified in the calling sequence is used for the high-order word, and the next sequential real-time variable is used for the low-order word. Thus, legal values for var are v1 to v13.

Examples: pulsesequence()

```
{
...
int SLIaddr; /* Address of SLI board */
...
SLIaddr = getval("address");
...
vsli(SLIaddr, SLI_SET, v1);
...
}
```

Notice that address is not a standard parameter, but needs to be created by the user if it is mentioned in a user pulse sequence (for details, see the description of the create command).

Related:	sli	Set SLI lines
	sp#off	Turn off specified spare line
	sp#on	Turn on specified spare line

Х

xgate	Gate pulse sequence from an external event		
Applicability:	All systems except MERCURY-VX, MERCURY, and GEMINI 2000.		
Syntax:	<pre>xgate(events) double events; /* number of external events */</pre>		
Description:	Halts the pulse sequence. When the number of external events has occurred, the pulse sequence continues.		
Arguments:	events is the number of external events.		
Examples:	<pre>xgate(2.0); xgate(events);</pre>		
Related:	rotorperiodObtain rotor period of MAS rotorrotorsyncGated pulse sequence delay from MAS rotor position		
xmtroff	Turn off observe transmitter		
Syntax:	<pre>xmtroff()</pre>		
Description:	Explicitly gates off the observe transmitter in the pulse sequence.		
Related:	xmtron Turn on observe transmitter		
xmtron	Turn on observe transmitter		

Syntax: xmtron()

Description: Explicitly gates on the observe transmitter in the pulse sequence. Transmitter gating is handled automatically by the statements obspulse, pulse, rgpulse, shaped_pulse, simpulse, sim3pulse, simshaped_pulse, sim3shaped_pulse, and spinlock. The obsprgon statement generally needs to be enabled with an explicit xmtron statement and followed by a xmtroff call. Related: xmtroff Turn on observe transmitter Set transmitter small-angle phase, rf type C, D xmtrphase Applicability: All systems except GEMINI 2000. Syntax: xmtrphase(multiplier) codeint multiplier; /* real-time AP variable */ Sets the phase of transmitter in units set by the stepsize statement. The Description: small-angle phaseshift is a product of multiplier and the preset step size for the transmitter. If stepsize has not been used, the default step size is 90°. If the product of the step size set by the stepsize statement and multiplier is greater than 90°, the sub-90° part is set by xmtrphase. Carryovers that are multiples of 90° are automatically saved and added in at the time of the next 90° phase selection (such as at the time of the next pulse or decpulse). xmtrphase should be distinguished from txphase. xmtrphase is needed any time the transmitter phase shift is to be set to a value that is not a multiple of 90°. txphase is optional and rarely is needed. Arguments: multiplier is a small-angle phaseshift multiplier and must be an AP variable. Examples: xmtrphase(v1); Related: dcplrphase Set small-angle phase of first decoupler, rf type C or D dcplr2phase Set small-angle phase of second decoupler, rf type C or D dcplr3phase Set small-angle phase of third decoupler, rf type C or D Set small-angle phase step size, rf type C or D stepsize

Ζ

zero_all_gradients Zero all gradients

Syntax:	<pre>zero_all_gradients()</pre>		
Description:	Sets the gradients in the x , y , and z axes to zero.		
Examples:	<pre>vagradient(3.0, 54. delay(0.001); zero_all_gradients(</pre>		
Related:	vagradient vagradpulse vashapedgradient vashapedgradpulse	Variable angle gradient Variable angle gradient pulse Variable angle shaped gradient Variable angle shaped gradient pulse	

zgradpulse	Create a gradient pulse on the z channel		
Applicability:	Systems with imaging or PFG module.		
Syntax:	<pre>zgradpulse(value,delay) double value; /* amplitude of gradient on z channel */ double delay; /* length of gradient in sec */</pre>		
Description:	Creates a gradient pulse on the z channel with amplitude and duration given by the arguments. At the end of the pulse, the gradient is set to 0.		
Arguments:	value is the amplitude of the pulse. It is a real number between -32768 and 32767 .		
	delay is any delay parameter, such as d2.		
Examples:	<pre>zgradpulse(1234.0,d2);</pre>		
Related:	dps_show rgradient vgradient	Draw delay or pulses for graphical display of a sequence Set gradient to specified level Set gradient to level determined by real-time math	

Chapter 4. UNIX-Level Programming

Sections in this chapter:

- 4.1 "UNIX and VNMR," this page
- 4.2 "UNIX: A Reference Guide," page 278
- 4.3 "UNIX Commands Accessible from VNMR," page 280
- 4.4 "Background VNMR," page 280
- 4.5 "Shell Programming," page 282

UNIX is among the most popular operating systems in the world today, with hundreds of books written on every aspect of UNIX, at every level. This manual does not attempt to replace that material, but attempts instead to provide a glimpse of the subject and then to guide you to resources that can paint a fuller picture.

4.1 UNIX and VNMR

Many VNMR software users do not need to have any contact with UNIX whatsoever. Although the UNIX operating system is running the workstation at all times, a user who wants to use only the Varian VNMR software package can do just that. In some installations, the system operator starts VNMR and different users simply sit down at the instrument and use the NMR software, just as in the earlier generation of NMR spectrometers. The worst that could happen is that the previous user logged out, requiring the next user to log back in with their name and password. After completing this login procedure, the VNMR software starts automatically, and again you do not need to have contact with UNIX if you don't wish to do so.

UNIX provides more than a hundred "tools" that can perform almost anything short of complex mathematical manipulations like a Fourier transform. For example, UNIX has commands to search through your files, to sort line lists, to tell you who is on the system, to run a program unattended at night, and much more. The more performance you want to get out of your computer, and the more you want to be able to do, the more it will benefit you to learn about UNIX.

Dozens of manuals are available for your Sun computer system, and surely you will not want to or be able to read them all. For those with no exposure to UNIX, however, we strongly recommend that you read any user's guides that accompanied your Sun workstation. After that, a book we have found to be particularly useful is *The UNIX System* by S. R. Bourne (Addison-Wesley). For coverage of the Solaris environment, a good book is *Guide to Solaris* by John Pew (ZD Press).

4.2 UNIX: A Reference Guide

A brief overview of the UNIX computer operating system and its associated commands appears below. For more information on UNIX, refer to the Sun manuals covering Solaris or to UNIX general references found at larger bookstores.

Command Entry

Single command entry	commandname
Command names	Generally lowercase, case-sensitive
Multiple command separator	; (semicolon) or new line
Arguments	commandname arg1 arg2

File Names

Typical (shorthand names usually used)	/vnmr/fidlib/fidld
Level separator	/ (forward slash)
Individual filenames	Any number of characters (256 unique)
Characters in filenames	Underline, period often used
First character in filename	First character unrestricted

File Handling Commands

Delete (unlink) a file(s)	rmfilenames
Copy a file	cp filename newfilename
Rename a file	mv filename newfilename
Make an alias (link)	ln filename1 filename2
Sort files	sort filenames
Tape backup	tar

Directory Names

Home directory for each user	Directory assigned by administrator
Working directory	Current directory user is in
Shorthand for current directory	. (single period)
Shorthand for parent directory	(two periods)
Shorthand for home directory	~ (tilde character)
Root directory	/ (forward slash)

Directory Handling Commands

Create (or make) a directory	mkdir directoryname
Rename a directory	mv dirname newdirname
Remove an empty directory	rmdir directoryname
Delete directory and all files in it	rm -r directoryname
List files in a directory, short list	ls directoryname

List files in a directory, long list	ls -l directoryname
Copy file(s) into a directory	cp filenames directoryname
Move file(s) into a directory	mv filenames directoryname
Print working (current) directory	pwd
Change current directory	cd newdirectoryname

Text Commands

Edit a text file using vi editor	vi filename
Edit a text file using ed editor	ed filename
Edit a text file using textedit editor	textedit filename
Display first part of a file	head filename
Display last part of a file	tail filename
Concatenate and display files	cat filenames
Compare two files	cmp filename1 filename2
Compare two files deferentially	diff filename1 filename2
Print file(s) on line printer	lp filenames
Search file(s) for a pattern	grep expression filenames
Find spelling errors	spell filename

Other Commands

Pattern scanning and processing	awk pattern filename
Change file protection mode	chmod newmode filename
Display current date and time	date
Summarize disk usage	du -k
Report free disk space	df-k filesystem
Kill a background process	kill process-id
Sign onto system	login username
Send mail to other users	mail
Print out UNIX manual entry	man commandname
Process status	ps
Convert quantities to another scale	units
Who is on the system	W
System identification	uname -a

Special Characters

Send output into named file	> filename
Append output into named file	>> filename
Take input from named file	< filename
Send output from first command to input of second command (pipe)	(vertical bar)
Wildcard character for a single character in filename operations	?
Wildcard character for multiple characters in filename operations	*

Run program in background	&
Abort the current process	Control-C
Logout or end of file	Control-D

4.3 UNIX Commands Accessible from VNMR

Several UNIX commands are accessible directly from VNMR, including the vi, edit, shell, shelli, and w commands.

Opening a UNIX Text Editor from VNMR

Entering vi(file) or edit(file) from VNMR invokes a UNIX text editor for editing the name of the file given in the argument (e.g., vi('myfile')). On the Sun workstation, a popup screen contains the editing window. On the GraphOn terminal, the main screen becomes the editing window. Exiting from the editor closes the editing window.

The most useful UNIX program you can learn is vi, the powerful UNIX text editor. UNIX provides at least two other text editors, ed and textedit, that are easier to learn than vi, but vi is the most widely used UNIX text editor and worth learning because of its many features. A text editor is necessary if you wish to prepare or edit text files, such as macros, menus, and pulse sequences (short text files such as those used to annotate spectra are usually edited in simpler ways)

Opening a UNIX Shell from VNMR

Entering the shell command from VNMR without any argument brings up a normal UNIX shell. On the Sun, a popup window is created. On the GraphOn terminal, the entire terminal is used. Entering shell with the syntax shell(command)<:\$file1\$file2,...>

executes the UNIX command line given, displays any text lines generated, and returns control to VNMR when finished. If return arguments *file1*, *file2*,... are present, the results of the command line are returned to the files listed, with each file receiving a single display line, for example:

```
shell('ls -t|grep May'):$filelist)
```

On a terminal, the command shelli(command) runs interactively the UNIX command line given as the argument. No return or output variables are allowed. Under window-based VNMR, shelli is identical to the shell command.

To display information about who is on UNIX, enter the w command from VNMR.

4.4 Background VNMR

Running VNMR commands and processing as a UNIX background tasks are possible by using Vnmr and vbg commands from UNIX.

Running VNMR Command as a UNIX Background Task

VNMR commands can be executed as a UNIX background task by using the command Vnmr -mback <-n#> command_string <&>

where -mback is a keyword (entered exactly as shown), -n# sets that processing will occur in experiment # (e.g., -n2 sets experiment 2), and command_string is a VNMR command or macro. If -n# is omitted, processing occurs in experiment 1. If more than one command is to be executed, place double quote marks around the command string; e.g., "printon dg printoff"

UNIX background operation (&) is possible, as in Vnmr -mback wft2da &. Usually it is a good idea to use redirection (> or >>) with background processing: Vnmr -mback -n3 wft2da > vnmroutput &

The UNIX shell script vbg (see below) is also available to run VNMR processing in the background.

All text output, both normal text window output and the typical two-letter prompts that appear in the upper right ("FT", "PH", etc.), are directed to the UNIX output window.

Note the following characteristics of the Vnmr command:

- Full multiuser protection is implemented. If user vnmr1 is logged in and using experiment 1, and another person logs in as vnmr1 from another terminal and tries to use the background Vnmr, the second vnmr1 receives the message "experiment 1 locked" if that person tries to use experiment 1. The second user can use other experiments, however.
- Pressing Control-C does *not* work: if you type the UNIX command shown, you cannot abort it with Control-C.
- Operation within VNMR is possible using the shell command; e.g., shell('Vnmr -mback -n2 wftda')
- Plotting is possible; e.g.,
 Vnmr -mback -n3 "pl pscale pap page"
- Printing is possible; e.g.,
 Vnmr -mback "printon dg printoff"

Running VNMR Processing in the Background

The UNIX shell script vbg runs VNMR processing in the background. The main requirements are that vbg must be run from within a UNIX shell and that no foreground or other background processes can be active in the designated experiment. From UNIX, vbg is entered in the following form:

vbg # command_string <prefix>

where # is the number of an experiment (from 1 to 9) in the user's directory in which the background processing is to take place, command_string is one or more VNMR commands and macros to be executed in the background (double quotes surrounding the string are mandatory), and prefix is the name of the log file, making the full log file name prefix_bgf.log (e.g., to perform background plotting from experiment 3, enter vbg 3 "vsadj pl pscale pap page" plotlog).

The default log file name is #_bgf.log, where # is the experiment number. The log file is placed in the experiment in which the background processing takes place. Refer to the *VNMR Command and Parameter Reference* for more information on vbg.

4.5 Shell Programming

The shell executes commands given either from a terminal or contained in a file. Files containing commands and control flow notation, called *shell scripts*, can be created, allowing users to build their own commands. This section provides a very short overview of such programming; refer to the UNIX literature for more information.

Shell Variables and Control Formats

As a programming language, the shell provides string-valued variables: \$1, \$2,.... The number of variables is available as \$# and the file being executed is available as \$0. Control flow is provided by special notation, including if, case, while, and for. The following format is used:

```
if command-list (not Boolean)
then command-list
else command-list
fi
case word in
pattern) command-list;;
...
esac
while command-list
do command-list
```

Shell Scripts

The shell scripts below show two ways a shell script might be written for the same command. In both scripts, the command name lower is selected by the user and the intent of the command is to convert a file to lower case, but the scripts differ in features.

The first script:

```
: lower --- command to convert a file to lower case
: usage lower filename
: output filename.lower
tr '[A-Z]' '[a-z]' < $1 > $1.lower
```

The second script:

esac

In the first script, only one form of input is allowed, but in the second script, not only is a second form of input allowed but a prompt explaining how to use lower appears if the user enters lower without any arguments. Notice that in both scripts a colon is used to identify lines containing comments (and that each script is carefully commented).

Chapter 5. Parameters and Data

Sections in this chapter:

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- 5.2 "FDF (Flexible Data Format) Files," page 290
- 5.4 "Creating and Modifying Parameters," page 298
- 5.5 "Modifying Parameter Displays in VNMR," page 304
- 5.6 "User-Written Weighting Functions," page 307
- 5.7 "User-Written FID Files," page 310

5.1 VNMR Data Files

Although a number of different files are used by VNMR to process data, VNMR data files use only two basic formats:

- Binary format Stores FIDs and transformed spectra. Binary files consist of a file header describing the details of the data stored in the file followed by the spectral data in integer or floating point format. Because of the different representations of integer and floating point numbers on different computer systems, binary files cannot be copied between VAX and Sun systems without a conversion step. On Sun systems, integers are 32-bits wide and are stored byte by byte, with the most significant byte at the lowest address of the full 32-bit word. On VAX systems, integers are stored with the least significant byte at the lowest address. The Sun system also uses the IEEE standard floating point format, whereas the VAX uses a slightly different format in which the floating point exponent is different. VNMR software contains routines to manipulate data (FIDs) that has been transferred between Sun and VAX systems.
- *Text format* Stores all other forms of data, such as line lists, parameters, and all forms of reduced data obtained by analyzing NMR spectra. The advantage of storing data in text format is that it can be easily inspected and modified with a text editor and can be copied from one computer to another with no major problems. The text on both Sun and VAX systems use the ASCII format in which each letter is stored in one byte.

Binary Data Files

Binary data files are used in the VNMR file system to store FIDs and the transformed spectra. FIDs and their associated parameters are stored as filename.fid files. A filename.fid file is always a directory file containing the following individual files:

- filename.fid/fid is a binary file containing the FIDs.
- filename.fid/procpar is a text file with parameters used to obtain the FIDs.
- filename.fid/text is a text file.

Chapter 5. Parameters and Data

In experiments, binary files store FIDs and spectra. In non-automation experiments, the FID is stored within the experiment regardless of what the parameter file is set to. The path ~username/vnmrsys/expn/acqfil/fid is the full UNIX path to that file. FIDs are stored as either 16- or 32-bit integer binary data files, depending on whether the data acquisition was performed with dp='n' or dp='y', respectively.

After an Fourier transform, the experiment file expn/datdir/data contains the transformed spectra stored in 32-bit floating point format. This file always contains complex numbers (pairs of floating point numbers) except if pmode='' was selected in processing 2D experiments. To speed up the display, VNMR stores also the phased spectral information in expn/datdir/phasefile, where it is available only after the first display of the data. In arrayed or 2D experiments, phasefile contains only those traces that have been displayed at least once after the last FT or phase change. Therefore, a user program to access that file can only be called after a complete display of the data.

The directory file expn for current experiment *n* contains the following files:

- expn/curpar is a text file containing the current parameters.
- expn/procpar is a text file containing the last used parameters.
- expn/text is a text file.
- expn/acqfil/fid is a binary file that stores the FIDs.
- expn/datdir/data is a binary file with transformed complex spectrum.
- expn/datdir/phasefile is a binary file with transformed phased spectrum.
- expn/sn is saved display number n.

To access information from one of the experiment files of the current experiment, the user must be sure that each of these files has been written to the disk. The problem arises because VNMR tries to keep individual blocks of the binary files in the internal buffers as long as possible to minimize disk accesses. This buffering in memory is not the same as the disk cache buffering that the UNIX operating system performs. The command flush can be used in VNMR to write all data buffers into disk files (or at least into the disk cache, where it is also available for other processes). The command fsave can be used in VNMR to write all parameter buffers into disk files.

The default directory for the 3D spectral data is curexp/datadir3d. The output directory for the extracted 2D planes is the same as that for the 3D spectral data, except that 2D uses the /extr subdirectory and 3D uses the /data subdirectory. Within the 3D data subdirectory /data are the following files and further subdirectories:

- data1 to data# are the actual binary 3D spectral data files. If the option nfiles is not entered, the number of data files depends upon the size of the largest 2D plane and the value for the UNIX environmental parameter memsize.
- info is a directory that stores the 3D coefficient text file (coef), the binary information file (procdat), the 3D parameter set (procpar3d), and the automation file (auto). The first three files are created by the set3dproc() command within VNMR. The last file is created by the ft3d program.
- log is a directory that stores the log files produced by the ft3d program. The file f3 contains all the log output for the f₃ transform. For the f₂ and f₁ transforms, there are two log file for each data file, one for the f₂ transform (f2.#) and one for the f₁ (f1.#). The file master contains the log output produced by the master ft3d program.

Data File Structures

A data file header of 32 bytes is placed at the beginning of a VNMR data file. The header contains information about the number of blocks and their size. It is followed by one or more data blocks. At the beginning of each block, a data block header is stored, which contains information about the data within the individual block. A typical 1D data file, therefore, has the following form:

```
data file header
header for block 1
data of block 1
header for block 2
data of block 2
```

The data headers allow for 2D hypercomplex data that may be phased in both the f_1 and f_2 directions. To accomplish this, the data block header has a second part for the 2D hypercomplex data. Also, the data file header, the data block header, and the data block header used with all data have been slightly revised. The new format allows processing of FIDs obtained with earlier versions of VNMR.The 2D hypercomplex data files with datafilehead.nbheaders=2 have the following structure:

```
data file header
header for block 1
second header for block 1
data of block 1
header for block 2
second header for block 2
data of block 2
```

• • •

All data in this file is contiguous. The byte following the 32nd byte in the file is expected to be the first byte of the first data block header. If more than one block is stored in a file, the first byte following the last byte of data is expected to be the first byte of the second data block header. Note that these data blocks are not disk blocks; rather, they are a complete data group, such as an individual trace in a experiment. For non-arrayed 1D experiments, only one block will be present in the file.

Details of the data structures and constants involved can be found in the file data.h, which is provided as part of the VNMR source code license. The C specification of the file header is the following:

```
struct datafilehead
/* Used at start of each data file (FIDs, spectra, 2D) */
{
long nblocks; /* number of blocks in file */
long ntraces; /* number of traces per block */
long np; /* number of elements per trace */
long ebytes; /* number of bytes per element */
long tbytes; /* number of bytes per trace */
long bytes; /* number of bytes per block */
short vers_id; /* software version, file_id status bits */
short status; /* status of whole file */
long nbheaders; /* number of block headers per block */
};
```

The variables in datafilehead structure are set as follows:

nblocks is the number of data blocks present in the file.

Chapter 5. Parameters and Data

- ntraces is the number of traces in each block.
- np is the number of simple elements (16-bit integers, 32-bit integers, or 32-bit floating point numbers) in one trace. It is equal to twice the number of complex data points.
- ebytes is the number of bytes in one element, either 2 (for 16-bit integers in single precision FIDs) or 4 (for all others).
- tbytes is set to (np*ebytes).
- bbytes is set to (ntraces*tbytes + nbheaders*sizeof(struct datablockhead)). The size of the datablockhead structure is 28 bytes.
- vers_id is the version identification of present VNMR.
- nbheaders is the number of block headers per data block.
- status is bits as defined below with their hexadecimal values. All other bits must be zero.

Bits 0–6: file header and block header status bits (bit 6 is unused):

0	S_DATA	0x1	0 = no data, 1 = data
1	S_SPEC	0x2	0 = FID, 1 = spectrum
2	S_32	0x4	*
3	S_FLOAT	0x8	0 = integer, 1 = floating point
4	S_COMPLEX	0x10	0 = real, 1 = complex
5	S_HYPERCOMPLEX	0x20	1 = hypercomplex

* If S_FLOAT=0, S_32=0 for 16-bit integer, or S_32=1 for 32-bit integer. If S_FLOAT=1, S_32 is ignored.

Bits 7–14: file header status bits (bits 10 and 15 are unused):

S_ACQPAR	0x80	0 = not Acqpar, 1 = Acqpar
S_SECND	0x100	0 = first FT, $1 = $ second FT
S_TRANSF	0x200	0 = regular, 1 = transposed
S_NP	0x800	1 = np dimension is active
S_NF	0x1000	1 = nf dimension is active
S_NI	0x2000	1 = ni dimension is active
S_NI2	0x4000	1 = ni2 dimension is active
	S_SECND S_TRANSF S_NP S_NF S_NI	S_SECND 0x100 S_TRANSF 0x200 S_NP 0x800 S_NF 0x1000 S_NI 0x2000

Block headers are defined by the following C specifications:

```
struct datablockhead
/* Each file block contains the following header */
{
short scale; /* scaling factor */
short status; /* status of data in block */
short index; /* block index */
short mode; /* mode of data in block */
long ctcount; /* ct value for FID */
float lpval; /* f2 (2D-f1) left phase in phasefile */
float rpval; /* f2 (2D-f1) right phase in phasefile */
float lvl; /* level drift correction */
float tlt; /* tilt drift correction */
};
```

status is bits 0–6 defined the same as for file header status. Bits 7–11 are defined below (all other bits must be zero):

7	MORE_BLOCKS	0x80	0 = absent, 1 = present
8	NP_CMPLX	0x100	0 = real, 1 = complex
9	NF_CMPLX	0x200	0 = real, 1 = complex
10	NI_CMPLX	0x400	0 = real, 1 = complex
11	NI2_CMPLX	0x800	0 = real, 1 = complex

Additional data block header for hypercomplex 2D data:

struct hypercmplxbhead

{		
<pre>short s_spare1;</pre>	/*	short word: spare */
short status;	/*	status word for block header $\star/$
<pre>short s_spare2;</pre>	/*	short word: spare */
<pre>short s_spare3;</pre>	/*	short word: spare */
long l_spare1;	/*	long word: spare */
float lpval1;	/*	2D-f2 left phase */
float rpval1;	/*	2D-f2 right phase */
float f_spare1;	/*	<pre>float word: spare */</pre>
float f_spare2;	/*	<pre>float word: spare */</pre>
};		

Main data block header mode bits 0–15:

Bits 0-3: bit 3 is currently unused

0	NP_PHMODE	0x1	1 = ph mode
1	NP_AVMODE	0x2	1 = av mode
2	NP_PWRMODE	0x4	1 = pwr mode
Bits 4	-7: bit 7 is currently un	used	
4	NF_PHMODE	0x10	1 = ph mode
5	NF_AVMODE	0x20	1 = av mode
6	NF_PWRMODE	0x40	1 = pwr mode
Dita 9	11. hit 11 is summantly	mused	

Bits 8–11: bit 11 is currently unused

8	NI_PHMODE	0x100	1 = ph mode
9	NI_AVMODE	0x200	1 = av mode
10	NI_PWRMODE	0x400	1 = pwr mode

Bits 12-15: bit 15 is currently unused

12	NI2_PHMODE	0x8	1 = ph mode
13	NI2_AVMODE	0x100	1 = av mode
14	NI2_PWRMODE	0x2000	1 = pwr mode

Usage bits for additional block headers (hypercmplxbhead.status)

U_HYPERCOMPLEX 0x2

1 = hypercomplex block structure

The actual FID data is typically stored as pairs of integers in either 16-bit format or 32-bit format. The first integer represents the real part of a complex pair (or the X channel from the perspective of quadrature detection); the second integer represents the imaginary component (or the Y channel). In phase-sensitive 2D experiments, "X" and "Y"

experiments are similarly interleaved. The format of the integers and the organization as complex pairs must be specified in the data file header.

VNMR Use of Binary Data Files

To understand how VNMR uses individual binary data files, consider the example of a simple Fourier transform followed by the display of the spectrum. The FT is performed with the command ft, which acts as follows:

- 1. Copy processing parameters from curpar into procpar.
- 2. If FID is not in the fid file buffer, open the fid file (if not already open) and load it into buffer.
- 3. Initialize the data file with the proper size (using parameter fn).
- 4. Convert integer FID into floating point and store result in data file buffer.
- 5. Apply dc drift correction and first point correction.
- 6. Apply weighting function, if requested.
- 7. Zero fill data, if required.
- 8. Fourier transform data in data file buffer.

At this point, the data file buffer contains the complex spectrum. Unless other FTs are done, which use up more memory space than assigned to the data file buffer, the data is not automatically written to the file expn/datdir/data at this time. Joining a different experiment or the command flush would perform such a write operation.

The ds command takes the following steps in displaying the spectrum:

- 1. If data is not in phasefile buffer or if the phase parameters have changed, ds tries to open the phase file (if not already open) and load data into the buffer (if it is there). If ds is unsuccessful, the data must be phased:
 - a. If the data is not in the data file buffer, ds opens the data file (if not already open) and loads it into the buffer.
 - b. ds initializes the phasefile buffer with the proper size (using the same parameter fn as used for last FT).
 - c. ds calculates the phased (or absolute value) spectrum and stores it in the phasefile buffer.
- 2. ds calculates the display and displays the spectrum.

The phasefile buffer now contains the phased spectrum. Unless other displays are done, which use up more memory space than assigned to the phasefile buffer, the data is not automatically written to the file expn/datdir/phasefile at this time. Joining a different experiment or entering the command flush would perform such a write operation.

Depending on the nature of the data processing, the two files data and phasefile will contain different information, as follows:

- After a 1D FT data contains a complex spectrum, which can be used for phased or absolute value displays.
- *After a 1D display* phasefile contains either phased or absolute value data, depending on which type of display had been selected.

- After a 2D FID display data contains the complex FIDs, floated and normalized for different scaling during the 2D acquisition. phasefile contains the absolute value or phased equivalent of this FID data.
- After the first FT in a 2D experiment data contains the once-transformed spectra. This is equivalent to the interferograms, if the data is properly reorganized (see f₁ and f₂ traces below). If a display is done now, phasefile contains phased (or absolute value) half-transformed spectra or interferograms.
- After the second FT in a 2D experiment data contains the fully transformed spectra, and after a display, phasefile contains the equivalent phased or absolute-value spectra.

Storing Multiple Traces

Arrayed experiments are handled in VNMR by storing the multiple traces of arrayed experiments in one file. To allow this, the file is divided into several blocks, each containing one trace. Therefore, in an arrayed experiment, the files fid, data, and phasefile typically contain the same number of blocks. The number of traces in an arrayed experiment is identical to the parameter arraydim. The only complication when working with such data files in arrayed experiments might be that there are "holes" in such files (in the UNIX version of VNMR only). The holes occur if not all FIDs are transformed or displayed. They do not present a problem as long as a user program just uses a "seek" operation to position the file pointer at the right point in the file and does not try to read traces that have never been calculated.

One can look at 2D experiments as a special case of an arrayed experiment; however, the situation is complicated by the fact that the data often has to be transposed. After the first FT, the resulting spectra are transposed to become the FIDs used for the second FT, and after the second FT, the user might want to work on traces in either the f_1 or f_2 direction. Furthermore, some types of symmetrization and baseline correction algorithms may have to work on traces in both directions at the same time. The situation is complicated by the fact that the "in place" matrix transposition of large data sets is a very complex operation, requiring many disk accesses and can therefore not be used in a system that has to transform large non-symmetric data sets in a short time.

"Out of place" transpositions are not acceptable for large data sets because they double the disk space requirements of the large 2D experiments. Therefore, VNMR software uses a storage format in the 2D data file that allows access to both rows and columns at the same time. Because of the proprietary nature and complexity of the algorithm involved, it is not presented here. The storage format is used only in datdir/data.

2D FIDs are stored the same way as 1D FIDs. Transformed 2D data is stored in data in large blocks of typically 256K bytes. This means that multiple traces are combined to form a block. Within one block, the data is not stored as individual traces but is scrambled to make access to rows and columns as fast as possible.

Phased 2D data is stored in phasefile in the same large blocks as in data, but the traces within each block are stored sequentially in their natural order. Both traces along f_1 and f_2 are stored in the same file. The first block(s) contain traces number 1 to fn along the f_1 axis; the next block(s) contains traces number 1 to fn1 along the f_2 axis. Note again, that phasefile will only contain data if the corresponding display operation has been performed. Therefore, in most typical situations, where only a display along one of the two 2D axes is done, phasefile will contain only the block(s) for the traces along f_1 or a 'hole' followed by the block(s) for the traces along f_2 . Furthermore, in large 2D experiments, where multiple blocks must be used to store the whole data, only a 'full' display will ensure that all blocks were actually calculated.

Header and Data Display

The VNMR commands ddf, ddff, and ddfp display file headers and data. ddf displays the data file in the current experiment. Without arguments, only the file header is displayed. Using ddf < (block_number,trace_number,first_number) >, ddf displays a block header and part of the data of that block is displayed. block_number is the block number, default 1. trace_number is the trace number within the block, default 1. first is the first data element number within the trace, default 1.

The ddff command displays the FID file in the current experiment and the ddfp command displays the phase file in the current experiment. Without any arguments, both display only the file header. Using the same arguments as the ddf command, ddff and ddfp display a block header and part of the data of that block is displayed. The mstat command displays statistics of memory usage by VNMR commands.

5.2 FDF (Flexible Data Format) Files

The FDF file format was developed to support the ImageBrowser, chemical shift imaging (CSI), and single-voxel spectroscopy (SVS) applications. When these applications were under development, the current VNMR file formats for image data were not easily usable for the following reasons:

- The data and parameters describing the data were separated into two files. If the files were ever separated, there would be no way to use or understand the data.
- The data file had embedded headers that were not needed and provided no useful purpose.
- There was no support or structure for saving multislice data sets or a portion of a multislice data set as image files.

FDF was developed to make it similar to VNMR formats, with parameters in an easy-tomanipulate ASCII format and a data header that is not fixed so that parameters can be added. This format makes it easy for users and different applications to manipulate the headers and add needed parameters without affecting other applications.

File Structures and Naming Conventions

Several file structure and naming conventions have been developed for more ease in using and interpreting files. Applications should not assume certain names for certain file; however, specific applications may assume default names when outputting files.

Directories

The directory-naming convention is <name>.dat. The directory can contain a parameter file and any number of FDF files. The name of the parameter file is procpar, a standard VNMR name.

File Names

Each type of file has a different name in order to make the file more recognizable to the user. For image files, the name is image[nnnn].fdf, where nnnn is a numeric string from 0000 to 9999. For volumes, the name is volume[nnnn].fdf, where nnnn is also a numeric string from 0000 to 9999. Programs that read FDF files should not depend on these names because they are conventions and not definitions.

Compressed Files

Although not implemented at this time, compression will be supported for the data portion of the file. The headers will not be compressed. A field will be put in the header to define the compression method or to identify the command to uncompress the data.

File Format

The format of an FDF file consists of a header and data:

- Listing 11 is an example of an FDF header. The header is in ASCII text and its fields are defined by a data definition language. Using ASCII text makes it easy to decipher the image content and add new fields, and is compatible with the ASCII format of the procpar file. The fields in the data header can be in any order except for the magic number string, which are the first characters in the header, and the end of header character <null>, which must immediately precede the data. The fields have a C-style syntax. A correct header can be compiled by the C compiler and should not result in any errors.
- The data portion is binary data described by fields in the header. It is separated from the header by a null character.

Listing 11. Example of an FDF Header

```
#!/usr/local/fdf/startup
int rank=2;
char *spatial_rank="2dfov";
char *storage="float";
int bits=32;
char *type="absval";
int matrix[]={256,256};
char *abscissa[]={"cm","cm"};
char *ordinate[]={"intensity"};
float span[]={-10.000000,-15.000000};
float origin[]={5.000000,6.911132};
char *nucleus[]=("H1", "H1"};
float nucfreq[]={200.067000,200.067000};
float location[]={0.000000,-0.588868,0.000000};
float roi[]={10.000000,15.000000,0.208557};
float orientation[]={0.000000,0.0000000,1.0000000,-1.000000,
0.000000,0.000000,0.000000,1.000000,0.000000};
checksum=0787271376;
<zero>
```

Header Parameters

The fields in the data header are defined in this section.

Magic Number

The magic number is an ASCII string that identifies the file as a FDF file. The first two characters in the file must be #!, followed by the identification string. Currently, the string is #!/usr/local/fdf/startup.

Data Set Dimensionality or Rank Fields

These entries specify the data organization in the binary portion of the file.

- rank is a positive integer value (1, 2, 3, 4,...) giving the number of dimensions in the data file (e.g., int rank=2;).
- matrix is a set of rank integers giving the number of data points in each dimension (e.g., for rank=2, float matrix[]={256,256};)
- spatial_rank is a string ("none", "voxel", "ldfov", "2dfov", "3dfov") for the type of data (e.g., char *spatial_rank="2dfov";).

Data Content Fields

The following entries define the data type and size.

- storage is a string ("integer", "float") that defines the data type (e.g., char
 *storage="float";).
- bits is an integer (8, 16, 32, or 64) that defines the size of the data (e.g., float bits=32;).
- type is a string ("real", "imag", "absval", "complex") that defines the numerical data type (e.g., char *type="absval";).

Data Location and Orientation Fields

The following entries define the user coordinate system and specify the size and position of the region from which the data was obtained. Figure 6 illustrates the coordinate system. Vectors that correspond to header parameters are shown in **boldface**.

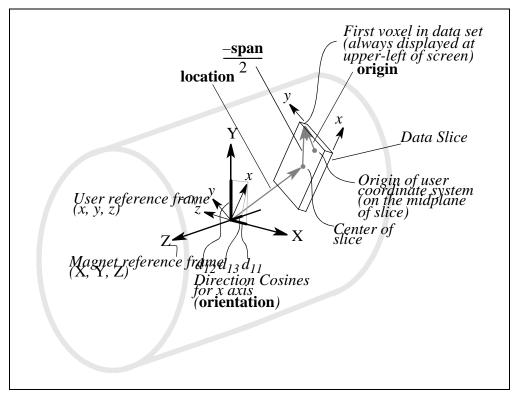


Figure 6. Magnet Coordinates as Related to User Coordinates.

• orientation specifies the orientation of the user reference frame (*x*, *y*, *z*) with respect to the magnet frame (X, Y, Z). orientation is given as a set of nine direction cosines, in the order:

 $\begin{array}{l} d_{11}, d_{12}, d_{13}, d_{21}, d_{22}, d_{23}, d_{31}, d_{32}, d_{33} \\ \text{where:} \\ x = d_{11}X + d_{12}Y + d_{13}Z \\ y = d_{21}X + d_{22}Y + d_{23}Z \\ z = d_{31}X + d_{32}Y + d_{33}Z \\ \text{and} \\ X = d_{11}x + d_{21}y + d_{31}z \\ Y = d_{12}x + d_{22}y + d_{32}z \\ Z = d_{13}x + d_{23}y + d_{33}z \\ \text{The value is written as nine floating point values grouped as three triads (e.g., float orientation[] = { 0 . 0 , 0 . 0 , 1 . 0 , -1 . 0 , 0 . 0 , 0 . 0 , 1 . 0 , 0 . 0 };). \\ location is the position of the center of the acquired data volume relative to the \\ \end{array}$

- location is the position of the center of the acquired data volume relative to the center of the magnet, in the user's coordinate system. The position is given in centimeters as a triple (three floating point values) of x, y, z distances (e.g., float location[]={10.0,15.0,0.208};).
- roi is the size of the acquired data volume (three floating point values), in centimeters, in the user's coordinate frame, not the magnet frame (e.g., float roi[]={10.0,15.0,0.208};). Do not confuse this roi with ROIs that might be specified inside the data set.

Data Axes

The data axes entries specify the user coordinates of data points. These axes do not tell how to orient the display of the data, but only what to call the coordinates of a given datum. There are no standard header entries to specify the orientation of the data display. Currently, data is always displayed or plotted in the same order that it is stored. The fastest data dimension is plotted horizontally from left to right; the next dimension is plotted vertically from top to bottom.

- origin is a set of rank floating point values giving the user coordinates of the first point in the data set (e.g., float origin[]={5.0,6.91};).
- span is a set of rank floating point values for the signed length of each axis, in user units. A positive value means the value of the particular coordinate increases going away from the first point (e.g., float span[]={-10.000, -15.000};).
- abscissa is a set of rank strings ("hz", "s", "cm", "cm/s", "cm/s2", "deg", "ppm1", "ppm2", "ppm3") that identifies the units that apply to each dimension (e.g., char *abscissa[]={"cm", "cm"};).
- ordinate is a string ("intensity", "s", "deg") that gives the units that apply to the numbers in the binary part of the file (e.g., char *ordinate[]={"intensity"};).

Nuclear Data Fields

Data fields may contain data generated by interactions between more than one nucleus (e.g., a 2D chemical shift correlation map between protons and carbon). Such data requires interpreting the term "ppm" for the specific nucleus, if ppm to frequency conversions are necessary, and properly labeling axes arising from different nuclei. To properly interpret ppm and label axes, the identity of the nucleus in question and the corresponding nuclear

Chapter 5. Parameters and Data

resonance frequency are needed. These fields are related to the abscissa values "ppm1", "ppm2", and "ppm3" in that the 1, 2, and 3 are indices into the nucleus and nucfreq fields. That is, the nucleus for the axis with abscissa string "ppm1" is the first entry in the nucleus field.

- nucleus is one entry ("H1", "F19", same as VNMR tn parameter) for each rf channel (e.g., char *nucleus[]={"H1", "H1"};).
- nucfreq is the nuclear frequency (floating point) used for each rf channel (e.g., float nucfreq[]={200.067,200.067};).

Miscellaneous Fields

- checksum is the checksum of the data. Changes to the header do not affect the checksum. The checksum is a 32-bit integer, calculated by the gluer program (e.g., int checksum=0787271376;).
- compression is a string with either the command needed to uncompress the data or a tag giving the compression method. This field is not currently implemented.

End of Header

A character specifies the end of the header. If there is data, it immediately follows this character. The data should be aligned according to its data type. For single precision floating point data, the data is aligned on word boundaries. Currently, the end of header character is <zero> (an ASCII "NUL").

Transformations

By editing some of the header values, it is possible to make a program that reads FDF data files to perform simple transformations. For example, to flip data left-to-right, set: span'₀=-span₀ origin'₀=origin₀-span'₀

Creating FDF Files

To generate files in the FDF format, the following macros are available to write out single or multislice images:

- For the current imaging software—including sequences sems, mems, and flash—use the macro svib(directory<, 'f' | 'm' | 'i' | 'o'>), where directory is the directory name desired (.dat is appended to the name), 'f' outputs data in floating point format (this is the default), 'm' or 'i' outputs data as 12-bit integer values in 16-bit words, and 'b' outputs data in 8-bit integer bytes.
- For older style SIS imaging sequences and microimaging sequences, use the macro svsis(directory<, 'f' | 'm'>), where directory, 'f', and 'm' are defined the same as svib.

Raw data from the FID file of the current experiment can be saved as an FDF file with the svfdf(directory) macro, where directory is the name of the directory in which to store the files (.dat is appended to the name). Data is saved in multiple files, with one trace per file. The files are named fid0001.fdf, fid0002.fdf, etc. The procpar file from the current experiment is also saved in the same directory.

Another way to create the FDF files is to edit or create a header defining a set of data with no headers and attach it to the data file with the fdfgluer program. Use the syntax fdfgluer header_file <data_file <output_file>> (from UNIX only).

This program takes a header_file and a data_file and puts them together to form an FDF file. It also calculates a checksum and inserts it into the header. If the data_file argument is not present, fdfgluer assumes the data is input from the standard input, and if the output_file name is not present, fdfgluer puts the FDF file to the standard output.

Splitting FDF Files

The fdfsplit command takes an FDF file and splits it into its data and header parts. The syntax is fdfsplit fdf_file data_file header_file (from UNIX only). If the header still has a checksum value, that value should be removed.

5.3 Reformatting Data for Processing

Sometimes, data acquired in an experiment has to be reformatted for processing. This is especially true for in-vivo imaging experiments where time is critical in getting the data so experiments are designed to acquire data quickly but not necessarily in the most desirable format for processing. Reformatting data can also occur in other applications because of a particular experimental procedure.

The VNMR processing applications ft2d and ft3d can accept data in standard, compressed, or compressed-compressed (3D) data formats. There are a number of routines that allow users to reformat their data into these formats for processing. The reformatting routines allow users to compress or uncompress their data (flashc), move data around between experiments and into almost any format (mf, mfblk, mfdata, mftrace), reverse data while moving it (rfblk, rfdata, rftrace), or use a table of values, in this case an AP table stored in tablib, to sort and reformat scans of data (tabc, tcapply).

In this section, standard and compressed data are defined, reformatting options are described, and several examples are presented. Table 39 summarizes the reformatting commands described in this section. Note that the commands rsapply, tcapply, tcclose, and tcopen are for 2D spectrum data; the remaining commands in the table are for FID data.

Standard and Compressed Formats

Usually when discussing standard and compressed data formats, *standard* means the data was acquired using the arrayed parameters ni and ni2, which specify the number of increments in the second and third dimensions; and *compressed* means using parameter nf to specify the increments in the second dimension.

For multislice imaging, standard means using ni to specify the phase-encode increments and nf to specify the number of slices and compressed means using nf to specify the phase-encode increments while arraying the slices.

Compressed-compressed means using nf to specify the phase-encode increments and slices for 2D or to specify the phase-encode increments in the second and third dimensions for 3D. In compressed-compressed data sets, nf can be set to nv*ns or nv*nv2, where nv is the number of phase-encode increments in the second dimension, nv2 is the number of phase-encode increments in the third dimension, and ns is the number of slices.

To give another view of data formats, which will help when using the "move FID" commands, each ni increment or array element is stored as a data block in a FID file and each nf FID is stored as a trace within a data block in a FID file.

Commands			
flashc*	Convert compressed 2D data to standard 2D format		
<pre>mf(<from_exp,>to_exp)</from_exp,></pre>	om_exp, >to_exp) Move FIDs between experiments		
mfblk*	Move FID block		
mfclose	Close memory map FID		
mfdata*	Move FID data		
<pre>mfopen(<src_expno,>dest_expno)</src_expno,></pre>	Memory map open FID file		
mftrace*	Move FID trace		
rfblk*	Reverse FID block		
rfdata*	Reverse FID data		
rftrace*	Reverse FID trace		
rsapply	Reverse data in a spectrum		
tabc<(dimension)>	Convert data in table order to linear order		
tcapply<(file)>	Apply table conversion reformatting to data		
tcclose	Close table conversion file		
tcopen<(file)>	Open table conversion file		
<pre>* flashc<('ms' 'mi' 'rare'<,traces><,echoes>)</pre>			
<pre>mfblk(<src_expno,>src_blk_no,</src_expno,></pre>	dest_expno,dest_blk_no)		
	o,src_start_loc,dest_expno, \		
<pre>dest_blk_no,dest_start_loc,n </pre>			
mftrace(<src_expno,>src_blk_no</src_expno,>	o,src_trace_no,dest_expno		
<pre>dest_blk_no,dest_trace_no) rfblk(<src_expno,>src_blk_no,dest_expno,dest_blk_no)</src_expno,></pre>			
rfdata(<src_expno,>src_blk_no,src_start_loc,dest_expno, \</src_expno,>			
dest_blk_no,dest_start_loc,num_points)			
<pre>rftrace(<src_expno,>src_blk_no,src_trace_no,dest_expno, \</src_expno,></pre>			
<pre>dest_blk_no,dest_trace_no)</pre>			

Table 39. Commands for Reformatting Data

Compress or Uncompress Data

The most common form of reformatting for imaging has been to use the flashc command to convert compressed data sets to standard data sets in order to run ft2d on the data. With the implementation of ft2d('nf', <index>), flashc is no longer necessary. However, use of flashc is still necessary for converting compressed-compressed data to compressed or standard formats.

Move and Reverse Data

The commands mf, mfblk, mfdata, and mftrace are available to move data around in a FID file or to move data from one experiment FID file to another experiment FID file. These commands give users more control in reformatting their data by allowing them to move entire FID files, individual blocks within a FID file, individual traces within a block of a FID file, or sections of data within a block of a FID file.

To illustrate the use of the "move FID" commands, Listing 12 is an example with code from a macro that moves a 3D dataset from an arrayed 3D dataset to another experiment that runs ft3d on the data. The \$index variable is the array index. It works on both compressed compressed and compressed 3D data.

The "reverse FID" commands rfblk, rftrace, and rfdata are similar to their respective mfblk, mftrace, and mfdata commands, except that rfblk, rftrace,

Listing 12. Code from a "Move FID" Macro

```
if (\$eqcon[3] = 'c') and (\$eqcon[4] = 'c') then
   "**** Compressed-compressed 3d ****"
   $arraydim = arraydim
   if ($index > $arraydim) then
     write('error','Index greater than arraydim.')
     abort
  endif
  mfblk($index,$workexp,1)
  jexp($workexp)
  setvalue('arraydim',1,'processed')
  setvalue('arraydim',1,'current')
  setvalue('array','','processed')
  setvalue('array','','current')
  ft.3d
   jexp($cexpn)
else if (\$eqcon[3] = 'c') and (\$eqcon[4] = 's') then
  "**** Compressed 3d ****"
  if (ni < 1.5) then
     write('error','seqcon, ni mismatch check parameters.')
     abort
  endif
  $arraydim = arraydim/ni
  if ($index > $arraydim) then
     write('error','Index greater than arraydim.')
     abort
  endif
  $i = 1
  k = index
  while ($i <= ni) do
     mfblk($k,$workexp,$i)
     $k = $k + $arraydim
     $i = $i + 1
  endwhile
  jexp($workexp)
  setvalue('arraydim',ni,'processed')
  setvalue('arraydim',ni,'current')
  setvalue('array','','processed')
  setvalue('array','','current')
  ft3d
   jexp($cexpn)
```

and rfdata also reverse the order of the data. The rfblk, rftrace, and rfdata commands were implemented to support EPI (Echo Planar Imaging) processing. Listing 13 is an example of using these commands to reverse every other FID echo for EPI data. Note that the mfopen and mfclose commands can significantly speed up the data reformatting by opening and closing the data files once, instead of every time the data is moved. The rfblk, rftrace, and rfdata commands can also be used with the "move FID" commands.

CAUTION: For speed reasons, the "move FID" and "reverse FID" commands work directly on the FID and follow data links. These commands can modify data returned to an experiment with the rt command. To avoid modification, enter the following sequence of VNMR commands before

```
manipulating the FID data:
cp(curexp+'/acqfil/fid',curexp+'/acqfil/fidtmp')
rm(curexp+'/acqfil/fid')
mv(curexp+'/acqfil/fidtmp',curexp+'/acqfil/fid')
```

Table Convert Data

VNMR supports reconstructing a properly ordered raw data set from any arbitrarily ordered data set acquired under control of an external AP table. The data must have been acquired according to a table in the tablib directory. The command for table conversion is tabc.

Reformatting Spectra

The commands rsapply, to reverse a spectrum, and tcapply, to reformat a 2D set of spectra using an AP table, support reformatting of spectra within a 2D dataset. The types of reformatting are the reversing of data within a spectrum and the reformatting of arbitrarily ordered 2D spectrum by using an AP table. These commands do not change the original FID data, and they may provide some speed improvement over the similar commands that operate on FID data. For 2D data, an ftld command should be applied to the data, followed by the desired reformatting, and then an ft2d command to complete the processing.

Listing 13. Example of Command Reversing Data Order

5.4 Creating and Modifying Parameters

VNMR parameters and their attributes can be created and modified with the commands covered in this section. The parameter trees used by these commands are UNIX files containing the attributes of a parameter as formatted text.

Parameter Types and Trees

The types of parameters that can be created are 'real', 'string', 'delay', 'frequency', 'flag', 'pulse', and 'integer (default is 'real'). In brief, the meaning of these types are as follows (for more detail, refer to the description of the create command in the VNMR Command and Parameter Reference):

- 'real' is any positive or negative value, and can be positive or negative.
- 'string' is composed of characters, and can be limited to selected words by enumerating the possible values with the command setenumeral.

- 'delay' is a value between 0 and 8190 (0 and 4095 on *GEMINI 2000*), in units of seconds.
- 'frequency' is positive real number values.
- 'flag' is composed of characters, similar to the 'string' type, but can be limited to selected characters by enumerating the possible values with the command setenumeral. If enumerated values are not set, the 'string' and 'flag' types are identical.
- 'pulse' is a value between 0 and 8190 (0 and 4095 on *GEMINI 2000*), in units of microseconds.
- 'integer' is composed of integers (0, 1, 2, 3,...),

The four parameter tree types are 'current', 'global', 'processed', and 'systemglobal' (the default is 'current'). Each type is described below:

- 'current' contains the parameters that are adjusted to set up an experiment. The parameters are from the file curpar in the current experiment.
- 'global' contains user-specific parameters from the file global in the vnmrsys directory of the present UNIX user.
- 'processed' contains the parameters with which the data was obtained. These parameters are from the file procpar in the current experiment.
- 'systemglobal' contains instrument-specific parameters from the text file /vnmr/conpar. The config program is used to define most of these parameters. All users have the same systemglobal tree.

Tools for Working with Parameter Trees

Table 40 lists commands for creating, modifying, and deleting parameters.

To Create a New Parameter

Use create(parameter<,type<,tree>>) to create a new parameter in a parameter tree with the name specified by parameter. For example, entering create('a','real','global') creates a new real-type parameter *a* in the global tree. type can be 'real', 'string', 'delay', ' frequency', 'flag', 'pulse', or 'integer'. If the type argument is not entered, the default is 'real'. tree can be 'current', 'global', 'processed', or 'systemglobal'. If the tree argument is not entered, the default is 'current'. See the section above for a description of parameter types and trees. Note that these same arguments are used with all the commands appearing in this section.

To Get the Value of a Parameter

The value of most parameters can be accessed simply by using their name in an expression; for example, sw? or r1=np accesses the value of sw and np, respectively. However, parameters in the processed tree cannot be accessed this way. Use

getvalue(parameter<, index><, tree>) to get the value of any parameter, including the value of a parameter in a processed tree. To make this easier, the default value of tree is 'processed'. The index argument is the number of a single element in an arrayed parameter (the default is 1).

Commands			
<pre>create(parameter<,type<,tree>>)</pre>	Create a new parameter in parameter tree		
<pre>destroy(parameter<,tree>)</pre>	Destroy a parameter		
destroygroup(group<,tree>)	Destroy parameters of a group in a tree		
display(parameter '*' '**'<,tree>)	Display parameters and their attributes		
<pre>fread(file<,tree<,'reset' 'value'>>)</pre>	Read in parameters from a file into a tree		
<pre>fsave(file<,tree>)</pre>	Save parameters from a tree to a file		
getvalue(parameter<,index><,tree>)	Get value of parameter in a tree		
groupcopy(from_tree,to_tree,group)	Copy group parameters from tree to tree		
<pre>paramvi(parameter<,tree>)</pre>	Edit parameter and its attributes using vi		
prune(file)	Prune extra parameters from current tree		
<pre>setdgroup(parameter,dgroup<,tree>)</pre>	Set the Dgroup of a parameter in a tree		
setenumeral*	Set values of a string parameter in a tree		
<pre>setgroup(parameter,group<,tree>)</pre>	Set group of a parameter in a tree		
setlimit*	Set limits of a parameter in a tree		
setprotect*	Set protection mode of a parameter		
<pre>settype(parameter,type<,tree>)</pre>	Change type of a parameter		
setvalue*	Set value of any parameter in a tree		
<pre>* setenumeral(parameter,N,enum1,enum2,enumN<,tree>)</pre>			
<pre>setlimit(parameter,maximum,minimum,step_size<,tree>) or</pre>			
<pre>setlimit(parameter, index<, tree>) seture</pre>			
setprotect(parameter,'set' 'on' 'off',value<,tree>) setvalue(parameter,value<,index><,tree>)			
servarue(parameter, varue, INDEX), t	TCC~)		

Table 40. Commands for Working with Parameter Trees

To Edit or Set Parameter Attributes

Use paramvi (parameter<, tree>) to open the file for a parameter in the UNIX vi text editor so that you can edit the attributes. To open a parameter file with an editor other than vi, use paramedit(parameter<, tree>). Refer to entry for paramedit in the VNMR Command and Parameter Reference for information on how to select a text editor other than vi. The format of a stored parameter is described in the next section.

Several parameter attributes can be set by the following commands:

- setlimit(parameter,maximum,minimum,step_size<,tree>) sets the maximum and minimum limits and stepsize of a parameter.
- setlimit(parameter, index<, tree>) sets the maximum and minimum limits and the stepsize, but obtains the values from the index-th entry of a table in conpar.
- setprotect(parameter,'set'|'on'|'off',bit_vals<,tree>) sets the protection bits associated with a parameter. The keyword 'set' causes the current protection bits to be replaced with the set specified by bit_vals(*listed in the VNMR Command and Parameter Reference*). 'on' causes the bits specified in bit_vals to be turned on without affecting other protection bits. 'off' causes the bits specified in bit_vals to be turned off without affecting other protection bits.
- settype(parameter, type<, tree>) changes the type of an existing parameter. A string parameter can be changed into a string or flag type, or a real parameter can be changed into a real, delay, frequency, pulse, or integer type.
- setvalue(parameter,value<,index><,tree>) sets the value of any parameter in a tree. setvalue bypasses normal range checking for parameter entry. It also bypasses any action that would be invoked by the parameter's protection bits.

- setenumeral(parameter, N, enum1, enum2, ..., enumN<, tree>) sets possible values of a string-type or flag-type parameter in a parameter tree.
- setgroup(parameter,group<,tree>) sets the group (also called the Ggroup) of a parameter in a tree. The group argument can be 'all', 'sample', 'acquisition', 'processing', 'display', or 'spin'.
- setdgroup(parameter,dgroup<,tree>) sets the Dgroup of a parameter in a tree. The dgroup argument is an integer. The usage of setdgroup is set by the application. Only the experimental user interface uses this command currently.

To Display a Parameter

Use display(parameter | ' *' | ' * ' < , tree>) to display one or more parameters and their attributes from a parameter tree. The first argument can be one of the following three options: a parameter name (to display the attributes of that parameter, ' *' (to display the name and value of all parameters in a tree), or ' **' (to display the attributes of all parameters in a tree.

To Move Parameters

Use groupcopy(from_tree,to_tree,group) to copy a set of parameters of a group from one parameter tree to another (it cannot be the same tree). group is the same keywords as used with setgroup.

The fread(file<, tree<, 'reset' | 'value'>>) command reads in parameters from a file and loads them into a tree. The keyword 'reset' causes the tree to be cleared before the new file is read; 'value' causes only the values of the parameters in the file to be loaded. The fsave(file<, tree>) command writes parameters from a parameter tree to a file for which the user has write permission. It overwrites any file that exists.

To Destroy a Parameter

The destroy(parameter<, tree>) command removes a parameter from a parameter tree while the destroygroup(group<, tree>) command removes parameters of a group from a parameter tree. The group argument uses the same keywords as used with the setgroup command. If the destroyed parameter was an array, the array parameter is automatically updated.

To remove leftover parameters from previous experimental setups, use prune instead. The prune(file) command destroys parameters in the current parameter tree that are not also defined in the parameter file specified.

Format of a Stored Parameter

To use the create command to create a new parameter, or to use the paramvi and paramedit commands to edit a parameter and its attributes, requires knowledge of the format of a stored parameter. If an error in the format is made, the parameter may not load. This section describes the format in detail.

The format of stored parameters changed somewhat starting with version 4.2 of VNMR. To make the changeover automatic, parameters in the format prior to VNMR 4.2 are automatically updated when they are retrieved and saved in working with an experiment. If you wish, you can also use the macro parfix to manually update parameters. For example, the commands rtp('mypars') parfix svp('mypars') update a parameter set named mypars.

Chapter 5. Parameters and Data

The stored format of a parameter is made up of three or more lines:

• Line 1 contains the attributes of the parameter and has the following fields (given in same order as they appear in the file):

name is the parameter name, which can be any valid string.

subtype is an integer value for the parameter type: 0 (undefined), 1 (real), 2 (string), 3 (delay), 4 (flag), 5 (frequency), 6 (pulse), 7 (integer).

basictype is an integer value: 0 (undefined), 1 (real), 2 (string).

maxvalue is a real number for the maximum value that the parameter can contain, or an index to a maximum value in the parameter parmax (found in

/vnmr/conpar). Applies to both string and real types of parameters.

minvalue is a real number for the minimum value that the parameter can contain or an index to a minimum value in the parameter parmin (found in

/vnmr/conpar). Applies to real types of parameters only.

stepsize is a real number for the step size in which parameters can be entered or index to a step size in the parameter parstep (found in /vnmr/conpar). If stepsize is 0, it is ignored. Applies to real types only.

Ggroup is an integer value: 0 (ALL), 1 (SAMPLE), 2 (ACQUISITION), 3 (PROCESSING), 4 (DISPLAY), 5 (SPIN).

Dgroup is an integer value. The specific application determines the usage of this integer.

protection is a 32-bit word made up of the following bit masks, which are summed to form the full mask:

Bit	Value	Description
0	1	Cannot array the parameter
1	2	Cannot change active/not active status
2	4	Cannot change the parameter value
3	8	Causes _parameter macro to be executed (e.g., if parameter is named sw, the macro _sw is executed when sw is changed)
4	16	Avoids automatic redisplay
5	32	Cannot delete parameter
6	64	System parameter for spectrometer or data station
7	128	Cannot copy parameter from tree to tree
8	256	Cannot set array parameter
9	512	Cannot set parameter enumeral values
10	1024	Cannot change the parameter's group
11	2048	Cannot change protection bits
12	4096	Cannot change the display group
13	8192	Take max, min, step from /vnmr/conpar parameters parmax, parmin, parstep.

active is an integer value: 0 (not active), 1 (active). intptr is not used (generally set to 64).

• Line 2, or the group of lines starting with line 2, list the values of the parameter. The first field on line 2 is the number of values the parameter is set to. The format of the rest of the fields on line 2 and subsequent lines, if any, depends on the value of

basictype set on line 1 and the value entered in the first field on line 2:

If basictype is 1 (real) and first value on line 2 is any number, all parameter values are listed on line 2, starting in the second field. Each value is separated by a space.

If basictype is 2 (string) and first value on line 2 is 1, the single string value of the parameter is listed in the second field of line 2, inside double quotes.

If basictype is 2 (string) and first value on line 2 is greater than 1, the first array element is listed in the second field on line 2 and each additional element is listed on subsequent lines, one value per line. Strings are surrounded by double quotes.

• Last line of a parameter file lists the enumerable values of a string or flag parameter. This specifies the possible values the string parameter can be set to. The first field is the number of enumerable values. If this number is greater than 1, all of the values are listed on this line, starting in the second field.

For example, here is how a typical real parameter file, named a, is interpreted (the numbers in parentheses are not part of the file but are line references in the interpretation):

```
(1) a 31 1e+30 -1e+30 0 0 1 0 1 64
(2) 24.126400
(3) 0
```

This file is made up of the following lines:

- 1. The parameter has the name a, subtype is 3 (delay), basictype is 1 (real), maximum size is 1e+30, minimum size is -1e+30, stepsize is 0, Ggroup is 0 (ALL), Dgroup is 1 (ACQUISITION), protection is 0 (cannot array the parameter), active is 1 (ON), and intptr is 64 (not used).
- 2. Parameter a has 1 value, the real number 24.126400.
- 3. Parameter a has 0 enumerable values.

As another example, here are the values in a file for the parameter tof:

```
(1) tof 5 1 7 7 7 2 1 8202 1 64
(2) 1 1160
(3) 0
```

The tof file is made up of the following lines:

- 1. The parameter has the name tof, subtype is 5 (frequency), and basictype is 1 (real). To read the next 3 values, we must jump to the protection field. Because the protection word value is 8202, which is 8192 + 8 + 2, then bit 13 (8192), bit 3 (8), and bit 1 (2) bitmasks are set. Because bit 13 is set, the maximum size, minimum size, and stepsize values (each is 7) are indices into the 7th array value in the parameters parmax, parmin, and parstep, respectively, in the file conpar. Because bit 3 is set, this causes a macro to be executed. The bit 1 bitmask (2) is also set, which means the active/not active status of the parameter cannot be changed. For the remaining fields, Ggroup is 2 (ACQUISITION), Dgroup is 1 (ACQUISITION), active is 1 (ON), and intptr is 64 (not used).
- 2. Parameter tof has 1 value, the real number 1160.
- 3. Parameter tof has 0 enumerable values.

The following file is an example of a multielement array character parameter, beatles: (1) beatles 2 2 8 0 0 2 1 0 1 64

```
(2) 4 john(3) paul
```

```
george
ringo
(4) 0
```

The beatles file is made up of the following lines:

- 1. The parameter has the name of beatles, subtype is 2 (string), basictype is 2 (string), 800 is max min step (not really used for strings), Ggroup is 2 (acquisition), Dgroup is 1 (ALL), protection is 0, active is 1 (ON), 64 is a terminating number.
- 2. There are four elements to this variable; therefore, it is arrayed. john is the first element in the array.
- 3. paul, george, and ringo are the other three elements in the array.
- 4. 0 (zero) is the terminating line.

5.5 Modifying Parameter Displays in VNMR

The VNMR display commands and macros—dg, dg1, dg2, dgs, and ap—are controlled by template parameters specifying the content and form of the information displayed. The template parameters have the same name as the respective command or macro; for example, the display created by the dg command is controlled by the parameter dg in the experiment's current parameter set.

To modify an existing template parameter, such as dg, enter paramvi('dg') to use the vi text editor, or enter paramedit('dg') to use the text editor set by the UNIX environmental variable vnmreditor. Users can also create a new template parameter (e.g., newdg) and then display it with the command dg('newdg').

Display Template

A display template can have a single string or multiple strings. The first number on the second line of a stored parameter indicates the number of string templates. If the number is 1, the display template is a single string; otherwise, a value greater than 1 indicates the template is multiple strings. Figure 7 shows an example of a single-string display template (actually the parameter dg) and the resulting display.

```
dg 2 2 1023 0 0 4 1 6 1 64
1 "1:ACQUISITION:sfrq:3,tn,at:3,np:0,sw:1,fb:0,bs:0,ss:0,pw:1,p1:1,d1:3,d2:3,tof
:1,nt:0,ct:0;2:SAMPLE:date,solvent,file;2:DECOUPLING:dn,dof:1,dm,dmm,dmf,dhp:0,d
1p:0,homo;2(ni):2D ACQUISITION:sw1:1,ni:0;3:PROCESSING:cf(nf):0,lb:2,sb:3,sbs(sb
):3.gf:3.gfs(gf):3.awc:3.lsfid:0.phfid:1.wtfile.proc.fn:0.math..werr.wexp.wbs.wn
t;4(ni):2D PROCESSING:1b1:2,sb1:3,sbs1(sb1):3,gf1:3,gfs1(gf1):3,awc1:3,wtfile1,p
roc1,fn1:0;4:FLAGS:i1,in,dp,hs;4:SPECIAL:temp:1;
n
   ACQUISITION
                               SAMPLE
                                                     PROCESSING
                                                                               FLAGS
sfrq
             399,952
                                  March 8.
                                             \sim
                                                1h
                                                                        i 1
                        date
                                                            not used
                                                                                            n
tn
                   Η1
                                        1993
                                                sb
                                                            not used
                                                                        in
                                                                                            n
                2 305
                        solvent
                                        cdc13
                                                            not used
                                                                        dp
at
                                                gf
                                                                                            Ч
               29952
np
                        file
                                          exp
                                                awc
                                                            not used
                                                                        hs
                                                                                           nn
                             DECOUPLING
sω
              6497.7
                                                lsfid
                                                            not used
                                                                              SPECIAL
fb
                 3600
                        dn
                                           Η1
                                                phfid
                                                            not
                                                                used
                                                                        temp
                                                                                    not used
bs
            not
                used
                        dof
                                         74.7
                                                wtfile
                                                                   ft
ss
                    0
                        dm
                                          nnn
                                                proc
                 23.0
pω
                        dmm
                                            С
                                                fn
                                                            not used
                                          200
p1
                    0
                        dmf
                                                math
                                                                     i
                        dhp
d1
                    0
                                            0
d2
                    0
                        dlp
                                           20
                                                werr
                                                              logain
              1100.0
                        homo
tof
                                                wexp
                                            n
                   16
                                                wbs
nt
                    0
ct
                                                wnt
```

Figure 7. Single-String Display Template with Output

In a single-string template, the string always starts with a double quote and then repeats the following information for each column in the display:

- Column number (e.g., 2)
- Condition for display of column (optional, e.g., "4(ni)", see below).
- Colon
- Column title (e.g., 2D ACQUISITION)
- Colon
- Parameters to appear in column, separated by commas (for notation, see below)
- Semicolon

At the end of the string is another double quote. Spaces *cannot* appear anywhere in the string template except as part of a column title.

Column titles are often in upper case, but need not be, and are limited to 19 characters. More than one title can appear in the same column (such as shown above, SAMPLE and DECOUPLING are both in column 2).

Parameters listed in "plain" form (e.g., tn, date, math) are printed either as strings or in a form in which the number of decimal places displayed varies depending on the value of the parameter.

To display a specific number of digits past the decimal place, the desired number is placed following a colon (e.g., sfrq:3,at:3,sw:0). Extra commas can be inserted to skip rows within a column (e.g., math, , werr, wexp,).

The maximum number of columns is 4; each column can have 17 lines of output. Since this includes the title(s), fewer than 17 parameters can be displayed in any one column. The entire template is limited to 1024 characters or less.

As an alternative to a single-string template, which tends to be difficult to read, a template can written as multiple strings, each enclosed in double quotes. The first number indicates the number of strings that follow. Each string must start with a column number. Figure 8 contains the display template for the parameter dg2, which is a typical example of a multiple-string template

```
6 "1:1st DECOUPLING:dfrq:3,dn,dpwr:0,dof:1,dm,dmm,dmf:0,dseq,dres:1,homo;"
"2(numrfch>2):2nd DECOUPLING:dfrq2:3,dn2,dpwr2:0,dof2:1,dm2,dmm2,dmf2:0,dseq2,dr
es2:1,homo2;"
"2(numrfch>3):3rd DECOUPLING:dfrq3:3,dn3,dpwr3:0,dof3:1,dseq3,dres3:1,homo3;"
"3(ni2):3D ACQUISITION:d3:3,sw2:1,ni2:0,phase2:0;"
"3(ni2):3D DISPLAY:rp2:1,lp2:1;"
"4(ni2):3D PROCESSING:lb2:3,sb2:3,sbs2(sb2):3,gf2:3,gfs2(gf2):3,awc2:3,wtfile2,p
roc2,fn2:0;"
```

Figure 8. Multiple-String Display Template

The conditional statement in this example (e.g., "(numrfch >2)") is covered below.

The title field can contain a string variable besides a literal. If the variable is a real variable, or not present, or equal to the null string, the variable itself is used as the title (e.g., mystrvar[1]=Example Col 1'and mystrvar[2]=Example Col 2').

Default Display Templates

The settcldefault<(<default><, sequence>)> macro selects the display templates to use as the default for a pulse sequence:

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- Without any arguments, settcldefault prompts for the name of a set of display templates to use for the default displays for the current pulse sequence. The current pulse sequence is defined by the parameter seqfil.
- If a single argument is given, it is used as the name of the display templates for the default displays of the current pulse sequence (e.g., settcldefault('cosy') uses the cosy display templates as the default displays for experiments using the pulse sequence defined by seqfil).
- If a second argument is given, it is used in the place of seqfil to define which pulse sequence will use the default displays of the first argument (e.g., settcldefault('default2d', 'HMQC8') uses the default2d display templates for HMQC8 experiments.

In general, 1D experiments do not need to define a default set of templates because a set already exists. A good default set for *GLIDE*-style 2D experiments is default2d. These experiments generally have capital letters in their names (e.g., HSQC, NOESY). A good default set for older style 2D experiments is defaultold2d. These experiments generally do not have capital letters in their names (e.g., mqcosy, tocsy).

Conditional and Arrayed Displays

Use of parentheses allows the conditional display of an entire column and/or individual parameters. If the real parameter within parentheses is not present, or is equal to 0 or to 'n', then the associated parameter or section is not displayed. In the case of string parameters, if the real number is not present, or is equal to the NULL string or the character 'n', then the associated parameter or section is not displayed. The following examples from the dg template above demonstrate this format:

- pl(pl):1 means display parameter pl only when pl is non-zero.
- sbs(sb): 3 means display sbs only when sb is active (not equal to 'n').
- 4(ni):2D PROCESSING: means display entire "2D PROCESSING" section only when parameter ni is active and non-zero.

Note that if a parameter is arrayed, the display status is derived from the first value of the array. Thus, if pl is arrayed and the first value is 0, pl will not appear; if the first value is non-zero, pl will appear, with "arrayed" as its parameter value.

Similarly, a multiple variable expression can also be placed within the parentheses for conditional display of parameters. Each expression must be a valid MAGICAL II expression (see "Programming with MAGICAL," page 29) and must be written so there is no space between the last character of the expression and the closing parenthesis ")".

In summary, if a single variable expression is placed in the parentheses, it is FALSE under the following conditions:

- Variable does not exist.
- Variable is real and equals 0 or is marked inactive.
- Variable is a string variable equal to the NULL string or equal to the character 'n'.

Multiple variable expressions are evaluated the same as in MAGICAL II. If a variable does not exist, it is considered an error.

Examples of multiple parameter expressions include the following:

• 2(numrfch>2):2nd DECOUPLING: means display entire "2nd DECOUPLING" section only when numrfch (number of rf channels) is greater than 2.

• 3((myflag <> 'n') or ((myni > ni) and (mysw < sw))):My Section: means display entire "My Section" section only when myflag is not equal to 'n' or when myni is greater than ni and mysw is less than sw.

The asterisk (...*) is a "special parameter" designator that allows the value of a series of string parameters to be displayed in a single row without names. This is more commonly used with the parameters aig, dcg, and dmg, for example: aig*, dcg*, dmg*

For tabular output of arrayed parameters, square brackets ([...]) are used. For example: 1:Sample Table Output: [pw,p1,d1,d2];

Notice that all parameters in the column must be in the brackets; thus, the following is illegal:

1:Sample Table Output:[pw,p1,d1],d2;

Since arrayed variables are normally displayed with da, this format is rarely needed.

The field width and digit field options can be used to clean up the display. The first number after the colon is the field width. The next colon is the digit field. For example: 1:Sample Table Output:[pw:6:2,p1:6:2,d1:10:6,d2:10:6];

Here, the parameters pw and p1 are displayed in 6 columns with 2 places after the decimal point, while d1 and d2 are displayed in 10 columns with 6 places after the decimal point.

Output Format

For display, each parameter and value occupies 20 characters of space:

- Characters 1 to 8 are the name of the parameter. Parameters with names longer than 8 characters are permitted within VNMR itself but cannot be displayed or printed with dg or pap.
- Character 9 is always blank.
- Characters 10 to 18 are used for the parameter value. Any parameter value exceeding 9 characters (a file name is a common example) is continued on the next line; in this case, character 19 is a tilde "~", which is used to show continuation.
- Character 20 is always blank.

For printing with the pap command, which uses the ap parameter template, a "da" listing is printed starting in column 3, so that the template will typically specify only two columns of output. ap can specify more than two columns, but if any parameter is arrayed, the listing of that parameter will overwrite the third column. For printing, the maximum number of lines in each column is 64.

5.6 User-Written Weighting Functions

The parameter wtfile can be set to the name of the file containing a user-written weighting function. If the parameter wtfile (or wtfile1 or wtfile2) does not exist, it can be created with the commands

```
create('wtfile','flag')
setgroup('wtfile','processing')
setlimit('wtfile',15,0,0).
```

If wtfile exists but wtfile='' (two single quotes), VNMR does not look for the file: wtfile is inactive. To enable user-written weighting functions, set wtfile=filename, where filename is the name of the executable weighting

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function (enclosed in single quotes) that was created by compiling the weighting function source code with the UNIX shell script wtgen (a process described in the next section).

VNMR first checks if filename exists in wtlib subdirectory of the user's private directory. If the file exists there, VNMR then checks if the file filename.wtp, which may contain the values for up to ten internal weighting parameters, exists in the current experiment directory. If filename.wtp does not exist in the current experiment directory, the ten internal weighting parameters are set to 1.

VNMR executes the filename program, using the optional file filename.wtp as the source for parameter input. The output of the program is the binary file filename.wtf in the current experiment directory. This binary file contains the weighting vector that will be read in by VNMR. The total weighting vector used by VNMR is a vector-vector product of this external, weighting vector and the internal VNMR weighting vector, the latter being calculated from the parameters lb, gf, gfs, sb, sbs, and awc. The parameter awc still provides an overall additive contribution to the total weighting vector. Although the external weighting vector cannot be modified with wti, the total weighting vector can be modified with wti by modifying the internal VNMR weighting vector. Note that only a single weighting vector is provided for both halves of the complex data set—real and imaginary data points of the complex pair are always weighted by the same factor.

If the filename program does not exist in a user's wtlib subdirectory, VNMR looks for a text file in the current experiment directory with the name filename. This file contains the values for the external weighting function in floating point format (for example, 0.025, but not 2.5e–2) with one value per line. If the number of weighting function values in this file is less than the number of complex FID data points (that is, np/2), the user-weighting function is padded out to np/2 points using the last value in the filename text file.

Writing a Weighting Function

Weighting functions must follow this format, similar to pulse sequence programs: #include "weight.h"

The variable wtpntr is a pointer and must be dealt with differently than an ordinary variable such as delta_t.wtpntr contains the address in memory of the first element of the user-calculated weighting vector; *wtpntr is the value of that first element. The statement *wtpntr++=x implies that *wtpntr is set equal to x and the pointer wtpntr is subsequently incremented to the address of the next element in the weighting vector.

The following examples show using the filename program set by wtfile=filename

```
int i;
  for (i = 0; i < npoints; i++)
     *wtpntr++ = (float) (exp(-(delta_t*i*wtconst[0])));
  /* wtconst[0] to wtconst[9] are 10 internal weighting */
  /* parameters with default values of 1 and type float. */
  }

    Optional parameter file filename.wtp in the current experiment directory:

  0.35
           /* value placed in wtconst[0] */
  -2.4
           /* value placed in wtconst[1] */
           /* etc. */
  . . .
 Text file filename in the current experiment directory:
  0.9879 /* value of first weighting vector element */
  0.8876 /* value of second weighting vector element */
  -0.2109 /* value of third weighting vector element */
  0.4567 /* value of fourth weighting vector element */
           /* etc. */
  . . .
          /* value of last weighting vector element */
  0.1234
```

Compiling the Weighting Function

The macro/shellscript wtgen is used to compile filename as set by parameter wtfile into an executable program. The source file is filename.c stored in a user's vnmrsys/ wtlib directory. The executable file is in the same directory and has the same name as the source file but with no file extension. The syntax is for wtgen is wtgen(file<.c>) from VNMR or wtgen file<.c> from UNIX.

The wtgen macro allows the compilation of a user-written weighting function that subsequently can be executed from within VNMR. The shellscript wtgen can be run from within UNIX by typing the name of the shellscript file name, where the .c file extension is optional. wtgen can also be run from within VNMR by executing the macro wtgen with the file name in single quotes.

The following functions are performed by wtgen:

- 1. Checks for the existence of the bin subdirectory in the VNMR system directory and aborts if the directory is not found.
- 2. Checks for files usrwt.o and weight.h in the bin subdirectory and aborts if either of these two files cannot be found there.
- 3. Checks for the existence of the user's directory and creates this directory if it does not already exist.
- 4. Establishes in the wtlib directory soft links to usrwt.o and weight.h in the directory /vnmr/bin.
- 5. Compiles the user-written weighting function, which is stored in the wtlib directory, link loads it with usrwt.o, and places the executable program in the same directory. Any compilation and/or link loading errors are placed in the file errmsg in wtlib.
- 6. Removes the soft links to usrwt.o and weight.h in the bin subdirectory of the VNMR system directory.

The name of the executable program is the same as that for the source file without a file extension. For example, testwt.c is the source file for the executable file testwt.

5.7 User-Written FID Files

You can introduce computed data into your experiment by using the command makefid(input_file <, element_number, format>). The input_file argument, which is required, is the name of a file containing numeric values, two per line. The first value is assigned to the X (or real) channel; the second value on the line is assigned to the Y (or imaginary) channel. Arguments specifying the element number and the format are optional and may be entered in either order.

The argument element_number is any integer larger than 0. If this element already exists in your FID file, the program will overwrite the old data. If not entered, the default is the first element or FID. format is a character string with the precision of the resulting FID file and can be specified by one of the following:

'dp=n'	single precision (16-bit) data
'dp=y'	double precision (32-bit) data
'16-bit'	single precision (16-bit) data
'32-bit'	double precision (32-bit) data

If an FID file already exists, format is the precision of data in that file. Otherwise, the default for format is 32 bits.

The number of points comes from the number of numeric values read from the file. Remember it reads only two values per line.

If the current experiment already contains a FID, you will not be able to change either the format or the number of points from that present in the FID file. Use the command rm(curexp+'/acqfil/fid') to remove the FID.

The makefid command does not look at parameter values when establishing the format of the data or the number of points in an element. Thus, if the FID file is not present, it is possible for makefid to write a FID file with a header that does not match the value of dp or np. Since the active value is in the processed tree, you will need to use the setvalue command if any changes are needed.

Be aware that makefid can modify data returned to an experiment by the rt command. To avoid this, enter the following sequence of VNMR commands on the saved data before running makefid:

```
cp(curexp+'/acqfil/fid',curexp+'/acqfil/fidtmp')
rm(curexp+'/acqfil/fid')
mv(curexp+'/acqfil/fidtmp',curexp+'/acqfil/fid')
```

The command writefid(textfile<, element_number>) writes a text file using data from the selected FID element The default element number is 1. The program writes two values per line—the first is the value from the X (or real) channel, and the second is the value from the Y (or imaginary) channel.

Chapter 6. Customizing Graphics Windows

Sections in this chapter:

- 6.1 "Customizing the Sample Entry Form Window," this page
- 6.2 "Customizing the status Window," page 322
- 6.3 "Customizing the Interactive dg Window," page 324

Almost every aspect of VNMR graphics windows can be customized for local use. Many of these windows are written in the scripting language Tcl/Tk (tool command language/tool kit). This language allows considerable customizing by users of the windows and their functions.

To find out more about Tcl/Tk, refer to books such as *Tcl and the Tk Toolkit* by J. K. Ousterhout (Addison-Wesley, 1994) and *Effective Tcl/Tk Programming* by M. Harrison and M. McLennan (Addison-Wesley, 1998). For those who do not wish to learn Tcl/Tk, Varian has further simplified much of this customization through the use of .conf files.

6.1 Customizing the Sample Entry Form Window

The Sample Entry Form window is the interface to the enter program. The enter program is used to define experiments for an automation run. The Sample Entry Form window is covered from the user's viewpoint in the manuals *Getting Started*, *User Guide: Liquids*, and *Walkup NMR Using GLIDE*. In this section, we cover customizing the enter interface.

Almost everything about the enter interface can be modified by the user. This includes whether certain choices are presented and whether choices are presented as check boxes or require typed input. Requests for alternative information also can be added.

Window Configuration Files

The interface to the enter program is controlled by one of following configuration files supplied in the directory /vnmr/asm:

- auto.conf when defining an experiment for a current automation run.
- enter.conf when setting up an automation run with a Carousel, SMS, or NMS sample changer.
- entervast.conf when setting up an automation run with the VAST accessory.
- enterlcnmr.conf when setting up an automation run with the LC-NMR accessory.

The enter.conf file is duplicated in Listing 14, with the lines numbered for reference. Any line in the file that starts with a # is a comment line. The interface presented by this configuration file is shown in Figure 9.

Listing 14. Text of enter.conf File

```
1. # Enter configuration information
2.
3. # infields identifies the items that will be displayed by the
4. # enter program. The order of the listed items is the order
5. # in which they will be displayed.
6. set infields {loc user solvent exp textfield}
7.
8. # outfields identifies the items that will be output by the
9. # enter program. The order of the listed items is the order
10. # in which they will be output.
11. set outfields {loc user exp solvent textfield userdir data stat separator}
12.
13. # Available input styles include info, radio, check, xradio, xcheck,
14. # xradiocustom, xcheckcustom, and textentry
15.
16. set loc(id) loc
17. set loc(label) "Sample Number"
18. set loc(menulabel) "Sample Number is "
19. set loc(style) radio
20. set loc(file) ""
21. set loc(min) 1
22. set loc(max) 50
23. set loc(numPerLine) 20
24. set loc(required) 1
25. set loc(output) SAMPLE#:
26. set loc(duplicates) 0
27. set loc(errormess) "No sample locations available"
28. set loc(errormess2) "Sample Tray is Completely Defined"
29.
30. # To select locations instead of allowing a choice
31. # uncomment the following lines
32. # set loc(label) "Insert Sample at location "
33. # set loc(output) SAMPLE#:
34. # set loc(style) info
35. # set loc(output) SAMPLE#:
36. # set loc(value) $nextLoc
37. # set loc(usenextloc) 1
38.
39. set user(id) user
40. set user(label) "User identification"
41. set user(menulabel) "User identification is "
42. set user(style) xradio
43. set user(file) users
44. set user(numPerLine) 6
45. set user(required) 1
46. set user(output) USER:
47.
48. # The following five lines set USER automatically.
49. # If you do not want USER to appear on the enter screen,
50. # remove user from infields. If you uncomment the following,
51. # this mode will be selected
52. #
53. # set user(id) user
54. # set user(label) "User identification is "
55. # set user(style) info
56. # set user(output) USER:
57. # set user(value) "$env(USER)"
```

Listing 14. Text of enter.conf File (continued)

```
58.
59. set solvent(id) solvent
60. set solvent(label) "Solvent Selection"
61. set solvent(menulabel) "Solvent Selection is "
62. set solvent(style) xradio
63. set solvent(file) solvents
64. set solvent(numPerLine) 4
65. set solvent(required) 1
66. set solvent(output) SOLVENT:
67.
68. set exp(id) exp
69. set exp(label) "Experiment Selection"
70. set exp(menulabel) "Experiment Selection is "
71. set exp(style) radio
72. set exp(file) experiments
73. set exp(numPerLine) 6
74. set exp(required) 1
75. set exp(output) MACRO:
76.
77. # The following three lines allow customization of experiments
78. # set exp(style) xradiocustom
79. # set exp(label2) "Selected Experiment"
80. # set exp(col) 40
81.
82. set textfield(id) textfield
83. set textfield(label) "Text\t"
84. set textfield(style) textentry
85. set textfield(file) ""
86. set textfield(col) 40
87. set textfield(required) 0
88. set textfield(output) TEXT:
89.
90. set userdir(id) userdir
91. set userdir(output) USERDIR:
92. set userdir(value) "$env(vnmruser)"
93.
94. set data(id) data
95. set data(output) DATA:
96.
97. set stat(id) stat
98. set stat(output) "STATUS:"
99. set stat(value) "Queued"
100.
101. set separator(id) separator
102. set separator(output) ------
103.
104. # Button Definitions
105. # Possible cntrls are addExp, saveExp, saveAndExit, addSaveAndExit, quit
106. # Automation controls are autoSample,autoSampleNoExit,priortySample,quit
107.
108. set cntrls {addExp saveAndExit quit}
109. # if you prefer a two button exit mechanism, uncomment the next line
110. # set cntrls {addSaveAndExit quit}
111. # if you prefer a one button exit mechanism, uncomment the line below
112. # In this case, the label for quit should be reset to "Exit"
113. # set cntrls {saveExp quit}
114.
```

Listing 14. Text of enter.conf File (continued)

```
115. set addExp(id) addExp
116. set addExp(label) "Add Entry"
117.
118. set saveExp(id) saveExp
119. set saveExp(label) "Save Entry"
120
121. set saveAndExit(id) saveAndExit
122. set saveAndExit(label) "Exit and Save"
123.
124. set addSaveAndExit(id) addSaveAndExit
125. set addSaveAndExit(label) "Exit and Save"
126
127. set autoSample(id) autoSample
128. set autoSample(label) "Add Sample"
129.
130. set autoSampleNoExit(id) autoSampleNoExit
131. set autoSampleNoExit(label) "Add Sample"
132.
133. set priortySample(id) priortySample
134. set priortySample(label) "Priority Sample"
135. set priortySample(passwd) ""
136.
137. set quit(id) quit
138. set quit(label) "Quit"
139.
140. # list of files from which excluded locations are taken
141. # the files names are relative to the directory of the enter file
142. set exList {}
143. set locList {}
144.
145. # show and edit can be yes or no
146. # content can be all or new
147. # num sets the number of entries to be shown in the scrolling window
148. # col sets the width of the scrolling window (in characters)
149. set results(show) no
150. set results(edit) no
151. set results(content) all
152. set results(num) 3
153. set results(col) 60
```

Setting Which Selections Are Displayed

On line 6, the infields parameter specifies which selections are displayed by enter and in what order. The default requests five selections, named loc, user, solvent, exp, and textfield. Most of the names chosen are arbitrary, but as you will see, subsequent definitions depend on the names set here. Also, while names such as xj and kld could also work, their meaning is not obvious. You might, however, want to add a name such as notebook. We use notebook as an example later in this chapter. Note that the loc and exp names are not arbitrary. These two input selections have been given special characteristics that require specific attributes.

Setting the Content of the Output File

On line 11, the outfields parameter specifies which items are written by enter into its output file and in what order they are written. This output file contains all the information

needed to run an experiment and is referred to as the enterQ file, even though at the time it is built, its name is arbitrary. When the output file is finally submitted as the set of experiments by the autogo command, it is copied into the automation directory and named enterQ.

The default enter program requests nine selections—named loc, user, exp, solvent, textfield, userdir, data, stat, and separator—to be written into the enterQ file. Some of the items in outfields match items in infields, and some do not. Also, the order that the items are written does not need to match the order of the items in infields.

Setting Name Attributes

The characteristics of each name used by infields and outfields needs to be defined. Each name is defined by a series of attributes. The attributes are fixed. They include an id, label, menulabel, style, file, numPerLine, required, output, and duplicates. There are also some attributes that depend on the value of other attributes. These include min, max, errormess, and usenextloc.

The syntax of setting attributes is shown on lines 16 to 27. The word set is a command that takes two arguments. The first argument is a parameter name and the second is a value. For example, the line

set loc(id) loc

sets the parameter loc(id) to the word loc. The id attribute should match the name of the item. The value of the label attribute is displayed at the top of the window pane used for that selection.

The label Sample Number shown in Figure 9 is controlled by the line set loc(label) "Sample Number"

– Sample Entry Form r				
Sample Number				
1 2 3 4 5 6 7 8 9 1	1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20			
21 22 23 24 25 26 27 28 29 3	30 31 32 33 34 35 36 37 38 39 4	0		
41 42 43 44 45 46 47 48 49 5	50			
	User identification			
vnmr1				
Solvent Selection				
CDC13 D20 Benzene DMSO				
Acetone Cyclohexane Tol	uene Methanol			
	Experiment Selection			
H1	C13	F19		
P31	HC	H-gCOSY		
H-TOCSY	H-gHSQC	H-gCOSY-gHSQC		
H-gCOSY-HSQC-gHMBC	H-gCOSY-HSQC-gHMBC-HSQCTOXY	H-COSY-C-DEPT-HETCOR		
H-COSY-C-APT	H-TOCSY-NOESY	H-TOCSY-ROESY		
H-TOCSY-HMQC	H-TOCSY-HMQC			
Text				
Customize Parameters Add Entry Exit and Save Quit				
Number of samples submitted: 0				

Figure 9. Default Interface (enter Program)

Note that if a parameter name is to be set to more than one word, the words need to be enclosed in double quotes (").

The menulabel attribute is currently unused.

Setting the Types of Widgets

The style attribute defines the type of widget used to select information. Available input styles include info, radio, check, xradio, xcheck, textentry, xradiocustom, and xcheckcustom.

The info style is used when information is presented to the user but the user cannot make a selection. This style is not used in the default enter.conf file but is used in two alternative interfaces that are commented out.

- The first, on lines 31 to 36, changes how the sample location is presented. In the default interface, a user presses a button to select a tray number. In the commented out interface, the user is presented with a location number into which the sample must be placed.
- The second, on lines 52 to 56, changes the way user identification is selected. In the default interface, a user presses a button to select a user name. In this interface, the user id is displayed for informational purposes but cannot be changed.

The radio and check styles are identical in function but different in appearance. The radio style presents a button with a label inside of the button. The check style presents a small box that can be checked, and the label is printed along side. For both radio and check styles, multiple selections can be made. The Sample Number and Experiment Selection window panes use the radio style.

Stylistically, xradio and xcheck styles are the same as the radio and check styles, respectively. The difference is that xradio and xcheck provide for exclusive selection of a choice. That is, if you press choice a and then choice b, choice a is deselected. The User identification and Solvent Selection window panes are examples of the xradio style.

If the style for the exp parameter is changed from radio to xradio, then the user can only select a single experiment. In the default setup, a user can select multiple experiments on a single sample location. A user can also select one or more experiments on a number of sample locations. When multiple samples and experiments are selected, then enterQ is ordered to minimize robot usage by finishing all experiments on a sample before putting the next sample into the magnet. If the style of the loc selection is changed from radio to xradio, the user can select only a single location.

The Sample Location buttons use the right mouse button to facilitate selecting multiple locations. The left mouse button selects and deselects an item, just as it does for all the check boxes. A single click of the right mouse button on one of the location check boxes selects that location and all preceding locations down to the next selected location. For example, a left mouse click on location 10 selects it. A right mouse click on 14 selects locations 14, 13, 12, and 11. A double click of the right mouse button on a location deselects that location and all preceding locations down to the first deselected location.

Alternate Interfaces

Figure 10 shows an interface in which all radio styles are changed to the check style and all xradio styles and changed to the xcheck check. Notice that the small box for the xcheck style (exclusive choice) is a diamond and the small box for the check style (multiple choice) is a square. If the textentry style is selected, a user simply inputs text.

🗁 Sample Ent	ry Form		
Sample	Number		
1 1 2 1 3 1 4 1 5 1 6	7 8 9 10		
	6 🗔 17 🗔 18 🗔 19 🗔 20		
	6 🗆 27 🗔 28 💷 29 🗔 30		
31 32 33 34 35 3	6 🔟 37 🛄 38 🛄 39 🛄 40		
	6 🔟 47 🔟 48 🔟 49 🔟 50		
User ident	tification		
💠 vnmr1			
Solvent Selection			
♦ CDC13 ♦ D20 ♦ Benzene ♦ DMS0			
💠 Acetone 🛛 💠 Cyclohexane 🤜	🗸 Toluene 🛛 🕹 Methanol		
Experiment	Selection		
☐ H1	□ C13		
□ F19	⊒ P31		
⊐ HC	☐ H-gCOSY		
☐ H-TOCSY	⊒ H-gHSQC		
☐ H-gCOSY-gHSQC	☐ H-gCOSY-HSQC-gHMBC		
☐ H-gCOSY-HSQC-gHMBC-HSQCTOXY	☐ H-COSY-C-DEPT-HETCOR		
☐ H-COSY-C-APT	H-TOCSY-NOESY		
☐ H-TOCSY-ROESY	☐ H-TOCSY-HMQC		
Text			
Customize Parameters Add Entry Exit and Save Quit			
Castomize ranameters had fifting exit and save			
Number of samples submitted: 0			

Figure 10. Alternate Interface (enter Program)

A col attribute defines how much space to make available for character input. You set the col attribute to the maximum number of characters you expect. The textfield parameter uses this style have allocates space to enter 40 characters.

The xradiocustom style is a hybrid of the xradio style and the textentry style. Similarly, the xcheckcustom style is a hybrid of the xcheck style and the textentry style. These two styles provide a set of xradio or xcheck buttons that initialize the textentry field. The textentry field can subsequently be edited. This is useful for users who like to customize standard experiments.

For example, if the H1 experiment button is pressed, the h1 macro is written into the textentry field. You might then add temp=40 to the textentry field. If the xradiocustom or the xcheckcustom styles are selected, two additional attributes are needed. A label2 attribute specifies a second label to be printed in front of the textentry field. A col attribute defines how much space to make available for character input. These styles are not used in the default enter.conf file but are used in an alternative interface that is commented out. Lines 77 to 79 will select this alternative xradiocustom interface. Figure 11 shows the interface with this selection.

File Attribute

The file attribute must be present for any parameter listed in infields. If file is set to a name, then a file of that name in the /vnmr/asm directory is read to specify the choices available. The user, exp, and solvent parameters specify a file for their set of choices. These files are pairs of lines. The first line is a label that will be displayed as a choice. The second line of each pair is the string that will be output into the file generated

-		Sai	mple Entry Form			•
	Sample Number					
1 2 3 4						
21 22 23 24	25 26 27 28 2	29 30 31 32 3	33 34 35 36 37 3	38 39 4	40	
41 42 43 44	45 46 47 48 4	19 50				
		Use	r identificatio	n		
vnmr1						
		So	lvent Selection	ı		
CDC13	D20	Benzene	zene DMSO			
Acetone	Cyclohexane	Toluene	uene Methanol			
		E×pe	eriment Selectio	on		
H1 C13			F19			
P31		HC	НС		H-gCOSY	
H-TOCSY		H-gHSQC	H-gHSQC		H-gCOSY-gHSQC	
H-gCOSY-HSQC-gHMBC		H-gCOSY	H-gCOSY-HSQC-gHMBC-HSQCTOXY		H-COSY-C-DEPT-HETCOR	
H-COSY-C-APT H-TOCSY-NOESY			H-TOCSY-ROESY			
H-TOCSY-HMQ	H-TOCSY-HMQC					
Selected Experiment AuHexp						
Text temp=40	Text temp=40					
Customize Parameters Add Entry Exit and Save Quit						
Number of sa	Number of samples submitted: 0					

Figure 11. Second Alternate Interface (enter Program)

by the enter command. If the file attribute is set to a null string, the min and max attributes can be selected for choices of integers. This is used by the loc selection.

The numPerLine attribute provides some control over the layout of the enter program. This attribute specifies how many choices are presented on a line. You may notice that the numPerLine attribute for the loc selection differs between Figure 9 and Figure 10.

The required attribute specifies whether a particular selection must be made. In the default configuration file, the required attribute for textfield is set to 0. This means that users do not need to enter descriptive text in order to submit an experiment. Changing the value of the required attribute to 1 enforces entry of descriptive text.

The output attribute specifies the title of a line in the enterQ file. Every parameter listed in outfields must have an output attribute. Parameters listed in infields that have a style of radio, check, xradio, xcheck, textentry, xradiocustom, or xcheckcustom have the selected choice printed after the value of the output attribute. Other parameters can define an attribute named value, the value of which is printed after the value of the output attribute in the enterQ file.

The loc parameter has several special attributes:

- The duplicates attribute specifies whether a user can duplicate a location that is present in a preexisting file. By default, this is not allowed. The locations defined in the preexisting files are shaded out in the location window pane and are not selectable. For example, notice locations 2 and 6 in Figure 9, Figure 10, and Figure 11.
- The errormess attribute specifies an error message to be displayed when a sample tray is filled. If this message is set, no more samples are accepted. If errormess is set to a null string (''), sample locations that are finished can be reused. The null setting is useful for continuous "walkup" operation.

- The errormess2 attribute specifies an error message to be displayed in the continuous walkup mode (i.e., errormess is set to a null string) when all sample locations are used.
- The usenextloc attribute is an initialization step only; it is not customizable.

Button Definitions

The buttons at the bottom of the enter window are partially configurable. The choices available are addExp, saveExp, saveAndExit, addSaveAndExit, and quit. Choices appropriate to automation runs are autoSample, autoSampleNoExit, and prioritySample.

- The addExp selection, when pressed, copies the currently defined experiments into a temporary file. The user still has the choice of ending the session by pressing either the saveAndExit button or the quit button.
- The saveAndExit selection appends the temporary file created by pressing the addExp button to the enterQ output file, deletes the temporary file, and then causes the enter program to exit.
- The saveExp button, when pressed, copies the currently defined experiments into a temporary file, appends the temporary file to the enterQ output file, and then deletes the temporary file.
- The addSaveAndExit button does exactly the same things as the saveExp button and then it causes the enter program to exit.
- The autoSample button submits the currently defined experiment directly to an automation run and then exits the enter program.
- The autoSampleNoExit button functions the same as the autoSample button except autoSampleNoExit does not cause the enter program to exit.
- The prioritySample button submits the currently defined experiment to the front of the queue of an automation run and then exits the enter program.
- The quit button deletes the temporary file and then exits.

In the default case, the user can create a lot of experiments with the addExp button, but not actually add them to the enterQ file until the saveAndExit button is pressed.

As an alternative, a two-button exit scheme might be preferred by some. In this case, an addSaveAndExit button and a quit button would be present. The addSaveAndExit button writes the experiments to a temporary file, appends the temporary file to the enterQ output file, deletes the temporary file, and then exits. In effect, it is the combination of the addExp button and the saveAndExit button.

A third alternative is to use the saveExp and quit buttons. In this case, the only way to exit from the enter program is with the quit button. After pressing the saveExp button, there is no way to cancel those experiments. Figure 11 shows this alternative.

The cntrls parameter on line 107 specifies the buttons and their order. The names are important in this case. The alternate scheme is selected by removing the comment symbol (#) in line 109. The second alternative scheme is selected by removing the # in line 112. The only other attribute that is configurable is the label for each button.

rtoutput and rtoutput2 Attributes

Buttons of type addExp, saveExp, addSaveAndExit, autoSampleNoExit, autoSample, and priortySample can have a rtoutput attribute. The value of the

rtoutput attribute is sent to VNMR for every sample added to the enter queue by the button.

The rtoutput attribute has access to all of the attributes of all the variables listed in the outfields variable. In addition, the value of each of the outfield variables is available as the val attribute.

For example, \$loc(val) contains the value of loc of the submitted experiment. Similarly, \$user(val), \$solvent(val), etc. will be set to the values selected by the user.

A variable \$filename is the name of the file where the output from the enter program will be written.

A second real-time output attribute can be specified by the rtoutput2 attribute, which has access to all the same variables as the rtoutput attribute. The distinction is that the action specified for rtoutput occurs for each sample submitted. A single press of the addExp button can cause many experiments to be submitted, if, for example, multiple experiments and/or multiple locations were specified. The rtoutput will occur once for each submitted experiment. The rtoutput2 action happens after all the rtoutput actions and only once for the entire group of samples submitted by a single button press.

An example is as follows:

```
set addExp(id) addExp
set addExp(label) "Add Entry"
set addExp(rtoutput) {write('alpha','loc=$loc(val)')}
set addExp(rtoutput2) {write('alpha','info written to file $filenam
```

If any $\$ variables are included in the value of the attribute, the value must be enclosed in braces $\{\,\}.$

Adding a Control Button that Sends a Command to VNMR

A control button can be made that sends a command to VNMR when the button is selected. For example, to add a hello button to the bottom of the Sample Entry Form window, add hello button to the cntrls line and then define the button in the enter.conf file. The control buttons have access a variable \$filename that is the name of the file where the output from the enter program will be written.

```
set cntrls {addExp saveAndExit quit hello}
set hello(id) vnmrexec
set hello(label) "hello"
set hello(rtoutput) "banner('hello')"
```

The id attribute must be vnmrexec and the rtoutput attribute will be sent to VNMR. If any \$ variables are included in the value of the attribute, the value must be enclosed in braces { }.

Using radio and check with set_rtoutput and unset_rtoutput Attributes

Selections of type radio and check have optional attributes set_rtoutput and unset_rtoutput. These attributes are magical commands that will be sent to VNMR when the button is selected and deselected, respectively. The value of the attribute can include any other attribute from that group.

Prepend a \$ character to the front of the attribute name to access the value of that attribute. In addition, four other variables are provided:

- \$index the index of the selected or deselected radio or check button.
- \$label the label of the selected or deselected radio or check button.
- \$value the value of the selected or deselected radio or check button.
- \$filename the name of the file where output from enter will be written.

For example

```
set loc(set_rtoutput) {write('alpha','$loc(label) $value selected')}
set loc(unset_rtoutput) {write('alpha','$loc(label) $value de-selected')}
```

If any \$ variables are included in the value of the attribute, the value must be enclosed in braces $\{\}$.

Using xradio and xcheck with rtoutput Attribute

Selections of type xradio and xcheck have an optional attribute rtoutput. This attribute is a magical command that will be sent to VNMR when the button is selected. The value of the attribute can include any other attribute from that group.

Prepend a \$ character to the front of the attribute name to access the value of that attribute. In addition, four other variables are provided:

- \$index the index of the selected xradio or xcheck button.
- \$label the label of the selected xradio or xcheck button.
- \$value the value of the selected xradio or xcheck button.
- \$filename the name of the file where output from enter will be written.

For example

```
set user(rtoutput) {write('alpha','$user(label) is $label with $value')}
```

If any \$ variables are included in the value of the attribute, the value must be enclosed in braces $\{\}$.

Sample Entry Control

The exList field in the configuration files is used to specify files that contain excluded sample locations. This is important for walkup automation, where sample locations are reused. The field is a list of file names. The contents of the files are searched for location definitions. For example, if the line SAMPLE#: 33 is one of the files, location 33 will be excluded. This is also useful to exclude certain locations that contain reference samples.

The current exList is set to {expl/sampleinfolocQ}. Relative path names are relative to the automation directory. Absolute path names can also be used. The entry expl/sampleinfo prevents the current location of the sample in the magnet from being used. The locQ entry causes all locations to be used before they are reused. Removing locQ from exList makes locations available for reuse as soon as all the experiments on that location are finished.

The locList is a single file that contains a list of locations that are submitted to an automation run. This file is used to recycle used locations for walkup automation and should not be altered. The difference between the files enter.conf and auto.conf

files is the selection of the button at the bottom of the window and the setting of the exList and locList parameters.

Adding a New Field

If you want to add a new field to the enter program, editing the enter.conf file is required. Suppose you want to have the users input a notebook number. If you have a list of possible notebook numbers, you could use a xcheck or xradio style of window pane.

Alternatively, you could have the user type in a notebook number, using the textentry style. Adding the following lines defines the window pane, using the textentry style. set notebook(id) notebook

```
set notebook(id) notebook
set notebook(label) "Note book Number"
set notebook(style) textentry
set notebook(col) 40
set notebook(col) 40
set notebook(output) NOTEBOOK:
set infields {loc user solvent exp notebook textfield}
set outfields {loc user exp solvent notebook textfield userdir data
stat separator}
```

Adding notebook to infields causes the notebook pane to appear in the enter program. Adding notebook to outfields causes its value to be written to the file when an entry is added. Note that in the example the notebook entry is specified as required. The specifications in the enter.conf file can be multiply defined. The last definition, in a top-to-bottom model, is the definition that is used. Therefore, adding the above lines to the button of the default enter.conf file has the effect of adding the notebook window pane. You could instead edit the infields and outfields definitions on lines 6 and 11 directly.

These changes add the notebook field to each entry in the enter queue for the automation run. The auto_au macro probably needs to be updated to take advantage of the new notebook field. You might set a VNMR parameter to the value of the notebook number. Or, in conjunction with the autoname parameter, you could imbed the notebook entry in the file name used to save the data.

New fields are the primary addition to the gilson.conf configuration file. Added were entries to specify the rack location on the sample changer (up to 5 rack locations are possible) and the zone location (each rack location can have up to 3 different zones). A specific configuration files for the status command (statgil.conf) is present to handle the extra outfields members.

6.2 Customizing the status Window

The status window displays the contents of the enterQ and doneQ files used to control automation:

- enterQ contains the list of experiments remaining to be submitted. This file is constructed by the enter program, which uses the outfields parameter to specify which items are written into the enterQ file.
- doneQ contains the list of experiments that either are currently active or are finished. This file is derived from the enterQ file.

Window Configuration File

The interface to status is usually controlled by the status.conf file., supplied in the /vnmr/asm directory. This file is duplicated in Listing 15, with the lines numbered for reference. Any line in the file that starts with a # is a comment line.

For status to work correctly, an outfields parameter must be specified that matches the outfields parameter used by enter as the initiator of the automation run. The

Listing 15. Text of the status.conf File

```
1. # Status configuration information
2.
3. # outfields identifies the items which will were output by the
4. # enter program. The order of the listed items must be the
5. # same as those used for the enter program
6. set outfields {loc user exp solvent textfield userdir data stat separator}
7.
8. # showfields identifies the items which will be displayed by the
9. # status program. They must be a subset of outfields. The order
10. # does not need to be the same as outfields
11. set showfields {user loc textfield}
12.
13. # Button Definitions
14. # Possible cntrls are rt locate and quit
15. set cntrls {rt locate quit}
16.
17. set rt(id) rt
18. set rt(label) "Retrieve Data"
19.
20. set locate(id) locate
21. set locate(label) "Find Entry"
22.
23. set quit(id) quit
24. set quit(label) "Quit"
25.
26
27. # num sets the number of entries to be shown in the scrolling window
28. # col sets the width of the scrolling window (in characters)
29. # logtitle sets the title above the Log window
30. # rows sets the number of rows in the Log window
31. # the selectcolor set the color of an entry which is selected with
32. # a mouse click. The other color parameters set colors of entries
33. # based on the STATUS: field for that entry.
34. # sort defines the way that the entries will be sorts. The choices
35. # are std, loc, user, or stat
36. set results(num) 8
37. set results(col) 60
38. set results(logtitle) "Log information"
39. set results(rows) 15
40. set results(selectcolor) pink
41. set results(errorcolor) red
42. set results(queuecolor) blue
43. set results(completecolor) black
44. set results(activecolor) magenta
45. set results(totalcolor) black
46. set results(sort) std
47. set results(sort) user
```

order of the items in the outfields parameter must also match that used by the enter program.

The status command displays a scrollable window with the separate experiments listed. Not all fields that define an enterQ entry need to be displayed in this window. The showfields parameter is a subset of the items in outfields. These are displayed in the order they are defined by the showfields parameter.

Defining Buttons and Window Attributes

Three buttons can be defined to be displayed below the scrolling list of experiments. The choices are rt, locate, and quit. The parameter cntrls is used to define to buttons and their order. The label on each button is controlled by the label attribute of each button definition.

When an entry in the scrolling window is clicked on with the left mouse button, a full summary of that entry is displayed below the buttons. The results parameter controls the details of the scrolling window and the summary display. Figure 12 shows the default status window.

The num attribute sets the number of experiments to be displayed in the scrolling window. This value, along with the number of items in the showfields parameter, determines the overall height of the status window.

The col attribute defines how much space to make available for character display. This attribute controls the overall width of the status window.

The logtitle attribute specifies the title to be displayed above the summary window.

Color is used by the status program to indicate the experiment status. Possible statuses are queued, active, complete, shimming, and error. Color selection for each status are made with the appropriate color attribute.

Two other color attributes are defined:

- selectcolor sets the color of the currently selected entry from the scrolling window. That is, the entry where the left mouse was clicked.
- totalcolor is the color of the number of total experiments shown at the top of the status command.

The sort attribute defines the default sorting criterion to be used to display the experiments in the scrolling window. The choices are to sort chronologically, which is the std sort, to sort by location numbers (loc), to sort by user names (user), or to sort by experiment status (stat). This attribute only defines the default sort. The locate button provides access to the other sort criteria.

6.3 Customizing the Interactive dg Window

The interactive dg window brings a new level of functionality to VNMR. This window is readily customizable and so can be designed for the specific needs of individual pulse sequences. The window consists of a series of panes. Any pane can be selected by clicking on the label tab normally found to the right of the window. Figure 13 shows this window.

Each pane of the window deals with settings and actions associated with a particular phase of operating the spectrometer. The most common display element on a pane is a labeled value of a setting. This value may be altered by clicking on it with the mouse, editing the value in the normal manner, and then either pressing Return or moving the mouse cursor to another value and clicking on that (shifting the focus).

_		Sa	mple Status				
Samples: (Complete				
LICER	2	0	5	0	8		A
SAMPLE#: TEXT:							
USER: SAMPLE#: TEXT:	5						
USER: SAMPLE#: TEXT:	6						
USER: SAMPLE#: TEXT:							
USER: SAMPLE#: TEXT:	15						
USER: SAMPLE#: TEXT:	21						
USER: SAMPLE#: TEXT:							
USER: SAMPLE#: TEXT:							
		Loş	g informat:	ion			
SAMPLE#:	6						Δ
USER: MACRO: SOLVENT:	h1 cdcl3						
TEXT: USERDIR: DATA: STATUS:	/usr24	/dan/tst	rsys ness/tcl/a	uto/0101			
Mon Jul 29 Mon Jul 29	15:25:5 15:26:5	4 1996: 5 1996:	Experiment Acquisitio	started n complet	e		
						j	
Retrie	eve Data		Find H	Intry		Quit	

Figure 12. Default Interface (status Program)

-				dg					· 🗆
Acquisition			Observe (Channel		Samp	le		Acq & Obs
Spect width	5998.8	Hz	Nucleus	HL		Date	Jul 29 96		
Acq. time	2.50183	sec	Spect Freq.	400.075	MHz	File	fid1d.fid		Decouplers
Acquired complex pts	15008		offset	0.0	Hz	Solvent	CDC13		Sequence
Recycle delay	1.0	sec	obs pulse	7.75	us	temperature	e 29	C	Flags & Cond.
Transients	16		power	55					Process
Steady state	0								Process
			Calibration	0		Channel	: Nucl.	Status	Process2
			pi/2 pulse	: 7.75	us	Observe	: H1		Display
			power	55		Decoupler	: H1	– nnn	<u> </u>
						Decoupler2	1 C C	-	display2
						Decoupler3	:	-	LCNMR/STARS
						Gradient Ty			Text
						oradient 1	the mud		Spare
									Setup EXP

Figure 13. dg Window

Chapter 6. Customizing Graphics Windows

Normally a setting displayed in dg is associated with a parameter. You can alter the setting by typing into the command line in the normal way or as outlined above

A number of editing operations can be used on an entry:

- A single click of the left mouse button positions the entry cursor between characters at about the mouse position. Typing characters insert them at this point. The backspace key deletes characters to the left of the cursor, and the Del key deletes characters to the right.
- Double-clicking the left mouse button highlights a string of characters bounded by white space or punctuation, such as a word. The highlighted characters can be deleted as a group or changed as a group by typing new characters.
- Triple-clicking highlights the entire entry. This spans multiple words. The action on deletion or overtyping is the same as the double click highlight.

Types of Fields

Many types of fields are available—titles, labels, entries, tabs, menus, buttons, check boxes, and more. Each type of field available is described in this section.

Titles

Titles are inactive, but identify groups of elements, normally below the title.

Labels

A label consists of two components—a character string and its current value. A label is noninteractive. An example of a label is "Completed transients 423".

Entries

An entry consists of three components—a character string (label), its current value and its units. The value field is interactive and is editable using the previous rules.

The unit field may be absent, may be fixed or may be selectable. If selectable, the selection is through a menu that is accessed by holding down the left mouse button on the field and then moving it to the desired new value before releasing it. Unit changes are local; they require no action from within VNMR.

Tabs

Each pane of dg has a tab associated with it. These tabs are normally on the right edge of the window. The currently displayed pane has its tab raised to the front. You can go to any other pane simply by clicking on its tab.

The tab labeled **Spare** typically has nothing of interest in its pane. The tab labeled **Text** is the text window of older versions of VNMR. It is here that commands such as dll display output. Commands dg, dgs etc. still work and display their traditional output on this pane.

As soon as the text displayed is greater than the size of the pane, a vertical scroll bar appear as an aide to navigation.

Menus

A menu consists of either one or two elements. Used on its own, a menu may have a character string (label) element and a choice bar. Used in conjunction with an "Entry," only

the choice bar is seen. The choice bar has a small rectangle embedded in it. The choice bar also shows the current choice.

The left mouse button drops down the menu of choices when depressed while the mouse is on the choice bar. Keep the button depressed and move the mouse to highlight the desired choice. Release the mouse button and this will make the choice.

Buttons

A button differs from a menu in a several ways. First, it has only one element, a bar with a text string in it. Second, when clicked on with the mouse, a button causes an action to occur in VNMR. An example is the button in the "FT & Post FT" pane marked "Transform". When pressed, an Ft is performed.

Titles are often buttons. You can tell if this is the case as inactive titles have no border.

Check Boxes

A check box can have one or two fields. They are often associated with entries, in which case they make the entry value active or inactive. The first field of a check box, if present, is a text string. The second field is the actual check box, which is a small square.

When checked, the small square is red and is sunken. When unchecked, it is gray and raised. The check box toggles between these two states with alternate mouse clicks on it. Generally, each check box is independent of all others.

Radio Buttons

Radio buttons are small diamonds arranged in vertical columns. Each row in a column has two fields, a text string and the actual radio button. When a radio button is selected, it is colored red and is sunken. When it is not selected, it is gray and raised.

Just like their namesake, adjacent radio buttons in a column are mutually exclusive. If you click on an unselected one, it becomes selected and the currently selected one becomes unselected. You will find radio buttons controlling mutually exclusive choices such as ph, av, and pwr.

Scales

Scales are slider bars. They have two or three fields. The first field is a text string. The second field is optional, but when present shows the current value of the slider. The third field is the slider itself.

There are two ways of altering the slider. The first is to grab the slider itself and drag it to the desired position in the trough. The other is to click in the trough itself. If you click in the trough with the middle mouse button, the slider moves to that position. Clicking in the trough with the left mouse button alters the slider in that direction by one unit. We have not used a slider in the sample panes, but an application could be setting phase parameters.

Scrolls

Scrolls are distinguished by two small boxes, side by side, one with an up arrow and the other with a down arrow. A scroll has three fields—a text string, the current value, and two arrows. You cannot see the set of choices that a scroll offers, only the currently selected value. Each click with the left mouse button on one of the arrows moves the selected value in the appropriate direction. A typical example of a scroll is in the selection of Fourier Number.

Selecting the New Interface

The primary program is named dg and resides in the tcl/bin directory of the vnmr system directory. This interface is selected by setting the UNIX environmental variable vnmrtext to the full path of the dg program. A typical setting would be setenv vnmrtext \$vnmrsystem/tcl/bin/dg

This line is in the .login file distributed with the software.

Deselecting the New Interface

You can run the noninteractive dg window by inserting a # character in front of the vnmrtext line.

Window Configuration Files

When the new interface is started, a dg.conf file specifies the general layout of the window (see Figure 13). This file exists in the user_templates/dg/default directory of the system directory. Listing 16 shows a default version of dg.conf (the lines are numbered for reference). Alternatively, if a user has a private copy of dg.conf in the user's directory vnmrsys/templates/dg/default, that copy is used.

The dg.conf file specifies the tabs, the associated label, and the configuration file for each window pane. If this file specifies only a single tab, then the actual tabs are not displayed and the specified configuration file is used for the single pane.

One special configuration file, dg.info, is present that mimics the behavior of the old dg window. The dgLocal (output, number) for the dg.info pane must be set to 1. The dgLocal (output, number) for all other panes must be set to 0.

Two other parameters in the dg.conf control the layout of the tabs and the overall geometry of the window. The dg.conf file must be edited by hand if you wish to make changes. Three parameters control the background color of entry elements if the parameter being displayed is arrayed, is set to "Not Active," or does not exist. Another parameter specifies whether the dg template configuration tool is available.

The window configuration files are checked for in the following order of priority:

- 1. In the user's vnmrsys/templates/dg directory, if an "Experiment Specific" configuration file exists in a directory named after the value of seqfil.
- 2. In the user's vnmrsys/templates/dg/default directory, which contains experiment-independent configuration files.
- 3. In the system's user_templates/dg directory, if an "Experiment Specific" configuration file exists in a directory named after the value of seqfil.
- 4. In the system's user_templates/dg/default directory, which contains experiment-independent configuration files.

Editing the Configuration Files

While the configuration files are simple text files, editing the files by hand is not recommended. A configuration tool is provided to construct the files. To activate the tool, hold down the Control key and click the left mouse button on the currently selected tab.

Two windows appear. The first window (see Figure 14) as a matrix of buttons labeled 1,1 1,2 1,3 etc. The name of the active configuration file is displayed in the title bar. This matrix

Listing 16. Text of dg. conf File

```
1. set dqLocal(title,1) "Acquisition"
set dqLocal(file,1) "dq.acq"
3. set dgLocal(output,1) 0
4.
5. set dqLocal(title,2) "Pre FT"
6. set dgLocal(file,2) "dg.process1"
7. set dqLocal(output,2) 0
8.
9. set dgLocal(title,3) "FT & Post FT"
10. set dgLocal(file,3) "dg.process2"
11. set dqLocal(output,3) 0
12.
13. set dqLocal(title,4) "Text"
14. set dqLocal(file,4) "dq.info"
15. set dgLocal(output,4) 1
16.
17. set dqLocal(title,5) "Spare"
18. set dgLocal(file,5) "dg.spare"
19. set dgLocal(output,5) 0
20.
21. set dgLocal(title,6) "Spare"
22. set dgLocal(file,6) "dg.spare"
23. set dgLocal(output,6) 0
24.
25. # Color for Arrayed entries
26. set dqLocal(ac) pink
27. # Color for Not Active entries
28. set dgLocal(off) gray80
29. # Color for Not defined entries
30. set dqLocal(nc) qray70
31. #set edit to yes or no to toggle configuration access
32. set dgLocal(edit) yes
33.
34. set dgLocal(side) vert
35. # Uncomment the following line to have the tabs appear across the top
36. # set dqLocal(side) horiz
37.
38. wm geometry . 925x350+0-0
```

window is used to select items and rearrange items. Each button in the matrix window represents a corresponding grid element in the dg pane. The buttons highlighted in pink indicate that some interaction item is present at that grid location. The first four characters of the label of the interaction are displayed.

To move items within the pane, hold the left mouse button down over one of the highlighted grid buttons, drag the mouse arrow, with the button still down, to a non-highlighted grid item, and then release the mouse button. The change is immediately shown in the dg pane.

To select grid items, click the left mouse button over one of the grid items in the matrix window. The currently selected item will blink in the matrix window. By selecting a grid item, you can either define or redefine the contents of that grid item.

The second window (see Figure 15) is used to define the interaction elements. At the top of this window, the Panel File: entry identifies the configuration file associated with the current dg pane. Below that is the Panel Title: and the Geometry of the DG window. This

				dg.a	cq				•
1,1	Acqu	1,3	1,4	Samp	1,6	1,7	Flag	Nucl	1,10
2,1	2,2	2,3	2,4	Date	2,6	2,7	inte	2,9	2,10
Spec	3,2	3,3	MHz	Solv	3,6	3,7	inte	3,9	3,10
0bs	4,2	4,3		File	4,6	4,7	32 b	4,9	4,10
Acq.	5,2	5,3		5,5	5,6	5,7	homo	5,9	5,10
Acq.	6,2	6,3	6,4	Deco	6,6	6,7	6,8	6,9	6,10
Spec	7,2	7,3		Nucl	7,6	7,7	Cond	7,9	7,10
8,1	8,2	8,3	8,4	Dec	8,6	8,7	bloc	8,9	8,10
Obs.	9,2	9,3		Dec	9,6		fid	9,9	9,10
ро	10,2	10,3	10,4	10,5	10,6	10,7	exp.	10,9	10,10
Recy	11,2	11,3		Dec	11,6	11,7	erro	11,9	11,10
12,1	12,2	12,3	12,4	mod	12,6	12,7	12,8	12,9	12,10
Tran	13,2	13,3	13,4	mod	13,6	13,7	Spec	13,9	13,10
CO	14,2	14,3	14,4	pow	14,6	14,7	temp	14,9	
Stea	15,2	15,3	15,4	90 p	15,6		15,8	15,9	15,10
Bloc	16,2	16,3	16,4	pow	16,6	16,7	16,8	16,9	16,10

Figure 14. Matrix Window (dg Program)

-	Display Gr	roups		r 🗆
	Panel File:	dg.acq		
	Panel Title:	Acquisition		
	Geometry of DG window:	925x350+0-0		
Rows: 16 🛁	Columns: 10 🖃			
Current element:	1,9			
Type of element:	scroll -			
Row extent:	1 -			
Column extent:	3 -			
Justify:	left =			
Label of element:	Nucleus			
Choices:	H1 F19 P31 C13			
Value of choices:				
Units:				
Color of label:	black			
Width of element:	3			
Scale Tcl pars:				
Vnmr Variables:	tn			
Vrumr Gmd:	tn=' \$VALUE'			
Vrumr Gmd2:				
Tcl Cmd:	\$tn			
Show Condition:				
Refresh Display	Exit	🔳 s2pul	Specific	Save Display

Figure 15. Interaction Elements Window (dg Program)

information comes from the dg.conf file. At the bottom of the window are several buttons. The Refresh Display button causes any changes you may make to be displayed in the Dg pane. However, those changes are only temporary and will go away when the configuration window goes away, either by pressing the Exit button or by selecting another tab from the Dg pane.

To save changes, the only way is to press the Save Display button in the lower right-hand conner of the window. To the left of this button is a selection to specify if the configuration file is "Experiment Specific" where Experiment will be substituted with the current value of seqfil.

- If Experiment Specific is selected, the file is saved in an Experiment directory, where Experiment is substituted with the current value of the seqfil parameter.
- If Experiment Specific is not selected, the file is saved in the default directory. These are subdirectories of the /vnmr/user_templates/dg directory or the user's vnmrsys/templates/dg directory.

If you have write permission in the vnmr system directories, you are presented a choice of System and User. Selecting one or the other saves the configuration files in the directories /vnmr/user_templates/dg or the user's vnmrsys/templates/dg directory. If you do not have write permission in the vnmr system directories, you do not see this choice.

In all cases, the name of the file is shown in the Panel File entry at the top of the window. Note that the file name is editable and can be used to create new configuration files. In order for them to become active, you need to add an appropriate entry into the dg.conf file.

As already mentioned, the geometry of the dg pane is defined in the dg.conf file. Entering a new value in the geometry field of the configuration window, and then pressing Refresh Display causes the dg window to resize and reposition to the new geometry. Alternatively, the mouse can be used to resize and reposition the dg window. Whenever the mouse enters and then leaves the area of the screen covered by the dg window, the value of geometry in the configuration window is updated. Once the desired geometry is set, the value displayed in the configuration window should be copied into the proper line in the dg.conf file.

The dg pane is broken up into a grid of rectangles, as represented by the matrix window. The size of the grid in terms of the number of rows and columns is controlled by the Rows and Columns menus in the configuration window. The Rows represents how many items can be placed in a column. It basically defines the height of the dg window. There are different choices that can be made when deciding the number of rows and columns. This will be discussed after all the customizable elements are described.

Below the Rows and Columns menus is a label that identifies which element of the matrix window is selected. Below that is the Type of Element menu. This menu provides a list of all the different types of interaction items that can be placed at the current location. If a pink highlighted button is selected from the matrix window, this menu displays the current item at that location.

The next two rows are Row Extent and Column Extent menus. Interaction items can be defined to be larger than a single grid rectangle. Increasing the Row Extent of an item causes it to occupy a corresponding number of grid rectangles below the currently selected rectangle. Increasing the Column extent of an item causes it to occupy a corresponding number of grid rectangles to the right of the currently selected rectangle.

The Justify menu selects whether the item is aligned along the left edge of its grid space, centered within the grid space, or aligned along the right edge of the grid space.

Below this menu are twelve entry fields. These are used to define the label and actions of the interaction items. Each type of interaction item has its own set of adjustable characteristics. Entry fields that are not appropriate for the selected type of element are shaded and you can not enter a value in the shaded field.

Interaction Elements

The Type of Element choices and the associated characteristics define the actions of the dg pane. The available elements are none, title, label, button, entry, check, radio, menu, menu2, scale, scroll and list. For each of these elements, the Row Extent, Column Extent, and Justify options are available.

Also for each of these elements, the Color of Label choice is available. It must be filled in with the name of any legitimate X-windows color. The UNIX command showrgb lists the available color names. If an unknown color name or no color name is present, it defaults to black

None Element

The none element removes any interaction item from the selected grid rectangle.

Title Element

The title element places a non-interactive title at the selected grid rectangle. The available characteristics are the following:

Label of element:	The text string to be displayed as the title. While this field is
	optional, the title element is invisible if it is empty.

The title item is useful to explore the effect of Row Extent and Column extent. If you input a fairly long text line as the title and then press Refresh Display, only a portion of the text is displayed. Increase the value of Row Extent from the menu and more text is displayed. Increase the Column Extent and the title can be positioned between rows of the grid.

Label Element

The label element places a noninteractive label at the selected grid rectangle. The label is different from a title in that the value of a parameter can be displayed and the display is updated in the parameter value changes. However, you cannot change the parameter directly with this item. The available characteristics are the following:.

Label of element:	Text string to be displayed to the left of the parameter value. This field is optional.
Units:	Text string to be displayed to the right of the parameter value. This field is optional.
Width of element:	Width of the field that the parameter value is displayed. This field is optional, but is automatically set to 8 if no value or an illegal value is entered.
Vnmr Variables:	List of VNMR variables that are used to construct a value to be displayed. This can be zero or more parameter names.
Tcl Cmd:	A Tcl expression that is evaluated to determine the value that is displayed by this label item. Any legitimate Tcl expression is allowed.

To access the values of any VNMR parameters specified in the Vnmr Variables list, prepend a dollar sign (\$) to the parameter name. For example, the value of sfrq is \$sfrq.

The following examples show Tcl expressions possible for Tcl Cmd:

hello	A simple string that will not be updated and is not very useful It would be better to use a title for this case.
[expr \$np/2.0/\$sw]	An expression to calculate acquisition times. Parameters np and sw need to be listed as Vnmr Variables is order to get access to their values.
[expr acos(-1)]	A calculator for pi.
\$ct	Probably the most common use. The value of a VNMR parameter is displayed and updated as it changes. ct needs to be listed as Vnmr Variables to get access to its value. During an acquisition, this value would be updated as block-size transfers of data occur.

Button Element

The button element is the first interactive item. It provides a mechanism to send any MAGICAL command to VNMR. As a mouse button passes over a button, the button changes color to indicate that it is an active item. The available characteristics are the following.

Label of element:	Text string to be displayed inside the button. This field is optional.
Width of element:	Width of the button. This field is optional. The actual width depends on this entry and the value of the Justify field. If any value greater than zero is set in this field, a button of roughly that many characters is shown. If the entry is set to zero, a default size based on the Label of element field is used. If the field is empty (or a non-real value is input), it behaves as if the value of zero were set, provided Justify is set to left or right. If Justify is set to center, an empty field or a non-real value causes the button to occupy the entire width of the selected grid rectangle.
Vnmr Cmd:	MAGICAL expression or command executed when the button is pressed. The field is optional, however; if nothing is specified, nothing happens when the button is pressed.

Entry Element

The entry element is similar to label, except that a value is not only displayed but can be directly altered. The available characteristics are the following

Label of element:	Text string to be displayed to the left of the parameter value. This field is optional.
Units:	Text string to be displayed to the right of the parameter value. This field is optional.
Width of element:	Width of the recessed entry field. In this field, the parameter value is displayed and entered. This field is optional but is automatically set to 8 if no value or an illegal value is entered.
Vnmr Variables:	List of VNMR parameters used in the following Vnmr Cmd and Tcl Cmd fields. This can be zero or more parameter names.
Vnmr Cmd:	MAGICAL expression sent to VNMR. Any specified VNMR parameters can be used. Their value is accessed by prepending a dollar sign (see example below). One special variable is also available. That is the value of the typed in entry. The value is accessed by the keyword \$VALUE.
Tcl Cmd:	Tcl expression that is evaluated to determine the value displayed by this entry item. Any legitimate Tcl expression is allowed.

Show Condition:	Tcl expression that is evaluated to determine whether the value
	background should be grayed out. If it evaluates to false, the color
	specified in dg.conf by dgLocal(off) is used.

To access the values of any VNMR parameters specified in the Vnmr Variables list, prepend a dollar sign (\$) to the front of the parameter name. The basic example for setting a Vnmr variable would be the following:

Vnmr Variables:	bs
Vnmr Cmd:	bs=\$VALUE
Tcl Cmd:	\$bs
Show Condition:	[vnmrOn bs]

The Vnmr Variables field requests access to the VNMR parameter bs. The Vnmr Cmd field constructs a MAGICAL expression where bs is set to the value entered into this entry widget. The Tcl Cmd field states how the value displayed in the entry field is determined.

When a value is entered, the field is updated according to the instructions in the Tcl Cmd field. If a nonsense value is entered, or if parameter recalculation occurs, the displayed value should be redisplayed based on VNMR parameters, not some internal state of that entry field. If the Tcl Cmd field is left blank, the entry field is cleared after the Vnmr Cmd is sent. The Vnmr Cmd is sent if the Return key is pressed in the entry window or the mouse arrow is clicked on some other widget so that the focus leaves the entry window.

Check Element

The check element selects and de-selects some mode or state, often as a yes or no selection. It is presented as a small square box to the left of a label. The box is depressed and colored if it is selected. The available characteristics are the following:.

Label of element:	Text string to be displayed to the right of the check box. This field is optional.
Vnmr Variables:	List of VNMR parameters used in the following Vnmr Cmd, Vnmr Cmd2, and Tcl Cmd fields. This can be zero or more parameter names.
Vnmr Cmd:	MAGICAL expression sent to VNMR whenever the check box is selected. Any specified VNMR variables can be used.
Vnmr Cmd2:	MAGICAL expression sent to VNMR whenever the check box is deselected. Any specified VNMR parameters can be used.
Tcl Cmd:	Tcl expression that is evaluated to determine whether or not the check box should be identified as selected or de-selected.

The prototype example for using a check box would be the following, which selects or deselects experiment interleaving:

Vnmr Variables:	il
Vnmr Cmd:	il='y'
Vnmr Cmd2:	il='n'
Tcl Cmd:	[expr {\$il == "y"}]

In the example, the Vnmr Variables field requests access to the VNMR parameter il. The Vnmr Cmd field constructs a MAGICAL expression where il is set to 'y' when the check box is selected. The Vnmr Cmd2 field constructs a MAGICAL expression where il is set to 'n' when the check box is deselected. The Tcl Cmd field determines, based on the current value of il, whether the check box should be shown as selected or deselected. It is the use of the value of il in this expression (as \$il) that requires il to be in the Vnmr Variables entry. The syntax of the Tcl Cmd field is standard Tcl syntax. Whatever the expression, it should return a 1 if the check box is to be selected; 0, otherwise.

Radio Element

The radio element gives a number of choices, only one of which can be selected. Whenever one is selected, the others are deselected. The choices are presented as small diamonds to the left of a label, and the choices are presented in a column of rows. This is one item where it is useful to use the Row extent so that each choice has its own row. The radio element is probably the most difficult item to program correctly. The available characteristics are the following:.

Label of element:	Set of text strings to be displayed to the right of the radio diamonds. If the label for a given choice is more than one word, it must be enclosed in double quotes. It must be filled in with at least two labels.
Value of choices:	List of values the variable VALUE (accessed as \$VALUE) will be set to. The number of values must match the number of labels. If a value is more than a single word, it must be enclosed in double quotes.
Vnmr Variables:	List of VNMR parameters used in the following Vnmr Cmd and Tcl Cmd fields. This can be zero or more parameter names.
Vnmr Cmd:	MAGICAL expression sent to VNMR whenever one of the radio boxes is selected. Any specified VNMR parameters can be used. The variable \$VALUE is set to the value in the Value of choices list of the selected choice.
Tcl Cmd:	Tcl expression that is evaluated to determine which radio selection should be identified. The return value of the expression must match one of the choices in the Value of choices list.

The radio buttons are useful when making exclusive choices among more than two items. If the choice is between two items, the check box is more appropriate. A prototype example for using radio buttons is the following, which selects one of three alternatives for temperature error handling:

Label of element:	"Ignore errors" "Warn on error" \backslash
	"Abort on error"
Value of choices	n w y
Vnmr Variables:	tin
Vnmr Cmd:	tin='\$VALUE'
Tcl Cmd:	\$tin

Note the single quotes around \$VALUE in the Vnmr Cmd field. This is standard MAGICAL syntax for setting string parameters. The single quotes are not part of the value of the string. That is, the value of \$tin is simply n, w, or y and not 'n', 'w', or 'y'.

The alternative of setting

Value of choices:	'n' 'w' 'y'
Vnmr Cmd:	tin=\$VALUE

could be used but then the Tcl Cmd field is much more complicated. The value of \$tin does not match the characters with single quotes. Simply using '\$tin' as the value of Tcl Cmd is not a valid Tcl expression.

The next example shows the flexibility of this interface. However, it does take familiarity with Tcl to decipher the value of Tcl Cmd. The result of this definition is a series of radio buttons that implement all of the jexp commands.

Label of element:	Exp1 Exp2 Exp3 Exp4 Exp5 Exp6 Exp7 \ Exp8 Exp9	
Value of choices:	1 2 3 4 5 6 7 8 9	
Vnmr Variables:	curexp	
Vnmr Cmd:	jexp\$VALUE	
Tcl Cmd:	string range \$curexp [expr	
	<pre>\[string length \$curexp]-1] end]</pre>	

Note that the substitution of \$VALUE is not as a parameter in a MAGICAL expression but to complete a MAGICAL command name. The result of the Tcl Cmd field is to return the last character of the curexp parameter, which will match one of the Value of choices list.

It is often the ease in which a Tcl Cmd entry can be constructed that determines what entries are put in the Value of choices field. For example, a second way to implement the same function as the jexp example above is with the following:

Label of element:	Expl Exp2 Exp3 Exp4 Exp5 Exp6 Exp7 \Exp8 Exp9
Value of choices:	exp1 exp2 exp3 exp4 exp5 exp6 exp7 \exp8 exp9
Vnmr Variables:	curexp
Vnmr Cmd:	j\$VALUE
Tcl Cmd:	[file tail \$curexp]

Some might claim the second Tcl Cmd expression is simpler.

Menu2 Element

The menu2 element gives a number of choices in a drop-down menu. A label can be displayed to the left of the menu2 button, and the current selection is displayed inside the menu2 button. This button is distinguished from the button element by a second, small rectangle imbedded in the button. The available characteristics are the following:

Label of element:	Text string to be displayed to the left of the menu box. This field is optional.
Choices:	Set of text strings to be displayed in the drop-down menu. If the text for a given choice is more than one word, it must be enclosed in double quotes. It must be filled in with at least one choice. The label of the currently selected choice is displayed in the menu box.
Value of choices:	List of values the variable VALUE (accessed as \$VALUE) will be set to. The number of values must match the number of choices. If a value is more than a single word, it must be enclosed in double quotes.
Vnmr Variables:	List of VNMR parameters to be used in the following Vnmr Cmd and Tcl Cmd fields. This can be zero or more parameter names.
Vnmr Cmd:	MAGICAL expression that is sent to VNMR whenever an item is selected from the drop-down menu. Any specified VNMR parameters can be used. The variable \$VALUE is set to the value in the Value of choices list of the selected choice.

Tcl Cmd:	Tcl expression that is evaluated to determine which choice should
	be identified and displayed in the menu2 button. The return value
	of the expression must match one of the choices in the Value of
	choices list.

The menu2 element is useful when making exclusive choices among several items. If the choice is among two items, a check box is useful; three or four items can be handled by radio buttons. For more items, the menu2 item is useful because the entire list of choices is only displayed where you are making a selection. Note that the menu2 item differs from the standard Tcl/Tk menu item in that it supports a multiple-column display of choices if more than ten choices are specified.

The following example selects one of several decoupler modulation schemes:

Label of element:	modulation
Choices:	ccc ccw cww www ccg ccp
Value of choices:	ccc ccw cww www ccg ccp
Vnmr Variables:	dmm
Vnmr Cmd:	dmm='\$VALUE'
Tcl Cmd:	\$dmm

Scale Element

The scale element adjusts a parameter with a slider. A label and the current value of the scale can be displayed to the left of the scale. The size of the scale item often requires a Row extent of 2 and a Column extent: of 2 or more. The value of the scale can be changed by clicking mouse button 1 or 2 in the scale or dragging the slider. The available characteristics are the following:

Label	of	element:	Text string to be di is optional.	isplayed to the left of the menu box. This field
Width	of	element:	width is 0, the valu selected, the label	eserved to display the value of the scale. If the ue is not displayed. If the center justification is and value are aligned along the left edge and d along the right edge of the grid rectangle.
set here. In g		set here. In genera	has many configuration options. These can be l, an option is a keyword preceded by a minus a value. Scales include the following options:	
			-from	Value corresponding to left or top of scale
			-to	Value corresponding to right or bottom of scale
			-tickinterval	Spacing between numerical values below or to left of scale. A 0 removes all values
			-resolution	Value specifying resolution of values. A value greater than zero causes the scale value to be an even multiple of the resolution. The default value is 1, which gives integer resolution.
			-showvalue	Set to 0 or 1 to show the scale value above or to the right of the slide. The default is 0, for no.
			-orient	Set to v for a vertical scale or h for a horizontal scale. h is default. If v is chosen, the Row extent value of the item probably needs to be increased.

	-length	Length of the scale in the long direction. The value is in arbitrary units.
	-width	Width of the scale in the narrow direction. The value is in arbitrary units. The default is 10.
Vnmr Variables:	List of VNMR parameters used in the following Vnmr Cmd and Tcl Cmd fields. This can be zero or more parameter names.	
Vnmr Cmd:	MAGICAL expression sent to VNMR whenever a mouse button is released in the scale item. Any specified VNMR parameters can be used. The variable \$VALUE is set to the value of the scale.	
Tcl Cmd:	Tcl expression that is evaluated to determine the value of the scale. Any legitimate Tcl expression is allowed. To access the values of any VNMR parameters specified in the Vnmr Variables list, prepend a dollar sign (\$) to the front of the parameter name.	

The scale element is a useful mechanism to modify a numerical parameter. It prevents errors in parameter entry. Its weakness is that it takes up a fair amount of area and is not always easily manipulated by dragging the slider with the left mouse button to a new value. However, clicking anywhere in the slider trough with the middle mouse button sets the scale to that value. Also, clicking inside the trough on either side of the slider with the left mouse button changes the scale value by one (resolution) unit.

The following example provides adjustment of the temperature:

Label of element:	temp
Width of element:	3
Scale Tcl pars:	-to 100 -from 0 -tickinterval 20 \-length 180
Vnmr Variables:	temp
Vnmr Cmd:	temp=\$VALUE
Tcl Cmd:	\$temp

If you wanted the scale value to move with the slider, the value of Width of element field could be set to 0 and a -showvalue 1 option could be added to the Scale Tcl pars field.

Scroll Element

The scroll element adjusts a parameter with a up-down buttons. A label and the current value of the scale can be displayed to the left of the scroll buttons. The scroll can be used for any list of items. In contrast to a menu2 item, you can only see the current value with a scroll element. The available characteristics are the following:

Label of element:	Text string to be displayed to the left of the scroll buttons. This field is optional.
Choices:	Set of text strings to be scrolled through. If the text for a given choice is more than one word, it must be enclosed in double quotes. It must be filled in with at least two choices.
Width of element:	Amount of space reserved to display the value of the scroll. If the width is 0, the value is not displayed. If the center justification is selected, the label and value are aligned along the left edge and the scroll is aligned along the right edge of the grid rectangle.
Vnmr Variables:	List of VNMR parameters to be used in the following Vnmr Cmd and Tcl Cmd fields. This can be zero or more parameter names.

Vnmr Cmd:	MAGICAL expression sent to VNMR whenever the scroll updates to the next item in the list. Any specified VNMR parameters can be used. The variable \$VALUE is set to the value of the scroll.
Tcl Cmd:	Tcl expression that is evaluated to determine the value of the scroll. Any legitimate Tcl expression is allowed. To access the values of any VNMR parameters specified in the Vnmr Variables list, prepend a dollar sign (\$) to the front of the parameter name.

The scroll element is a useful mechanism to modify a numerical or string parameter. It prevents errors in parameter entry. This item is most useful if there is an obvious up-down notion about the parameter. An example with Fourier Numbers is the following:

Label of element:	Fourier Number
Choices:	128 256 512 1024 2048 4096 8192 \16384 32768 65536 131072
Width of element:	6
Vnmr Variables:	fn
Vnmr Cmd:	fn=\$VALUE
Tcl Cmd:	\$fn

Tips for dg Design

The key to designing dg panes is to have a clear understanding of the operation of the two entries Vnmr Cmd and Tcl Cmd. The contents of these two fields are passed as strings via the Tcl set command in the form set dgTemplate {string}.

What VNMR Sees

In the case of Vnmr Cmd, the string is sent to VNMR for evaluation. Thus, the final string needs to be something that makes sense to MAGICAL. However, along the way, Tcl gets a look at the string and may well do some evaluation and substitution.

As an example, in the simple case where Vnmr Cmd is something like tof=\$VALUE, Tcl substitutes the contents of VALUE (a Tcl variable) in the string for \$VALUE. Thus, the final string is something like tof=493.5, assuming that the value entered was 493.5.

More complex mixtures of MAGICAL and Tcl can be used. For example, if [vnmrSize pp] then pp=\$VALUE*[vnmrUnits pp] endif

The effect of this command is discussed later.

An issue that arises is where to use a local MAGICAL variable such as a. Unless something special is done, Tcl intercepts a and looks to substitute it by the contents of a Tcl variable a. This will probably fail! The solution is to escape the b by using the syntax a instead of a. The b is then passed to MAGICAL.

What TCL Sees

For Tcl Cmd, the string is eventually evaluated and the results displayed. So we can think of this as the value being displayed as being dgTemplate once it is evaluated by Tcl. The value displayed normally comes from VNMR.

Consider the situation where you might enter a negative value for spectral width. You can type a negative value and it shows until you either press Return or move the mouse focus. At this point, the negative number is sent to VNMR. MAGICAL catches this and will

correct the error (it sets sw to 100). The corrected value is then returned to the Tcl Cmd, so that the value displayed will change to the corrected one.

Common Constructs

In this section, we look at some strategies for the Vnmr Cmd and Tcl Cmd entries.

The simplest case is that of a numeric value for a parameter such as tof:

Vnmr Cmd:	tof=\$VALUE
Tcl Cmd:	\$tof

Where we expect a string, the \$VALUE should be in single quotes, for example

Vnmr Cmd:	tn='\$VALUE'
Tcl Cmd:	\$tn

This avoids the need for the user to quote the entry.

When entering numeric fields, the question of precision and of decimal places may arise. If you want to display an integer, a trick is required if any math is involved. Here is one example that introduces two concepts.

Vnmr Cmd:	np=\$VALUE*2
Tcl Cmd:	[expr \$np/2]

In this case, we wish to display the number of complex points. This is, of course, np/2. 0. The Vnmr Cmd entry is straightforward. Tcl Cmd requires some explanation. Tcl needs to be told when math is involved. This is done with the expr command. We need the square brackets [...] to tell Tcl to evaluate the expression in [...] first. Each term in the expression is best separated by blanks. Finally, by dividing by 2 rather than 2.0, we do integer math rather than real math, so that the result is an integer displayed as 8000 rather than 8000.00

In some cases, we want to display some decimal places, but not necessarily all available. For example, if sb=2/3, the value of sb is 0.6666666...

Tcl Cmd: [format "%.3f" \$sb]

This displays sb with 3 decimal places.

A more complex example can be found with fn.

Vnmr Cmd:	fn=\$VALUE*2
Tcl Cmd:	[expr{(\$fn > 2000) ? [format "%dk"
	[expr \$fn / 2000]] : \$fn / 2}]

This complex expression checks to see if fn is greater than 1024. If fn>1024, it is displayed as nk, but if not, the display is the full number of complex points.

This introduces the Tcl expression for true and false. The expression in parentheses (...) is evaluated for truth (or the value 1). If found true, the result is the value of the expression between the question mark (?) and the colon (:); otherwise, the result is the value of the expression that follows the colon.

Allowing the units of an entry to change requires some more Tcl. Take sw for example. We may wish to display and enter this either as Hz or as ppm.

Vnmr Cmd:	sw=\$VALUE*[vnmrUnits sw]
Tcl Cmd:	[expr \$sw / [vnmrUnits sw]]

The Tcl procedure vnmrUnits takes the string sw (note, not \$sw) as an argument and returns a scaling factor for sw. The scaling factor is chosen through an adjacent menu2 widget. The key definitions for this widget are the following.

Choices:	Hz ppm
Value of choices:	1 4
Vnmr Variables:	SW
Vnmr Cmd:	<pre>setdgroup('sw',\$VALUE)</pre>
Tcl Cmd:	[vnmrDgroup sw]

The values that can be set in Dgroup are shown in the table for Dgroup and factor. Note that in Tcl, vnmrDgroup returns the key and vnmrUnits returns the scaling factor.

When the factor is not one already recognized by dg, a slightly different procedure is used. An example is temp.

Vnmr Cmd:	<pre>temp=\$VALUE- [expr {([vnmrUnits temp] \</pre>
Tcl Cmd:	<pre>[expr \$temp + (([vnmrUnits temp] \</pre>

The Tcl ternary if is again used, here to convert between the two temperature scales.

Many variables can be set to a "not used" condition by setting the variable to 'n'. This can be indicated by using the "Show Condition" characteristic of an entry element. An example is lb.

Vnmr Cmd:	lb=\$VALUE
Tcl Cmd:	\$lb
Show Condition:	[vnmrOn lb]

When lb='n', the background of the value box is a darker gray (or whatever color is specified in dg.conf by dgLocal(off). Note that the background is set dark if the condition is FALSE.

When we deal with a variable such as sbs, a more complex condition may be needed.

Show Condition: [expr ([vnmrOn sb] && [vnmrOn sbs])]

Here, the sbs background is dark when either sb or sbs is 'n'.

Overall Design of Panes

We have used a number of design criteria for our sample panes. It is recommended that you stick to the following design rules in order to maintain as much consistency as possible. Think of the person who will use the pane when you are not around to explain it!

- Avoid labels that are just parameter names. Try to use concise natural language to describe the value rather than leaving the user to look it up a manual. For example, "Spectral Width" is much better than "sw". Don't over-use capital letters in labels. "Spectral width" is better than "SPECTRAL WIDTH"
- Group parameters in logical blocks. For example, group decoupling parameters together.
- Try to always display a parameter in about the same spot on the same pane. Don't make the user hunt all over a pane (or many panes).
- Use color, but use it wisely. We have used "blue" for titles, "seagreen" for important fields and "indianred" for alert conditions. These colors are easy to read and somewhat

muted but still convey some sense of meaning. Remember that some people are colorblind and that a particular color (such as red) may not always carry the same connotations for others.

- Try not to clutter the pane. There is no need to fill every cell in the matrix. Use space to highlight regions of interest on the pane.
- We have chosen a 16 x 10 matrix. The first column of entries is 3 columns wide with a fourth for menus of units. The other columns of entries are, in general, 3 matrix columns wide, including the units.
- Keep things neat. Watch the size of value boxes. Most entry fields in the samples have a width of 7 and are justified "center." This allows everything to line up neatly.
- The definition file dg.conf is not mutable. This means that the tabs must serve all pulse sequences that a user may wish to use. Plan the number of panes and their function to satisfy the most complex experiment. Then the panes can be depopulated for simpler pulse sequences. Again, remember, keep each parameter in the same place in the same pane throughout. If it is not relevant, do not display it.
- Use the visual cues provided to indicate function. Titles are not interactive, buttons are. Labels are not interactive, entries are. Radio buttons require the user to choose one of the available options. Check boxes do not require a choice—none, some or all of the options can be selected.
- Let VNMR and MAGICAL do as much of the work as possible. The manipulations done by Tcl should only be those associated with the display and entry functions. Excessive use of Tcl adds another layer of complexity that someone will have to untangle later.

Utilities for Accessing VNMR Parameters.

Tcl procedures are available to provide access to VNMR parameter attributes. Each procedure available takes the VNMR parameter name as an argument. The procedures include vnmrOn, vnmrSize, vnmrUnits, vnmrDgroup, vnmrMax, and vnmrMin.

vnmrOn

The vnmrOn procedure returns 1 if the VNMR parameter is Active; 0 if Not Active.

vnmrSize

The vnmrSize procedure returns the number of array values for the parameter. If the parameter is not arrayed, it returns 1. If the parameter does not exist, it returns 0.

vnmrUnits

The vnmrUnits procedure returns a scaling factor based on the current Dgroup attribute of a parameter. The table on the right lists the Dgroup value and scaling factor.

Dgroup	Factor
1	1
2	1e3
3	1e6
4	reffrq
5	reffrq1
6	reffrq2

vnmrDgroup

The vnmrDgroup procedure returns the value of the Dgroup attribute of the parameter.

vnmrMax

The vnmrMax procedure returns the value of the maxvalue attribute of the parameter.

vnmrMin

The vnmrMin procedure returns the value of the minvalue attribute of the parameter.

Sending a Tcl Script

The command tcl(script) sends a Tcl (Tool Command Language) script to the Tcl version of the dg window. Any legal Tcl script can be sent. Sending the value of curexp to this dg window causes the window to update itself. The value of seqfil is also used to determine which configuration files to use to update the window. The bootup macro and the jexp macros use the following command for this purpose:

tcl('set seqfil '+seqfil+';set curexp '+curexp)

If the Tcl version of the dg window is not active, the tcl command does nothing.

Chapter 6. Customizing Graphics Windows

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