VnmrJ 2.2B Installation and Administration

Varian NMR Systems
With VnmrJ 2.2B Software
Pub. No. 01-999341-00, Rev. B 0107

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Varian NMR spectrometer systems with workstations running VnmrJ 2.2B software

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VnmrJ Installation and Administration

- "Overview of this Manual," next
- "Conventions in This Manual," page 12

Overview of this Manual

The VnmrJ Installation and Administration manual contains the following main parts:

VnmrJ Installation

Install the operating system before installing VnmrJ:

- Linux

Refer to the OS for hardware setup and OS installation instructions. Proceed to the instructions in Chapter 1, "VnmrJ Installation," page 13 of this manual after the OS is installed.

VnmrJ Configuration

Configure the software for the spectrometer as described in Chapter 2, "System Configuration," page 19 after VnmrJ is installed.

VnmrJ Administration

VnmrJ and NMR spectrometer administration.

- Chapter 3, "VnmrJ Administration," page 27, describes VnmrJ administration functions and the *VnmrJ Admin* interface.
- Chapter 4, "VnmrJ Printers and Plotters," page 47 describes setting up of printers using VnmrJ administration functions and the *VnmrJ Admin* interface.
- Chapter 5, "Automated Hardware," page 53 provides general instructions for configuring the software to control automated hardware such as sample handlers and automated probe tuning.
- Chapter 6, "VnmrJ Accounting Administration," page 55, describes how the use the VnmrJ accounting tool.

VnmrJ User Account and Hardware Administration

- Chapter 7, "VnmrJ User Account Administration," page 65 procedures executed within a user account to set up or customize the user account functions
- Chapter 8, "System Calibrations," page 77, describes the liquids NMR system calibrations.
- Chapter 9, "Magnet and Spectrometer Maintenance," page 97, describes NMR spectrometer hardware and magnet preventative maintenance.

The appendixes provide some reference information about the NMR console, printers, VnmrJ Locator, and the VnmrJ Browser.

Additional Information

Additional information related to VnmrJ installation and administration is contained in the appendixes.

Conventions in This Manual

The following notational conventions are used throughout VNMR manuals:

- Typewriter-like characters identify VNMR and UNIX commands, parameters, directories, and file names in the text of the manual:

  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:

  `Self Test Completed Successfully.`

- User input is usually shown in bold type:

  ```
  # mount /dev/cdrom /media
  # cd media
  # ./load.nmr
  ```

- Input or output that depends on local use is shown in italics:

  `Login:` **`root`**
  `Password:` ***`root_password`***

- Optional input is shown by angled brackets:

  `seqgen s2pul<.c>` means that `seqgen s2pul.c` and `seqgen s2pul` are 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 is 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.

- Pressing the Return key is required at the end of almost every command or line of text typed on the keyboard. Use of the Return key is mentioned only in cases where it is *not* used. This convention avoids repeating the instruction “press the Return key” throughout most of this manual.

Chapter 1. VnmrJ Installation

Sections in this chapter:

- 1.1 "Operating System," this page
- 1.2 "OS Patches," page 13
- 1.3 "Setting Up for VnmrJ Installation," page 14
- 1.4 "Installing VnmrJ," page 14
- 1.5 "VnmrJ Installation Options," page 16
- 1.6 "Installing VnmrJ Online Manuals," page 17
- 1.7 "VnmrJ Patches," page 18

This chapter describes how to install operating system (OS) patches, the VnmrJ software, and online help. Install the Operating Systems (OS) and all patches must be installed before installing VnmrJ.

1.1 Operating System

VnmrJ 2.2B is support only on Redhat Linux® — Red Hat Enterprise Linux WS v.4 (and latest V.4 update). Refer to *Linux Installation for VnmrJ* (Pub. No. 01-999268-00) for installation and configuration instructions.

1.2 OS Patches

VnmrJ ships with several CD-ROMs. Required patches for the OS (if any) are included on one of the CD-ROMS or as part of the OS distribution. Install OS any OS patches before installing VnmrJ for proper VnmrJ operation. Patches for the VnmrJ software are available at the Varian NMR User Page at `http://www.varianinc.com`. Click **NMR** in the list of *Scientific Instruments*, click **User Page** in the *NMR Resources* section, click on *Software Patches*, click on the appropriate software version, and enter the login name and password when requested. Follow the on screen instructions.

1. Log in as root.
2. Verify that the following conditions are true before installing patches:
   - VnmrJ is not running.
   - No users are logged on to your system (use the `who` command).
   - The NMR console is idle.
3. Proceed to the next section, 1.3 "Setting Up for VnmrJ Installation," page 14.

1.3 Setting Up for VnmrJ Installation

CAUTION: You must exit all running programs of VnmrJ and stop the `proc` family from running. Use the command `su acqproc`. The installation of VnmrJ automatically creates a link of `/vnmr` to the VnmrJ home directory.

1. Do one of the following:
   - New installation — continue with step 4.
   - Upgrade of current software — continue with step 2.
2. Exit all instances of VnmrJ.

   Do not delete the current version of the software, see "Files Automatically Transferred on Systems with VnmrJ or VNMR Installed," page 16.
3. Stop all `proc` family processes - use **`su acqproc`**.

   Refer to 2.4 "Creating the Acqproc User," page 24 for instructions on creating the `acqproc` user if this user does not exist.
4. **Stop** if the latest OS patches are not installed or continue with step 5 if all OS patches are installed.

   Follow the instructions in section 1.2 "OS Patches," page 13 before proceeding with VnmrJ installation if all OS patches are not installed.
5. Log in as `root` or use the `su` command to become root.

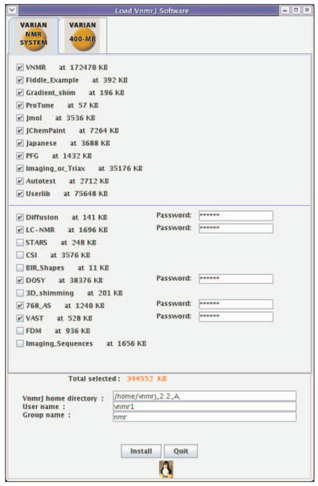
   Do not switch user to root using su –.
6. Open a terminal window and continue with 1.4 "Installing VnmrJ," page 14

1.4 Installing VnmrJ

1. Insert the VnmrJ CD and in a terminal window enter:

   ```
   cd /media/cdrecorder
   ./load.nmr
   ```

A prompt for the root password is displayed if the current user is not root. The installation window opens (Figure 1).



VNMRS 400-MR

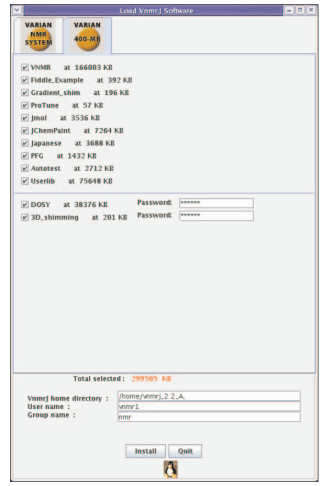


Figure 1. Installation Windows

a. Click on the either the **VARIAN NMR SYSTEM** or the **400-MR** tab to select the correct software options for the system.

   Section 1.5 “VnmrJ Installation Options,” page 16 lists and describes the available options. Some options require a password.

   Options can be installed at any time after VnmrJ is installed. Insert the CD, repeat the installation procedure, and select (check the box) only the options to be installed and remove checks from all other boxes.

b. Enter a name for the VnmrJ administrator in the **User name** field. The default user name is `vnmr1`.

   The installation program uses the directory and user account for the VnmrJ owner. The account and directory are created if they not do exist.

c. Enter a OS group name of the *VnmrJ* administrator **Group name**. The default is `nmr`.

d. Enter a new path for the **VnmrJ home directory**. As an example, replace `VnmrJ_2.2B` with an appropriate name.

CAUTION: **Avoid overwriting the current version of VnmrJ. Make sure that the path in the *VnmrJ home directory* entry is different from previous versions of VnmrJ; otherwise, the installed version of VnmrJ will be overwritten. Do not use *vnmr* as the directory name.**

2. Click **Install**.

   Installation time depends on the number of options selected. During the installation a pop up window displays the progress. A beep sounds when the installation is complete and the **Cancel** button in the progress window changes to **Done**.

   The installation progress report is saved in `~vnmr1/vnmrsys/VnmrJMsgLog`

3. Click the **Done** button and the following messages appear:

```
If your system is a spectrometer:
 1. Exit all Vnmr/VnmrJ programs.
 2. Run /vnmr/bin/setacq
On all systems:
 1. Run /vnmr/bin/makeuser for every user
```

```
    You can use vnmrj adm for this
    See Configure->Users->Update users...
 2. In the VnmrJ interface from Edit (liquids) Tools (Imager)->System
settings...
    click System config
```

Running `setacq` and configuring user accounts are described in the next chapter: Chapter 2, “System Configuration,” on page 19.

Files Automatically Transferred on Systems with VnmrJ or VNMR Installed

The `/vnmr/conpar` file, `/vnmr/devicenames` file, and the following directories are copied to the new `/vnmr directory` if a previous version of VnmrJ or VNMR is installed:

shims	imaging/gradtables
probes	fastmap
probes	adm/users
imaging/decclib	adm/accounting
imaging/gradtables	asm/info
dicom/config	tune/
mollib	pgsgl
gshimlib	

1.5 VnmrJ Installation Options

The installation program enables you to select from a list of *general* and *password* options to be installed with VnmrJ.

- “General Options,” next
- “Additional VnmrS System Options,” page 17
- “Options Requiring a Password,” page 17

General Options

The following is a list of general options and descriptions. Click the box next to each option you want to load. A check mark appears to show that the option is selected.

Option	*Description*
VNMR	Loads the basic VnmrJ and VNMR packages.
Fiddle_Example	Loads example of fiddle reference deconvolution.
Gradient_shim	Loads software for gradient shimming.
ProTune	Loads software for automated probe tuning with AutoX probes.
Jmol	Loads integrated Jmol molecular viewing software.
JChemPaint	Loads integrated JChemPaint molecular editing software.
Japanese	Adds Japanese language support
PFG	Loads `seqlib`, `psglib` parameters and other files for PFG experiments.

AutoTest	Loads AutoTest software for automated system testing.
Userlib	Loads Userlib.

Additional VnmrS System Options

The VnmrS System has the following additional options available:

Option	*Description*
Imaging_or_Triax	Loads software for imaging or triple axis gradient.

Options Requiring a Password

The following is a list of options (and descriptions) that require a password. A password field is visible when the option is selected. Enter the password in the field (passwords are case-sensitive). The list of options presented is system dependent.

- "400MR System Options," page 17
- "VnmrS System Options," page 17

400MR System Options

Option	*Description*
DOSY	Loads DOSY experiment to separate resonances based on diffusion characteristics.
3D_shimming	Loads software for 3D gradient shimming.

VnmrS System Options

Option	*Description*
Diffusion	Software for running diffusion experiments.
LC-NMR	Software for driving LC-NMR experiments.
STARS	A software simulation package.
CSI	Loads files for Chemical Shift Imaging.
BIR_shapes	Loads BIR-shaped pulse statements for variable tip-angle adiabatic pulses.
DOSY	Loads DOSY experiment to separate resonances based on diffusion characteristics.
3D_shimming	Loads software for 3D gradient shimming.
768_AS	Loads software for 768 AS sample changer accessory.
VAST	Loads software for VAST sample changing accessory.
FDM	Loads software for FDM data processing methods.
Imaging_Sequences	Loads special pulse sequences for imaging.

1.6 Installing VnmrJ Online Manuals

VnmrJ either individual manuals or the entire manual set manuals can be installed onto the system or read directly from the *VnmrJ Online Manuals* CD (which must be then left in the CD drive). The appropriate manuals are loaded based on the `/vnmr/vnmrrev` file.

Use Acrobat Reader to view online manuals. Installing the Online Manuals copies the manual set and a copy of the Acrobat Reader to the hard drive.

Load *VnmrJ Online Manuals* and Online Help from a Terminal window as follows:

1. Log in as `root` or use the `su` command to become root. *Do not switch user to root using su –.*
2. Open a Terminal window.
3. Change to the `vnmrj_online` directory on the CD-ROM:
   - Enter **`cd /media/cdrecorder`**
4. Look at the contents in the `vnmrj_online` directory:

   \# **`ls`**
5. Enter the following command:

   \#**`./install`**
6. Eject the CD-ROM after either installing the online manuals or reading them by entering the following commands in a terminal console window:

   \# **`cd /`**

   \# **`eject cdrom`**

1.7 VnmrJ Patches

The latest VnmrJ patches can be downloaded from the NMR User Pages www.varianinc.com/products/nmr/apps/vnmrusers.html, which are accessible to registered VnmrJ users. See 3.1 “VnmrJ User Pages on the Web,” page 27, for more information.

Check the Patch Level

1. Log in as `vnmr1`.
2. Open a terminal window and enter:
   `vnmr1>` **`ls /vnmr/adm/patch`**
   The installed patches are listed. The system returns `No such file or directory` if no patches are listed.

Download and Install a Patch

1. Log in as `vnmr1`.
2. Go to the VnmrJ User Pages Web page:

   www.varianinc.com/products/nmr/apps/vnmrusers.html
3. Navigate to the Software Patches page and find the appropriate patch.
4. Read the **Readme** file for the patch before downloading and installing the patch. Any patch specific instructions are specified in this file.
5. Follow the instructions in the **Readme** file.
6. Click on the patch name to download it.

Use the **`patchinstall`** script to install the patch.

Chapter 2. System Configuration

This chapter describes how to configure VnmrJ on your system. It includes the general, rf channel, and gradient configuration values for your system. Sections include:

- 2.1 “Setting Up the Host Computer for Data Acquisition,” page 19
- 2.2 “System Settings,” page 20
- 2.3 “Spectrometer Configuration,” page 22
- 2.4 “Creating the Acqproc User,” page 24
- 2.5 “Setting the Lock Frequency,” page 25

2.1 Setting Up the Host Computer for Data Acquisition

This section describes how to use the `setacq` command to establish communications between the host computer and the NMR console.

Skip this section if this installation is for data station or if setting up the host for data acquisition is delayed.

CAUTION: **Do not reboot or reset the NMR console until setacq has finished. The process may take eight or more minutes.**

1. Make sure the host computer is connected to the console and the console is on.
2. Log in as `root`.
3. Open a Terminal or Shell Tool and enter the following commands:

```
# cd /vnmr/bin
# ./setacq
```

   The system asks for the root password if the current log in is not `root`.

   `Expproc` will start and stop as needed.

   A message appears:

```
One moment please...
           Stopping Acquisition communication
```

   The system responds as follows if the user is not logged in as the system root user:

```
To run setacq you will need to be the system’s root user
Please enter this system’s root user password
Password:
```

   The system continues with the following:

```
The Network Port to Console = eth1, subnet = xxx.xxx.xxx
The Network Port to main net = eth0, subnet = yyy.yyy.yyy
```

```
Please make sure both console and PC are connected.
One moment please...
Stopping Acquisition communication
      The download step may take four to eight minutes
      Do not reboot the console during this process
downloading 9 files to the acquisition console.
downloading file 1 of 9
downloading file 2 of 9
downloading file 3 of 9
downloading file 4 of 9
downloading file 5 of 9
downloading file 6 of 9
downloading file 7 of 9
downloading file 8 of 9
downloading file 9 of 9

Starting Acquisition communications.
```

4. Wait for `setacq` to finish the update process. The update process may take eight or more minutes.

WARNING: **Do not reboot or interrupt the console during the update process or the console may be come inoperable.**

5. Wait for the following message:

   ```
   NMR Console software installation complete
   Starting Acquisition communications
   ```

6. The system prompts for a reboot if needed.

   `You must reboot the operating system for these changes to take effect`

   As root, reboot the workstation:

   `#` **`reboot`**

   Check that the Ethernet connections between the host computer and the console are properly connected and reboot the console if `setacq` repeatedly shows the message "`Console timed-out, is it connected?`".

   Use **Control–C** to stop the messages and return to the # prompt; then run `setacq` again once the host computer and the console are properly connected.

7. Continue with "System Settings," next.

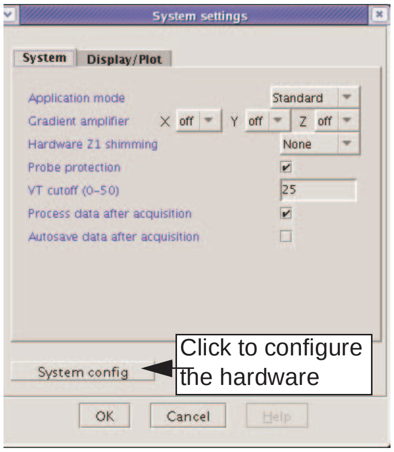
2.2 System Settings

The software must be configured using the VnmrJ System Settings window after it is installed. The System Settings window provides software settings that are used more often than general spectrometer settings. Typically vnmr1 is set to the experimental interface and the Systems Settings window displays the options as shown. Refer to the *VnmrJ Walkup* manual for the Systems Setting window options when the interface is set to walkup.

1. Log in as the VnmrJ administrator (e.g., `vnmr1`) and start VnmrJ.
2. Do the following:
   - All systems except imaging:

     Click **Edit** in the main menu after VnmrJ starts.
   - Imaging systems only:

     Click **Tools** in the main menu after VnmrJ starts.
3. Click on **System Settings** to open the System settings window.



The System Settings window has two tabs; **System** and **Display Plot**. The fields, drop down menus, and check boxes for each tab is shown below. Select the choices that are correct for the spectrometer system.

Tab	*Fields*
System	**Application mode** — Standard, Walkup, Imaging, LC-NMR, Autotest. **Gradient amplifier** — On/Off selection for each installed gradient axis. **Hardware Z1 shimming** — None for no Z1 shimming, Delay for Z1 shimming enabled during delay time, or Presat for Z1 shimming enabled during delay time preceding presat. **Probe protection** — check to enable. **Solids VT System** — check to enable **VT cutoff (0-50)** — specify VT cutoff temperature; 25^{o}C recommended. **Process data after acquisition** — check to enable. **Autosave data after acquisition** — check to enable.
Display/Plot	**Process data on drag-and drop from locator** — check to enable. **Set display from plotter aspect ratio (wysisyg)** — check to enable. **Spectrum updating during phasing (0-100)** — set the percentage of the display that is updated during interactive phasing. 100 is recommended. **Max # of pens** — number of plotter pens to use. **Show Tooltips** — check to enable. **Max # of items to show in Locator** - Set the number of items to show in the locator. Setting this to greater than 2000 starts to diminish the performance. **Display only matching items in locator** — check to enable. **Day Limit of files in Locator (neg = forever)** — Enter the cutoff age in days for keeping `.fid` and `.fdf` files in the locator database. Files are only removed from the database after reaching this age. Files remain on the disk and are not removed. A negative number means keep all files forever. Zero, means do not keep any `.fid` nor `.fdf` files except Varian files. An entry of 30 means remove files older than 30 days from the database. Refer to Appendix B, "Locator Administration," on page 119 for more information on working with the locator. **Turn Locator Off** - check to completely disable the Locator.

4. Continue with "Spectrometer Configuration," next.

2.3 Spectrometer Configuration

Use the Spectrometer Configuration window to configure NMR spectrometer hardware.

1. Click the **System config** button in the System Settings window.

   A VnmrJ Spectrometer Configuration window, similar to Figure 2, opens.

2. Check that the configuration values are correct for your system.

   Refer to Table 1, "General Configuration" on page 22 for more information on these values.

3. Configure each rf channel.

   Refer to Table 2, "RF Channels Configuration" on page 24 for information on each selection.

4. Click **OK** to save the system settings or **Cancel** to make no changes and close the System Settings window.

5. Exit and restart VnmrJ to enable acquisition features in the main menu if the system is changed from a datastation to a spectrometer.

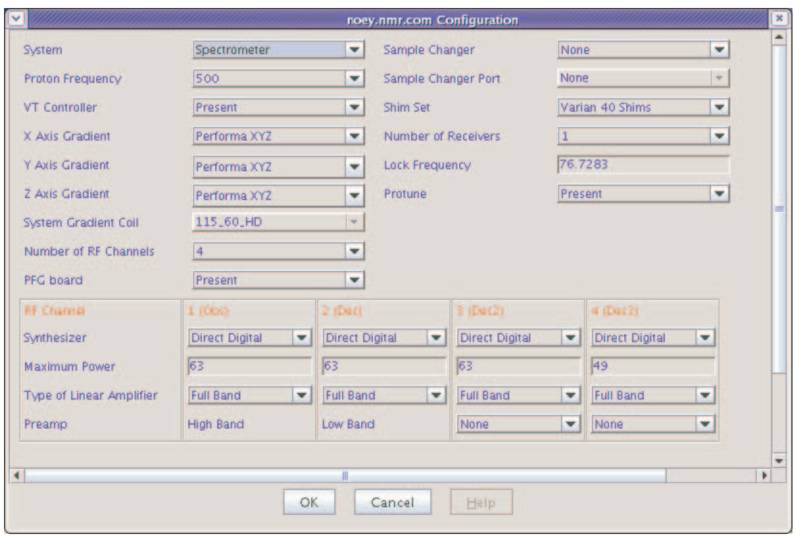


Figure 2. Spectrometer Configuration Window

Table 1. General Configuration

Label	*Choices*	*Explanation*
System	Spectrometer, Data Station	Sets whether function of the workstation is to control a spectrometer or to operate as a separate data station. VnmrJ does not allow acquisitions (the `go` command, its aliases, and related commands do not work) if Data Station is selected.
Proton Frequency	85, 100, 200, 300, 400, 500, 600, 700, 750, 800, 900, 3T, 4T	Sets ^{1}H frequency for spectrometer-type systems.
VT Controller	Not Present, Present	Sets whether a VT controller is present.

Table 1. General Configuration (continued)

Label	*Choices*	*Explanation*
X Axis Gradient, Y Axis Gradient, Z Axis Gradient	Not Present, Gradient Coordinate Rotator Performa I, Performa IV, Performa XYZ, Homospoil	Sets value of the spatial axis. Do the following for systems with: Waveform generator and a gradient control unit — verify that the gradient values are correct next to the labels X Axis, Y Axis, and Z Axis. Waveform generator present for an axis — set the value to WFG+GCU. PFG option installed — set the value to Performa I, Performa II, Performa III, or Performa IV; otherwise, set the value for the axis to None. Up to three gradients can be present, one for each spatial axis.
System Gradient Coil	None, Nano, Performa_1, Performa_2, Performa_XYZ	Selects the gradient coil configuration file that defines the current installed gradient coil (`sysgcoil`). The full list is in `/vnmr/imaging/gradtables`.
Number of RF Channels	1, 2, 3, 4, 5	Sets number of rf channels available (excluding the lock channel). Systems normally have 2, 3, or 4 rf channels: The first channel is for direct observation. The second channel allows decoupling or pulsing when decoupling. An optional third channel allows decoupling of a second nucleus. An optional fourth channel allows decoupling of a third nucleus. The minimum value you can select is 2. *Do not change this value to eliminate the use of a channel.* Refer to the descriptions of the parameters `dn2` and `dn3` in the *VnmrJ Command and Parameter Reference* for information on how to disable a channel.
PFG board	Present, Not Present	Sets whether the PFG Controller board is present.
	MicroImaging	Sets software for both Gradient and PFG.
Sample Changer	None, Carousel, SMS 50 Sample, SMS 100 Sample, VAST, NMS, LC-NMR, 768 AS	Sets the type of optional sample changer. Select None if no sample changer is present or to disable an attached sample changer. Refer to “Automated Hardware,” page 53 for more information.
Sample Changer Port	Not Used, Port A, Port B, Com1, Ethernet	Sets communications port used for the sample changer. Select Not Used if no sample changer is present.
Shim Set	Varian 14 Shims, Varian 15 Shims, Oxford 15 Shims, Varian 18 Shims, Varian 20 Shims, Varian 23 Shims, Varian 26 Shims Varian 28 Shims, Varian 29 Shims, Varian 35 Shims, Varian 40 Shims, Ultra 18 Shims, Ultra 39 Shims, Whole Body	Sets type of shims on the system.
Number of Receivers	1, 2, or 4	Sets the number of receivers available in the system.

Table 1. General Configuration (continued)

Label	*Choices*	*Explanation*
Lock Frequency	1 Hz to 160 MHz, in 0.1 Hz steps (enter the number directly)	The value should be the same as found in the procedure in section 2.5 "Setting the Lock Frequency," page 25, which is the nominal ^{2}H observe frequency. **To observe NMR signals, the value of Lock Frequency must be set correctly.**
ProTune	Present, Not Present	Select present if Protune hardware is installed and in use, see also "Setting Up ProTune," page 54.

Table 2. RF Channels Configuration

Label	*Choices*	*Explanation*
RF Channel		Number of rf channels displayed is determined by the value set in Number of RF Channels. Channels are RF Channel 1 (Obs) and RF Channel 2 to 5 (Dec).
Synthesizer	None, PTS320, PTS500, PTS620, PTS1000, Direct Digital, Varian 400	Sets the model of the PTS frequency synthesizer if present on the current rf channel. The model number is written on the front of the synthesizer. To make a selection for the Decoupler RF Channel with a fixed-frequency decoupler, select PTS*** for RF channels 1 and 2 (and all others, if present), where *** is the number written on the front of the synthesizer.
Maximum Power	0 to 63 for 63-dB attenuator, or -16 to 63 for 79-dB attenuator (enter number directly)	Sets the maximum power (upper limit) to the current rf channel to prevent damage from high power rf. The *decoupler* channel is usually set to **45** or **50** to prevent damage to the probe. *MR imaging systems* — enter **127**.
Type of Linear Amplifier	Full band, Low band, Broadband,	Sets type of amplifier on the current rf channel. Full Band indicates the channel uses a linear full-band amplifier. Low Band indicates the channel uses a linear low-band amplifier. Broadband indicates the channel goes to one amplifier for all frequencies. Contact your field service engineer if you have any questions about what class amplifiers are in your system. Refer to the `amptype` parameter in the *VnmrJ Command and Parameter Reference*.
Preamp	None, High band, and Low band	Select correct type based on system.

2.4 Creating the Acqproc User

Daemons, known as the proc-family, direct communications between the host computer and the console on systems that include a magnet installation (spectrometers systems, not data stations).

Create the user `acqproc` as follows:

1. Log in as `root`

2. Type the following command:

   # /vnmr/bin/makesuacqproc

   The system asks for the root password if the login is not root.

All users can enable or disable the daemons once `acqproc` is created by typing the following command:

`user>` **`su acqproc`**

2.5 Setting the Lock Frequency

This procedure is not required for imaging systems.

Set the lock frequency using the following procedure after VnmrJ is installed on system and the magnet is installed and ready for use. Use the true ^{2}H frequency for this procedure. This procedure is required during initial system installation and is repeated only if the magnet quenches or a large change in field strength occurs.

1. Make sure the magnet is at field.
2. Log in as the administrator, typically vnmr1.

   The `setlockfreq` macro will not use the values obtained to update `/vnmr/compar` if the logged in user does not have administrative privileges.
3. Insert a water sample is in the magnet.

   Tap water is an acceptable sample.
4. Load the Proton experiment.
5. Set **`sw=500000`** (`sw=2000000` for wideline systems).
6. Set **`tn='H1' lockfreq='n'`**.
7. Enter **`ga`**. The system is off resonance if no peaks are observed.

   Locate the water resonance by changing the value of `tof` (or array `tof`). Make changes of 200-kHz- to 400-kHz, so each spectral window overlaps its neighbors.
8. Center the located water resonance in the spectral window by placing the cursor on the line and entering **`movetof`**.
9. Acquire a spectrum with the line centered in the window.
10. Enter the command **`setlockfreq`**.

    `setlockfreq` calculates and sets the lock frequency parameter `lockfreq`.

Chapter 3. VnmrJ Administration

Sections in this chapter:

- 3.1 “VnmrJ User Pages on the Web,” this page
- 3.2 “Starting the VnmrJ Admin Interface,” this page
- 3.3 “VnmrJ Admin Interface,” page 28
- 3.4 “User Account Administration,” page 30
- 3.5 “User Defaults and Directories,” page 34
- 3.6 “Setting Data Saving Templates,” page 36
- 3.7 “Creating Operator Profiles,” page 36
- 3.8 “Walkup Account Administration,” page 39
- 3.9 “Imaging System Administration,” page 43
- 3.10 “Setting Up Automation Queue.,” page 44
- 3.11 “Viewing the File System,” page 45

This chapter covers the administration procedures executed using the VnmrJ Admin interface that apply to all user accounts at the time the user account is created or updated. Various administration functions need to be applied to multiple items or accounts. The instructions for account administration in this section are applied by selecting a single account or item.

3.1 VnmrJ User Pages on the Web

The VnmrJ User Pages offer an array of useful information for registered VnmrJ users, including:

- Software patches for VnmrJ and operating system
- Online manuals
- Varian NMR News — current issue and searchable archive
- FAQs and Bug lists
- User library — provides additional software such as BioPack
- Magnetic Moments newsletter archive
- Upgrade information

1. Go to:
   http://www.varianinc.com/products/nmr/apps/vnmrusers.html
2. Register as a VnmrJ user and to be eligible to access the User Pages
3. Click **Registration Form**.
4. Fill in the form and click **Submit**.

3.2 Starting the VnmrJ Admin Interface

Use one of the following procedures:

- Click on the VnmrJ Admin icon on the desk top if the current user is the administrator.
- Use a terminal window — useful if the current user is not the administrator:

  a. Log in to the workstation using the VnmrJ administrator user account or open a terminal window and change users to the VnmrJ administrator account.

  b. Enter **`vnmrj admin`** at the prompt.

  c. Enter the administrator password, if prompted, to start VnmrJ Admin, see Figure 3.

3.3 VnmrJ Admin Interface

VnmrJ Admin interface, see Figure 3, provides the tools for administering VnmrJ software and user accounts. The menus are described below.

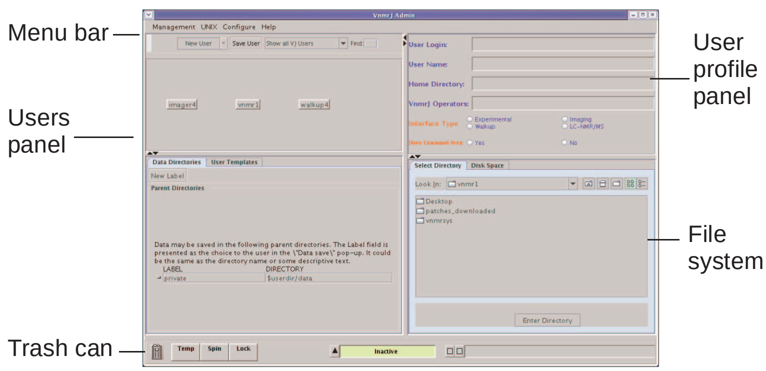


Figure 3. VnmrJ Administrator Window

Select administration functions from the menu bar.

- “Management,” page 28
- “UNIX,” page 29
- “Configure,” page 29
- “Help,” page 29

Management

Menu Item	*Description*
Users	Displays users in the users panel and makes available all the administrative functions, refer to “User Account Administration,” page 30.
Printers	Printer functions using popup window, refer to Chapter 4, “VnmrJ Printers and Plotters,” on page 47.
Cost/Time Accounting	VNMR ACCOUNTING window. Refer to Chapter 6 “VnmrJ Accounting Administration,” page 55.
Exit	Exit and close VnmrJ Admin.

UNIX

Menu Item	*Description*
File System	Popup window displays file system information, refer to "Viewing the File System," page 45 for more information and instructions.
Command window	Opens a operating system terminal window.

Configure

Menu Item	*Description*
Users	Select additional functions using popup windows: **Convert users** opens the *Change vnmr users to VnmrJ user* window. Refer to "Converting User Accounts to VnmrJ," page 33. **Defaults** opens the default values window. Refer to "User Account Defaults," page 34. **Update users** opens the *Update VnmrJ Users* window. Refer to "Updating User Accounts," page 34.
Operators	Add operators to the walkup account, see 3.8 "Walkup Account Administration," page 39. **Edit operators** opens the *Modify Operators* window (Modify Operators tab). Refer to "Adding Operators to a User Account," page 39. **Delete operators** opens the *Modify Operators* window (Delete Operator tab). Refer to "Deleting Operators from User Accounts," page 43. **Reset password** opens the *Reset Operators Password* window. Refer to "Resetting Operator Password," page 40. **Preferences** opens the *Preferences* window for setting the default operators password and for selecting a default login icon. Refer to "Setting Operator Default Password," page 40.
Automation	Set up automation queue options using this popup window, see "Setting Up Automation Queue.," page 44.
Edit Profiles	Create and assign user profiles containing the protocols, rights and tools "Creating, Editing, Viewing, and Deleting Profiles," page 37.
Investigator List	Enter investigators in the popup window, refer to "Setting Up Investigator List," page 43.
Background Colors	Change the default background colors of the VnmrJ Admin windows.

Help

Menu Item	*Description*
VnmrJ Help	Opens the VnmrJ HTML help pages in a browser.
Admin Help	Opens the VnmrJ Administration HTML help pages in a browser.
Online Manuals (PDF) …	Opens the VnmrJ online manuals in PDF format.

3.4 User Account Administration

User accounts are created or set up from the VnmrJ Admin interface. A typical administration function is setting up new accounts and configuration of the VnmrJ interface according to the user's needs. Another administrative function is assigning a group of operators to a single user account–typically, for liquids system, the user and operators are working with a system that has an automated sample changer system.

- "VnmrJ Interfaces," page 30
- "Creating a Single New User Account," page 31
- "Creating Multiple New User Accounts," page 32
- "Changing the Interface of a User Account," page 32
- "Deleting a User Account," page 33
- "Restoring a User Account," page 33
- "Converting User Accounts to VnmrJ," page 33
- "Updating User Accounts," page 34

VnmrJ Interfaces

Each VnmrJ account can an be set up with an interface and privileges that are appropriate for the needs of the user. The main interfaces are:

- "Experimental," page 30
- "Walkup," page 30
- "Imaging," page 31

Experimental

The VnmrJ user requiring the full range of flexibility and experimental capabilities is typically set up with the Experimental interface.

Walkup

The walkup interface is designed for automated operation with a sample changer and for operation in an open access environment. There are two levels, the Walkup account owner and the Walkup operator level.

Walkup Account owner – The walkup administrator is the operating system login and therefor the owner of the account and any automation runs started while logged in. Operator login establishes the operator parameter and other properties set by through VnmrJ Admin, such as the user profile, panellevel, etc. All default operations that occur during an automation run (shimming, locking, etc.) are set up by this user before the automation run is started. Refer to the manual VnmrJ Walkup for a full description of the Walkup interface the administrator account functions.

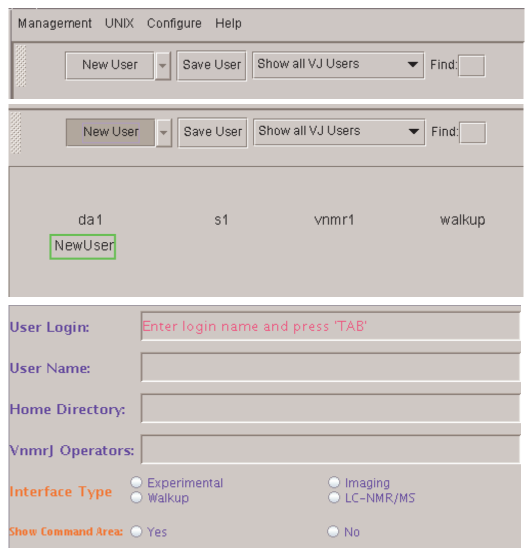
Walkup Operator – The walkup operator has VnmrJ access via a user name and password and is not a operating system login (the operator may have operating system level privileges for other accounts) and therefore does not own any of the files in the account. All default operations that occur during an automation run (shimming, locking, etc.) are first set up by the walkup administrator before the automation run is started. Refer to the manual VnmrJ Walkup for a full description of the Walkup interface the operator account functions. See also: "Walkup Account Administration," page 39.

Imaging

The imaging interface provides the user with the full range of functions necessary for the acquisition of MRI data, design imaging sequences, build study protocols, and process and imaging data. See also: “Imaging System Administration,” page 43.

Creating a Single New User Account

This procedure creates a single new user account. To create multiple new user accounts, refer to the next section, “Creating Multiple New User Accounts,” page 32. The new user account will be set up using the default values set in User Account Defaults, see “User Account Defaults,” page 34.



1. Select **Management**.
2. Select **Users**.
3. Select **Show all VJ Users**.
4. Select **Management.**
5. Select **Users**.
6. Select **Show all VJ Users**.

   Click **New User**.

   NewUser appears with a box around it and the account’s profile is displayed in the User Profile Panel.
7. Fill in the **User Profile Panel** as appropriate.

   The **User Profile Panel** (by default) has five sections; see “User Account Defaults,” page 34 to view other fields, data dir etc.

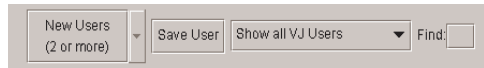
Field	*Description*
User Login:	*Enter login name and press ‘RETURN’* prompt is displayed in the user login field.
User Name:	Optional. Enter a user name.
Home Directory	New users with no operating system account: Setup is automatic and applies the user defaults (see “User Account Defaults,” page 34). Current users with an a operating system account: The user’s operating system account home directory is used.
Interface Type	Click the radio button to select **Experimental**, **Walkup**, **Imagining**, or **LC-NMR** interface type, Refer to “VnmrJ Interfaces,” page 30.
VnmrJ Operators	Optional. List other users with VnmrJ operation privileges (Walkup only).
Show Command Area	Click a **Yes** or **No** radio button to show or hide the command area.

8. Click **Save User**.

Creating Multiple New User Accounts

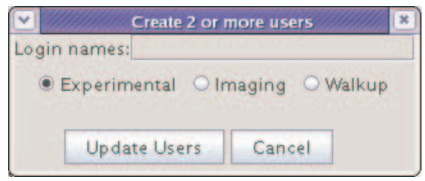
This procedure describes how to create multiple new user accounts. The new user accounts will be set up using the default values set in User Account Defaults, see “User Account Defaults,” page 34. Refer to “Creating a Single New User Account,” page 31, to create a single new user account.

1. Select **Management** from the main menu bar.



2. Select **Users**.
3. Click on next to **New User**.
4. Select **Multiple Users** from the drop down menu.
5. Click **New Users (2 or more)**.

   The **Create 2 or more users** window opens.



6. Enter the login names for each user. Separate each user name by a space.
7. Click on a **radio button** to select the interface assigned to these users.

   Refer to “VnmrJ Interfaces,” page 30.

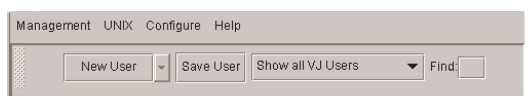
8. Click **Update Users**.

   The home directory is automatically setup (new users - no operating system account) based upon the user defaults (see “User Account Defaults,” page 34) or, if the user was first set up as a operating system account, the user’s operating system account home directory is used.

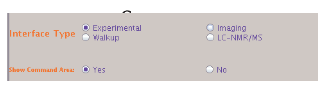
Changing the Interface of a User Account

Change the interface assigned to a user account as follows:

1. Select **Management** from the main menu bar.



2. Select **Users**.
3. Select **Show all VJ Users**.
4. Click on the user account to change.
5. Click on the radio button for the **Interface Type**.



7. Click on a **Yes** or **No** radio button for Show Command Area.
8. Click **Save User**.
9. Select **Configure**.
10. Select **Users**.
11. Select **Update** users to open the update users window.
12. Select the **user account** you just changed and click the **green arrow** to move the user into the **Update users** box.
13. Click **Update Users** to update all global parameters for the new interface.

Deleting a User Account

Use this procedure to delete a user account.

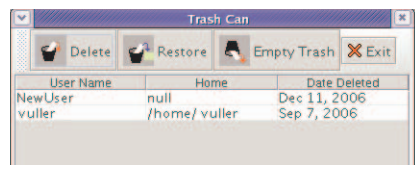
1. Select **Management**.
2. Select **Users**.
3. Select **Show all VJ Users**.
4. **Right-click** on the user account and select **Delete**.

   Only the user account is deleted; operators assigned to the account are not deleted. The operators can be assigned to other user accounts, see “Adding Operators to a User Account,” page 39 or deleted, see “Deleting Operators from User Accounts,” page 43.

   The home directory and VnmrJ files are not deleted and can be restored from the trash can only if the trash can has not been emptied.

Restoring a User Account

A deleted user account can be restored only if the trash can has not been emptied.

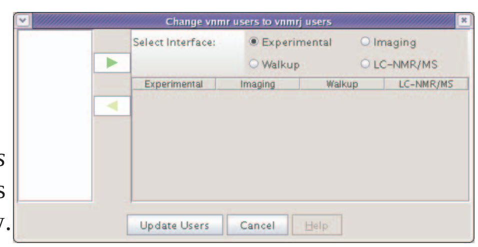


1. **Double-click** the **trash can** icon.

   The *Trash Can* window appears.
2. **Select** on the account to be restored by clicking it once.
3. Select **Restore**.
4. **Exit** the Trash Can window.

Converting User Accounts to VnmrJ

The VnmrJ Admin interface provides a tool for converting VNMR users to VnmrJ users

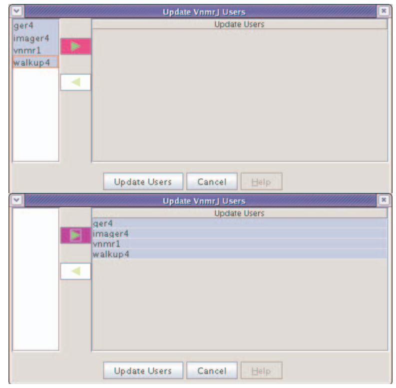


1. Select **Configure**.
2. Select **Users**.
3. Select **Convert users**.

   The *Change vnmrusers to VnmrJ users* window appears. VNMR user accounts are listed in the left side of the window.
4. Click on an interface type to sort by interface type.
5. Select a **VNMR account** to be converted.
6. Select the **interface type** and click the **green arrow**.
7. Hold the **Control** and **Shift** keys to make multiple selections of accounts with the same interface.
8. Repeat the previous step for other accounts using other interfaces.
9. Click **Update Users**.

Updating User Accounts

Use the Update VnmrJ Users window to update multiple VnmrJ user accounts. Use this procedure every time the software is upgraded or reloaded.



1. Select **Configure**.
2. Select **Users**.
3. Select **Update users**.

   The *Update VnmrJ users* window appears with VnmrJ user accounts listed on the left side of the window.
4. Click on an **interface** to sort by that interface.
5. Select the **accounts** to be updated.

   Hold the Control and Shift keys to select multiple accounts with the same interface.
6. Click the highlighted, green arrow to move the accounts to the *Update users* box.
7. Click **Update Users**.

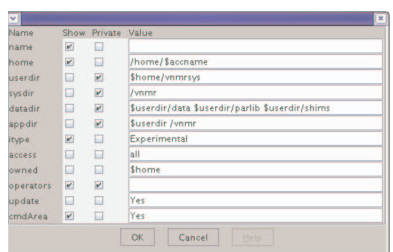
3.5 User Defaults and Directories

Use the VnmrJ Admin interface to set up user account defaults, templates, and directories.

- "User Account Defaults," page 34
- "User Directories," page 35

User Account Defaults

Review and configure user account default properties before creating a new user account. These properties apply to all new VnmrJ user accounts and typically are not be changed.



1. Select **Configure**.
2. Select **Users**.
3. Select **Defaults**.

   The *Defaults* window appears and shows the defaults that will be used when a new user account is established.

Field	*Description*
name	Full name of a user, e.g., Elsie Enemare
home	Home directory of a user
userdir	Directory that contains private VnmrJ files for a user
sysdir	System directory for VnmrJ
datadir	Path of the directories where user data is stored
appdir	Directory search path used to search for application-specific files

itype	The **`itype`** field specifies the user interface; Experimental, Walkup for automation and open access, or Imaging for imaging systems.
access	User's access level to other users' data
owned	Directories that are owned by the user
operators	Authorized account users. A system login is not required.
update	When creating users, `makeuser` is automatically run to update user preferences if the value is set to `Yes`. This setting is only for operating system or VnmrJ users who are already in the system
cmdArea	Show or do not show a command line.

4. Review the `home` field, which shows the path of a new user's home directory.

   The default is set to `/home/$accname`.

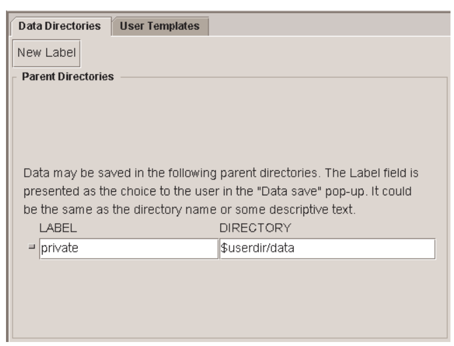
   The account name is `$accname` and `/export/home` is where the home directory of a new user account is located. This path is only used if the user is not a defined operating system user. The current home directory of existing operating system user is used.

   Replace `/home` with the directory path to the user's home directory if `/home` does not exist or if the home directory of a the user is located in another directory.
5. Review the `itype` field (the default interface type) for new VnmrJ users.
6. Click **OK** to save your changes or click **Cancel** o leave the settings unchanged.

User Directories

The default user directories are set up for each user. Additional user directories can be added or user directories deleted. These data directories are available to each user in **Save Data setup** where the user can select any of the data directories to use when saving data.

LABEL — template name that will appear in the users *Save Data Setup* popup.
Directory — Defines the construction of the file name.



1. Click **New Label**, which adds a blank row below the current user directories to create a new label.
2. Enter a directory in the blank cell in the column under **DIRECTORY** or select the cell and use the file browser.
3. Click the **Save User** button to save any changes made.
4. Select a directory and click the **Enter Directory** button.

   Refer to 3.11 "Viewing the File System," page 45.

3.6 Setting Data Saving Templates

VnmrJ provides data saving templates and designated data saving directories to control how data is saved.

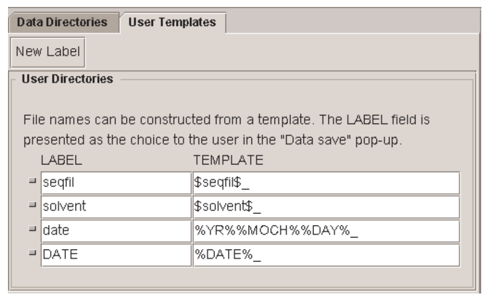
The default user templates are set up for each user. Additional user templates can be added or deleted. These user templates are accessed by the user when saving data in VnmrJ. All the templates for each user are available to them in **Save Data setup**, where the user can select any of their templates to use when saving data.

LABEL — template name that will appear in the users *Data Save* popup.

TEMPLATE — Defines the construction of the file name.

The default templates use by a user account when **Save data setup …** from the **File** menu is selected is set in the User Template window.

1. Click on the **User Template** tab in the VnmrJ Admin window to view, change, or add a new template.
2. Click the **New Template** button to add a new row.
3. Enter a **LABEL** name and **TEMPLATE** definition in the fields under the LABEL and TEMPLATE columns.
4. Click the **Save User** button to save any changes made.



3.7 Creating Operator Profiles

Operator profile is implemented for the Walkup account owner and operator. The system administrator creates and assigns a profiles containing the protocols, rights, and tools that are available to a specific operator or assigned to several operators.

Protocols are selected from the available `apptypes`. The standard liquids protocols include Std 1D, Homo 2D, Hetero 2D, Sel 1D, and Dosy 2D (if available). Any protocols within any `apptype` may be selected. Rights are selected from the available rights listed in Table 3.

Table 3. User Profile Rights and Options

Right	*Function or Action Allowed*
May Edit Password	Show the Edit Password item in the Tools menu.
Can Browse Anywhere	Give the operator access to all files in the file browser.
Enable Locator Update	Show the following items in the Tools menu: Update locator submenu, Import files to locator, Save/Delete custom locator statement.
Enable All Editors	Show all items in the Edit menu, and show the Create protocols submenu in the Tools menu.
Edit Own Profile	Show the Edit config profile item in the Edit menu.
Show Molecular Structures	Show the Molecular Structures submenu in the Tools menu.
Show All Acquisition Menus	Show the Acquisition menu.

Table 3. User Profile Rights and Options

Right	*Function or Action Allowed*
Show All Processing Menus	Show the Process menu.
Enable Calibrations	Tools menu, show the Standard Calibration Experiments, Probe Tuning, and Gradient Shimming menus.
May Tune Probe	Show the Manual Tune Probe item in the Tools menu.
Enable Automation Setup	Show the New Workspace, Save data setup, New automation run, and Create Plot Design items in the File menu; Show the Experiments menu; Show Update night queue start time and Auto Tune Setup in the Tools menu.
Show All Operators Studies	Show studies for all operators in the study queue.
Edit All Operators Studies	May edit studies for all operators. If selected, Show All Operators Studies must also be selected.
Remove New Sample Node	When a study is cleared using New sample in the Study Options menu, do not create a new sample node.
Can Edit Protocols	May edit or customize protocols in the study queue.
Select All Prescans	Select all prescans when an operator logs in.
Priority Sample	Show the priority sample check box in the study queue panel.
Can Exit VnmrJ	Operator may exit VnmrJ.

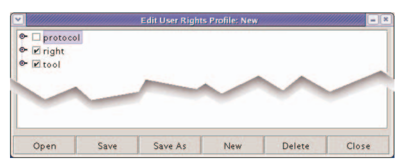
Tools are selected from the available tools list. This includes Locator, Browser, and Study Queue.

The following user profiles are provided:

- `AllLiquids` contains all liquids protocols, all rights, and all tools.
- `BasicLiquids` contains only a few protocols, a few rights, and all tools.

Creating, Editing, Viewing, and Deleting Profiles

1. Start VnmrJ Admin.
2. Click on **Configure** on the main menu.
3. Select **Edit Profile**. The Edit User Rights Profile window opens and displays the Profile named at the top of the window.



Creating a New Profile

1. Select **New** to create a new profile.
2. Use the file tree controls to expand or contract the file tree:

   Expand — click on the to change it to .

   Collapse — click on the to change it to .
3. Set Rights as follows:

   Allow —change the check box from ☐ to ☑.

   Not Allow — change the check box from ☑ to ☐.
4. Use the controls at the bottom of the Edit User Profile window to **Save** (uses existing file name), **Save As** (prompts for new file name), or **Close** (no change) the Edit User Profile window.

Editing or Viewing an Existing Profile

1. Select **Open** to edit an existing user rights profile.
2. Use the file tree controls to expand or contract the file tree:

   Expand — click on the to change it to .

   Collapse — click on the to change it to .
3. Do one of the following:
   - Close after viewing the profile — Go to step 5 and click on **Close**.
   - Continue and edit the profile — Continue with step 4.
4. Set Rights as follows:

   Allow —change the check box from to .

   Not Allow — change the check box from to .
5. Use the controls at the bottom of the Edit User Profile window to **Save** (uses existing file name), **Save As** (prompts for new file name), or **Close** (no change) the Edit User Profile window.

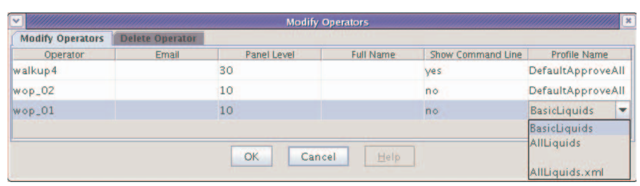
Deleting an Existing Profile

1. Click on the **Delete** button to bring up a profile browser.
2. Select the user profile to be deleted.
3. Click on the **Delete** button to delete or click on the **Cancel** button to exit without deleting any profiles.

Assigning Operator Profiles

Assign a named profile to an operator using the VnmrJ Admin interface as follows:

1. Start VnmrJ Admin.
2. Click on **Configure** on the main menu.
3. Select **Operators**.
4. Select **Edit Operators…** to open the Modify Operators window.



   The last column in the Modify Operators window is for assigning the operator or account owner a Profile Name. The default is DefaultApproveAll which is the same as the profile AllLiquids. Two profiles are provided; AllLiquids and BasicLiquids.
5. Click on the field under **Profile Name** for an operator to access the drop down menu of profiles.
6. Select a **Profile** for the operator rights.

   See "Creating, Editing, Viewing, and Deleting Profiles," page 37 if a custom profile is required.
7. Click OK to apply the selected profile.

Walkup Account Owner Control of Operator Rights

The Walkup Account Owner can further limit the experiments/protocols visible to operators assigned to the walkup account.

1. Log in as the Walkup Account owner.
2. Click on the **Edit** menu.
3. Select **Edit config profile...**

   A panel similar to one in "Creating, Editing, Viewing, and Deleting Profiles," page 37 opens. The operator level panel contains only protocols, no rights or tools.
4. Set the protocol access level:
   - **Checked** box — protocol **available** to an operator.
   - **Un-checked** box — protocol **unavailable** to the operator.
5. Click the **Save** button to save the changes in the operators protocol or discard the changes by closing the window.

3.8 Walkup Account Administration

These administrative functions are controlled at the VnmrJ Admin level. Additional Walkup administration functions are controlled by the Walkup account owner, see "Setting up the Walkup Account," page 68.

- "Adding Operators to a User Account," page 39
- "Setting Operator Default Password," page 40
- "Resetting Operator Password," page 40
- "Setting Panel Levels and Command Line Access," page 41
- "Adding Operators Email," page 41
- "Deleting Operators from User Accounts," page 43
- "Changing the Icon on the Operator Login Screen," page 43

Adding Operators to a User Account

VnmrJ operators can be added to user accounts. Operators are typically added to a Walkup account owner, that is a Walkup account that also has a operating system login. Typically, a Walkup account owner will set up an automation run that the operators will use. Operators can be VnmrJ-only operators or established VnmrJ users.

1. Click **Show all VJ Users** and select the user account to which you want to add operators.
2. Enter the name of each operator that will have NMR privileges in the selected account in the VnmrJ Operator field on the right panel.

   Separate each operator with a space. The operators can have a mixture of VnmrJ only operators and operators with both a operating system and VnmrJ account.

   Operators that are do not have a operating system account are assigned the default password, see "Setting Operator Default Password," page 40. Operators that have a operating system account use their operating system account password to access the VnmrJ operator interface
3. Click **Save User**.

Setting Operator Default Password

Set the default password for VnmrJ operators that *do not have* a operating system login as follows:

1. Select **Configure**.
2. Select **Operators**.
3. Select **Preferences**.

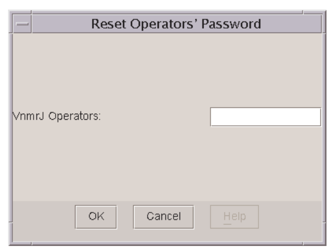
   The Preferences window appears.
4. Enter a **default password** in the password field for operators that do not have a operating system login.

   Operators with a operating system account login use the operating system account password to access the walkup operator interface. Operators, both with and without a operating system account, can change their passwords by selecting Change Password from the Tools menu on their interface, refer to *Walkup VnmrJ* manuals. Change Password will change the both the Operator and operating system login password, if a operating system account exists.
5. Click **OK**.

Resetting Operator Password

This applies only to operators that do not have a operating system (OS) account login.Refer to the OS manual(s) to reset the password for an operator/OS account.

Reset an operator's password to the default password set in "Setting Operator Default Password," page 40, by entering the operator name and clicking OK.



Modifying Operators

- "Opening the Modify Operators Window," page 40
- "Adding Operators Email," page 41
- "Setting Panel Levels and Command Line Access," page 41
- "Adding Operators Full Name," page 42
- "Viewing Command Line Access," page 42
- "Adding or Changing User Profiles," page 42

Opening the Modify Operators Window

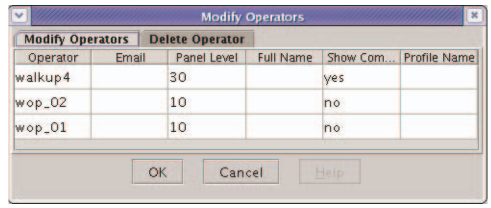
1. Start the VnmrJ Admin interface.
2. Select **Configure**.
3. Select **Operators**.
4. Select **Edit operators**.

   The *Modify Operators* window appears.
5. Select the **Modify Operators** tab.

Adding Operators Email

The operator is notified when a sample is finished if an email address is added. Edit or add an email address as follows.

1. Refer to "Opening the Modify Operators Window," page 40.
2. Edit or add an email address
3. Do one of the following:

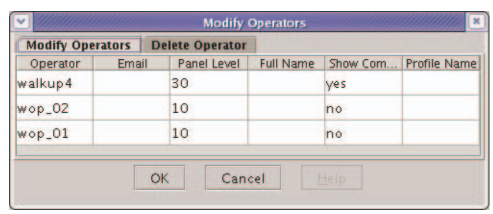


- Continue with "Setting Panel Levels and Command Line Access," page 41.
- Click **OK** to close the Modify Operators window.
- Click **Cancel** to exit the Modify Operators window and make no changes.

Setting Panel Levels and Command Line Access

Setting panel levels are set by the VnmrJ Administrator and determine which VnmrJ interface pages are available under the tabs in the parameter page area. Setting panel levels applies only to walkup account owners and walkup account operators. The default is 10 for operators and 30 for the account owner. Setting the panel level higher makes more pages are available. The only time panel level is changed is during the operator login process in the Walkup interface. The experimental and imaging VnmrJ accounts have a fixed panel level of 100.

1. Refer to "Opening the Modify Operators Window," page 40.
2. Change the panel level for any operator by entering a value in the Panel Level cell for the operator.



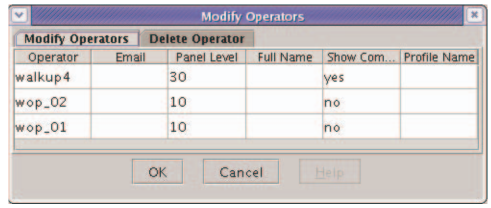
Panel level values and displayed pages are:

Value	*Display*
0-9	show minimum number of pages
10-29	No shim, lock, or processing, and minimal parameter control is available. This may be used for routine automation users and is typical for a basic Walkup user Shim and lock are available only if there is a no sample changer. Basic processing is available. Pages are not fully populated, allowing control of a few basic parameters.
30-100	All pages are available and fully populated. Typical setting for the system owner.

3. Enter **yes** in the field under Show Command Line to give each operator command line access. The default is **no** command line access.
4. Do one of the following:
   - Continue with "Adding Operators Full Name," page 42.
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

Adding Operators Full Name

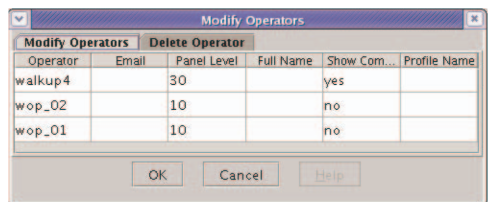
Edit or add a full name as follows.



1. Refer to "Opening the Modify Operators Window," page 40.
2. Edit or add the operators full name in the field below Full Name in the operator's row.
3. Do one of the following:
   - Continue with "Viewing Command Line Access," page 42
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

Viewing Command Line Access

The operator is notified when a sample is finished if an email address is added. Edit or add an email address as follows.

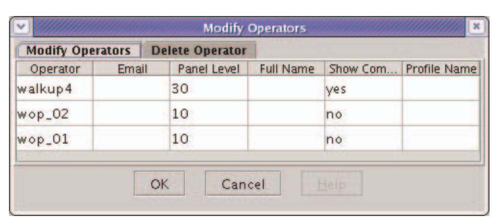


1. Refer to "Opening the Modify Operators Window," page 40
2. The command line access is displayed in the field below Show Command Line in the operator's row.

   Access to the command line is set by either "Setting Panel Levels and Command Line Access," page 41 or by "Adding or Changing User Profiles," page 42.
3. Do one of the following:
   - Continue with "Adding or Changing User Profiles," page 42.
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

Adding or Changing User Profiles

1. Refer to "Creating Operator Profiles," page 36 and either create or edit an existing user profile.
2. Close the Edit User Rights Profile window.
3. Write down the name or names of the user profiles that will be assigned to the operators.



4. Refer to "Opening the Modify Operators Window," page 40
5. Type the name of the profile (with no extension) in the field below Profile in the operator's row.
6. Do one of the following:
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

Deleting Operators from User Accounts

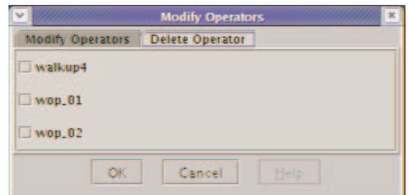
Operators can be removed from all accounts or from a single account.

- Deleting Operators from All Assigned Accounts on page 43
- Deleting An Operator from a Single Account on page 43

Deleting Operators from All Assigned Accounts

1. Select **Configure**.
2. Select **Operators**.
3. Select **Delete operators**.

   The Modify Operators window appears with the Delete Operators tab in front.

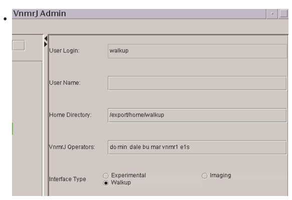


4. **Select the operators** to be removed and click **OK**.

Deleting An Operator from a Single Account

1. Click a user account to select it.

   The operators are listed in the right panel, in the VnmrJ Operators field.
2. Delete the operator(s) from the list.
3. Click **Save User**.



Changing the Icon on the Operator Login Screen

The default operator login window contains the Varian, Inc. logo, which is a GIF file. Change the logo as follows.

1. Select **Configure**.
2. Select **Operators**.
3. Select **Preferences** to display the Preferences window.
4. Enter the complete path to the GIF file.
5. Click **OK**.

3.9 Imaging System Administration

Do the following procedures:

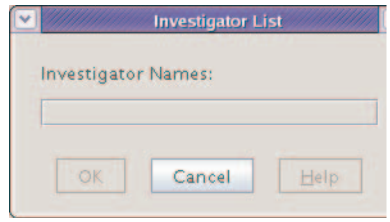
- Set the user account as an imaging experiment type (or imager), refer to "User Account Administration," page 30 for details.
- "Setting Up Investigator List," page 43

Setting Up Investigator List

This procedure is done using the VnmrJ Admin interface.

Investigators used in imaging are selected from the VnmrJ imaging investigator list in the imaging interface after adding investigator names.

1. Select **Configure**.
2. Select **Investigator List** to display the Investigator List window
3. Enter the names separated by spaces.
4. Click **OK**.



3.10 Setting Up Automation Queue.

This procedure applies to the Automation Queue used with the Walkup interface.

1. Select **Configure**.
2. Select **Automation**.

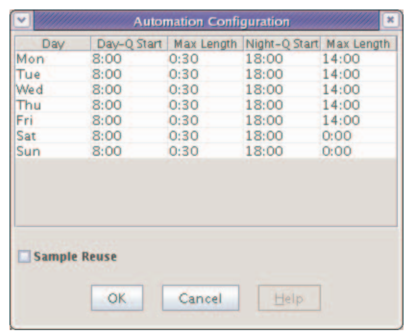
   The Automation Configuration window has the following columns:

   Day — Monday through Sunday

   Day-Q Start — time the daytime sample queue starts and the nighttime sample queue ends

   Max Length — time limit per sample for data acquisition during the daytime acquisition queue for the day of the week in the Day column

   Night-Q Start — nighttime sample queue start and daytime sample queue end time

   Max Length — time limit per sample for data acquisition during the nighttime acquisition queue for the day of the week in the Day column

   The DayQ button is grayed out for samples submitted during the daytime queue period that require acquisition times in excess day queue Max Length time. Click the NightQ button to run the sample during the night queue.

   Setting the Night-Q Start time the same as the Day-Q Start time or setting the Night-Q Max Length to 0:00 set the entire day as a continuation of the previous day's night queue.

3. Enter **times** in *hours:minutes* format and use a 24-hour clock.

   The clock is referenced to the workstation clock.

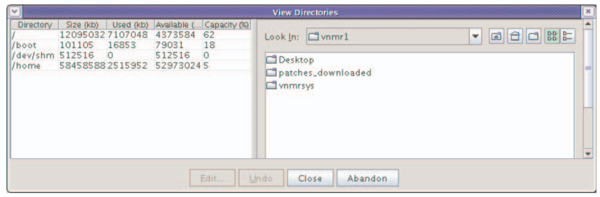
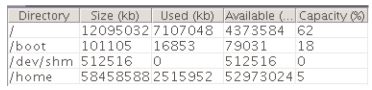
4. Select **Sample Reuse** to reuse sample numbers during an automation run.
5. Click **OK** to create the automation queue.

   Or click **Cancel** to close the window without creating an automation queue.

3.11 Viewing the File System

VnmrJ Admin interface lower right panel shows information about the operating system.

Select Directory tab has the following icons:

<table>
<tr><th>Icon/Button/Instruction</th><th>Description or Window</th></tr>
<tr><td>1. Select UNIX.
2. Select File System.
The View Directories window opens.</td><td>
</td></tr>
<tr><td>Disk space window</td><td>
<table>
<tr><th>Directory</th><th>Size (kb)</th><th>Used (kb)</th><th>Available (...</th><th>Capacity (%)</th></tr>
<tr><td>/</td><td>12095032</td><td>7107048</td><td>4373584</td><td>62</td></tr>
<tr><td>/boot</td><td>101105</td><td>16853</td><td>79031</td><td>18</td></tr>
<tr><td>/dev/shm</td><td>512516</td><td>0</td><td>512516</td><td>0</td></tr>
<tr><td>/home</td><td>58458588</td><td>2515952</td><td>52973024</td><td>5</td></tr>
</table>
Disk space window displays information about disk partitions, size, space used, space available, capacity available. The same information is displayed about any mounted network directories.
The same information is also shown when the Disk Space tab is in the VnmrJ Admin Interface is selected.</td></tr>
<tr><td></td><td>Change directory to selected directory.</td></tr>
<tr><td></td><td>Go to admin’s <code>/home</code> directory.</td></tr>
<tr><td></td><td>Create a new directory in the current directory.</td></tr>
<tr><td></td><td>List files with small icons</td></tr>
<tr><td></td><td>List files with small icons and details</td></tr>
<tr><td>Look In drop down menu</td><td>Select a directory from the drop down list.
Click on a directory in the directories window to select a directory. The directory is inserted in the empty directory field of user directories, see “User Directories,” page 35.</td></tr>
</table>

Chapter 4. VnmrJ Printers and Plotters

Sections in this chapter:

- 4.1 "Opening the ADD Printer/Plotter Window," this page
- 4.2 "Setting up Printers and Plotters," page 48
- 4.3 "Removing Printers and Plotters," page 50
- 4.4 "Viewing Installed Printers and Plotters," page 51

Printer and plotter management is done by the VnmrJ administrator (typically vnmr1), using ADD Printer/Plotter window, see Figure 4.

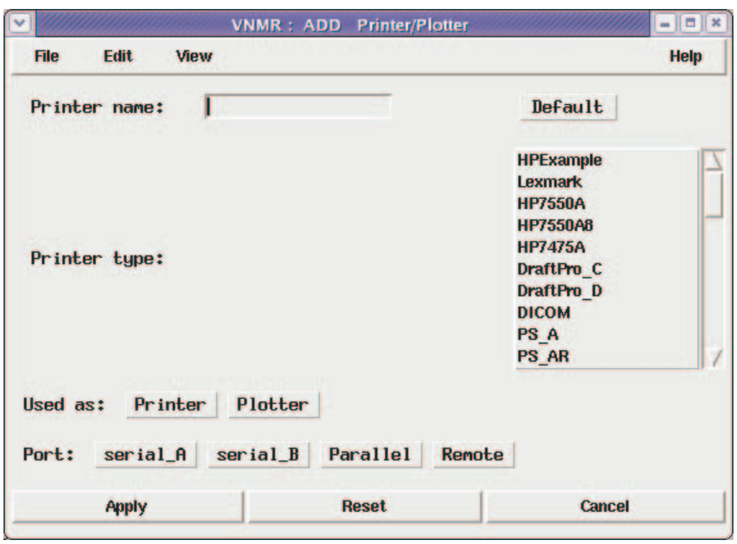


Figure 4. Add Printer / Plotter window

4.1 Opening the ADD Printer/Plotter Window

Open the ADD Printer/Plotter window from the VnmrJ Admin interface or a terminal.

Using VnmrJ Admin

1. Click on the **VnmrJ Admin** icon.
2. Click on **Management**.
3. Select **Printers...** to open the tool.

Using a Terminal Window

1. Open a terminal console window and enter **su** to become `root`.
2. Change to the `/vnmr/bin` directory.
   `#` **`cd /vnmr/bin`**
3. Type the command **`adddevices`** to open the tool.
   `#` **`./adddevices`**

4.2 Setting up Printers and Plotters

1. Select **Printer…** from the **File** menu in the VNMR:Add Printer/Plotter window to select a printer from a list of currently configured printers.
   `Quit` is the only option if there are no printers or plotter currently configured, continue with step 2.
2. Enter in the printer name in the **Printer name** field.
3. Select a VnmrJ printer or plotter type from the list by double-clicking on your choice from the scrolling list in the window. These types are described in Table 4.
4. Click the **Default** button if this device is to be the default printer.
   Designate one printer as the default printer.

Table 4. VnmrJ Printer and Plotter Types with Descriptions

VnmrJ Device Types	*Descriptions*
HP7475A	HP7475 plotter
HP7550A	HP7550 plotter using 11x17 inch paper
HP7550A8	HP7550 plotter using 8 1/2 x 11 inch paper
DeskJet_300	HP DeskJet using 300 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
DeskJet_300R	HP DeskJet using 300 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
DraftPro_C	HP DraftPro plotter using size C paper
DraftPro_D	HP DraftPro plotter using size D paper
DraftMaster_A	HP DraftMaster plotter using size A paper
DraftMaster_B	HP DraftMaster plotter using size B paper
DraftMaster_C	HP DraftMaster plotter using size C paper
DraftMaster_D	HP DraftMaster plotter using size D paper
DraftMaster_E	HP DraftMaster plotter using size E paper
LaserJet_150	HP LaserJet (or DeskJet) using 150 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
LaserJet_150R	HP LaserJet (or DeskJet) using 150 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LaserJet_300	HP LaserJet (or DeskJet) using 300 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.

Table 4. VnmrJ Printer and Plotter Types with Descriptions (continued)

VnmrJ Device Types	*Descriptions*
LaserJet_300R	HP LaserJet (or DeskJet) using 300 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_B_300R	HP LaserJet (or DeskJet) using 300 dpi, B-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_300R	HP LaserJet (or DeskJet) using 300 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_300R	HP LaserJet (or DeskJet) using 300 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LaserJet_4550	HP Color LaserJet using 600 dpi.
LaserJet_600R	HP LaserJet (or DeskJet) using 600 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_B_600R	HP LaserJet (or DeskJet) using 600 dpi, B-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_600R	HP LaserJet (or DeskJet) using 600 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
PS_A	PostScript printer using vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value is not recommended.
PS_AR	PostScript printer (e.g., PS4069) using horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
PS4079_HPGL	Lexmark PS4079 or PS4079plus using 11x17 inch paper in HPGL mode. HPGL mode is required for color output.
QuietJet_96	HP QuietJet using low 96 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
QuietJet_96R	HP QuietJet using 96 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
QuietJet_192	HP QuietJet using 192 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
QuietJet_192R	HP QuietJet using 192 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
ThinkJet_96	HP ThinkJet using 96 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
ThinkJet_96R	HP ThinkJet using 96 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
ThinkJet_192	HP ThinkJet using 192 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
ThinkJet_192R	HP ThinkJet using 192 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.

5. Next to **Used as**, select whether the devices will be used as a Printer or Plotter.
6. Next to **Port**, select how the device is connected to the host computer:
   - Serial port A — Click **/dev/term/a**.

Serial port B — Click **/dev/term/b**.

A list of Baud rates appears below the Port: selections. Select the appropriate baud rate for your device.

- Parallel port — Click **Parallel**.
- Remote printer — Click **Remote**.

  Two more fields appear below the **Port** selections.

  Remote host name— enter the name of the host that is connected to the printer to use. This host must known to your computer.

  Remote host OS — click the button that represents the OS of the remote host is running. If the remote host is running Solaris, IRIX, or AIX, click **System V**. If the remote host is running SunOS, click **BSD**.

7. Click **Apply** after filling in all the fields in the VNMR: Add Printer/Plotter window.

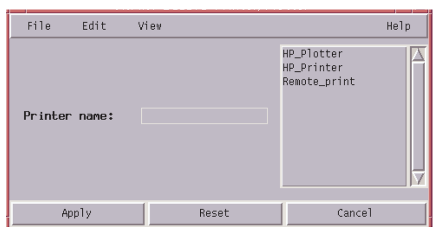
   The device is added to the VnmrJ `devicenames` file. The device is also added to appropriate places in operating system's printer service.

8. Add another printer or plotter by selecting **Edit**, then **Add Printer**, and repeating this procedure.

9. Click on **File** on the main menu of the VNMR: Add Printer/Plotter window and select **`Quit`** to close the window.

4.3 Removing Printers and Plotters

This section describes how to delete a printer or plotter that was added using the Add Printer/ Plotter tool. Printers added with the AdminTool will not be deleted. Use the AdminTool to delete unwanted printers.



1. Open the Add Printer/Plotter tool as described in "Opening the ADD Printer/ Plotter Window," page 47.

2. Select **Edit** from the main menu, then **Delete Printer**.

   The DELETE Printers/Plotters window appears. The list on the right side of the window shows the printers and plotters set up on the system.

3. Double-click the printer or plotter in the list to delete.

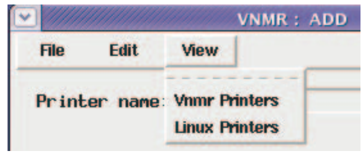
   The name of the device appears next to **Printer name**.

4. Click **Apply** to delete the printer or plotter.

4.4 Viewing Installed Printers and Plotters

This section describes how to view printers and plotters are installed on the system.

1. Open the Add Printer/Plotter tool, see "Opening the ADD Printer/Plotter Window," page 47.
2. Click the **View** menu.
3. Select **Vnmr Printers** from the **View** menu.



4. A list appears similar to the example in Figure 5.
5. Select **(operating system) Printers** from the **View** menu to view the operating system printers. A window similar to the example in Figure 6 appears. This window might pause for a few seconds as operating system obtains status information about various output devices and remote hosts.

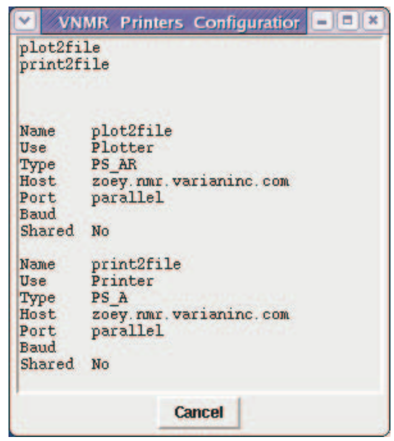


Figure 5. VnmrJ Printers View Window

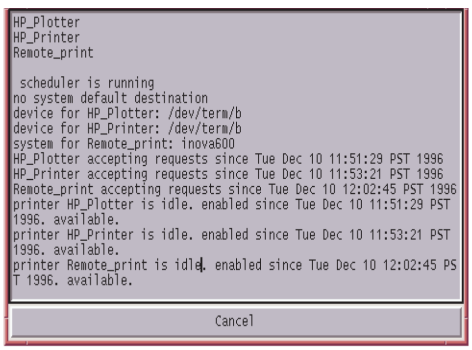


Figure 6. OS Printers View Window

Chapter 5. Automated Hardware

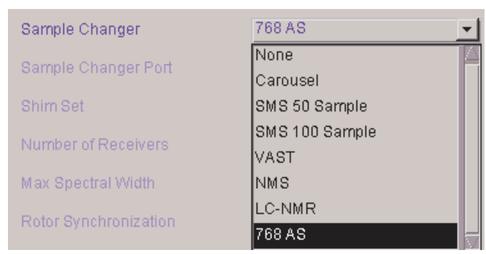
Sections in this chapter:

- 5.1 “Setting Up Automated Sample Handling,” page 53
- 5.2 “Setting Up ProTune,” page 54

This section provides general instructions for configuring the software when using the Walkup interface to control automated hardware such as sample handlers and automated probe tuning. Most of the set up procedures require system hardware administration access, typically as vnmr1, and some procedures require vnmrj system administrator access.

5.1 Setting Up Automated Sample Handling

1. Log in as the system hardware administrator, typically vnmr1.
2. Click on **Edit** on the main menu.
3. Select **System Settings**.
4. Click on the **System config** button.
5. Click on the drop down menu next to the Sample Changer field and select a sample changer option.



6. Click on the drop down menu next to the Sample Changer Port field.
7. Select a sample changer port:
   Click on the drop down menu next to the Sample Changer Port field.

SMS 50, 100, NMS, Carousel	Select Com1
768-AS	Select Ethernet
LC-NMR	Select Ethernet
Not used or no sample handler	Not Used

Operating and other instructions specific to an automated sample handing option are contained in one of the following manuals:.

Option	*Related manual*
SMS 50, 100, NMS, Carousel	*VnmrJ Walkup NMR*
768 AS	*768AS Sample Management System*
LC-NMR	*LC-NMR/MS*

8. Click **OK**.
9. Set up the day and night queue times, see “Setting Up Automation Queue.,” page 44.

5.2 Setting Up ProTune

Configuring the Software for ProTune

1. Log in as the system hardware administrator, typically vnmr1.
2. Click on **Edit** on the main menu.
3. Select **System Setting**s.
4. Click on the **System config** button.
5. Select **Present** from the drop down menu next to the Protune field.
6. Continue with "Loading ProTune chan# and motor# Persistence Files," page 54.

Loading ProTune chan# and motor# Persistence Files

AutoX probes ship with a CD containing Persistence files (six chan# and six motor#) specific to that probe. These files characterize the probe for the ProTune accessory and are used the first time the probe is automatically tuned.

Load the Persistence files as follows:

1. Insert the CD with probe Persistence files into the CD ROM drive.
2. Open a terminal window and do one of the following:

   Locate the system probe file.

   a. type
      ```
      cd /vnmr/probes
      ls
      ```
   b. Write down the <name of probe file>.
   c. Continue with step 3.

   Create a probe system file

   a. Follow the procedure in "Setting Up the Probe Calibration File," page 85.
   b. type
      ```
      cd /vnmr/probes
      ls
      ```
   c. Verify and write down the <name of probe file>.
   d. Continue with step 3.

3. type
   ```
   cd /vnmr/tune
   mkdir <name of probe file>
   ```
4. Change to the CDROM directory and type one of the following:
   ```
   cd /media/cdrecorder
   ```
5. Copy the Persistence files from the CDROM to the probe directory you made:

   Type: `cp * /vnmr/tune/ProbeName`
6. Verify that the files were copied.

Type: `ls /vnmr/tune/ProbeName`

The new `ProbeName` directory should contain six chan# files (chan#0 through chan#5) and six motor# files (motor#0 through motor#5).

Protune software copies the probe Persistence files to the directory; `~user/vnmrsys/tune,` the first time it is run by a user. The directory is created if it does not already exist. A database of reference values is maintained in the local directory.

Chapter 6. VnmrJ Accounting Administration

Sections in this chapter:

- 6.1 "VnmrJ Accounting Tool," this page
- 6.2 "VnmrJ Accounting Procedures," page 59

6.1 VnmrJ Accounting Tool

The VnmrJ Accounting tool provides NMR administrators with an easy way to keep a log of VnmrJ users. The program gives you the following capabilities:

- Create groups of console users with single-rate or multi-rate billing.
- Calculate special rates on days identified as holidays on a calendar.
- Show and print lists and accounting reports.

Opening the Accounting Tool

The accounting tool window, similar to the one shown in Figure 7, can be opened from either the *VnmrJ Admin* interface or from a terminal window.

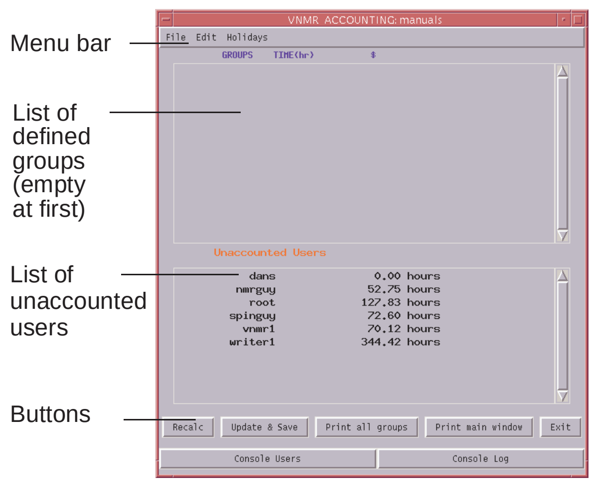


Figure 7. VNMR Accounting Window

Opening from the *VnmrJ Admin* interface:

1. Click **Management** in the main menu.
2. Select **Cost/Time Accounting**.

Opening from an OS terminal window:

1. Open a terminal window and log in as **`root`**.
2. Enter the command: **`/vnmr/bin/vnmr_accounting`**

Note: Users other than `root` can look at the accounting tool entries by opening a terminal window and starting the program but they cannot make changes to the data.

Navigating the VNMR Accounting Tool

The VNMR Accounting tool, shown in Figure 7, consists of:

- "Menu Bar," next
- "Lists of Groups and Unaccounted Users," page 58
- "Buttons," page 58

Menu Bar

The top of the window has a menu bar with the following options, each of which can be clicked to show a submenu:

File	Select printer and print options or exit the accounting program.
Edit	Add or delete groups and users.
Holidays	Assign holidays for billing purposes.

Lists of Groups and Unaccounted Users

The middle of the window has two panes listing accounting groups and unaccounted users:

Defined Groups	The upper pane shows a list of accounting groups defined by the program, with the amount of time and the charges for each group. This list only appears if all users have been added to a group.
Unaccounted Users	Users who have not been added to a group appear in the lower list. The first time the accounting program is run only unaccounted users are listed because no groups have yet been added and the accounting window is similar to Figure 7. The first column identifies the VNMR user. The second column lists the total amount of time, in minutes, that user was logged on to the system. Use of VNMR by unaccounted users is reported as time-only because these users have no cost structure associated with them.

Buttons

The bottom of the window has two rows of buttons:

Recalc	Recalculates all accounts.
Update & Save	Saves all accounting information in the directory `/var/adm` and resets accounting logs.
Print All Groups	Prints a summary of charges for each group.
Print Main Window	Prints a summary of all charges.
Exit	Exits the accounting program.
Console Users	Displays a list of console users. Double-clicking on a line in the display opens a detailed window showing the user's activity.
Console Log	Displays a window of system use, sorted chronologically.

6.2 VnmrJ Accounting Procedures

- "Setting Up Billing Rates," next
- "Adding Users to Groups," page 63
- "Calculating Billing Information," page 61
- "User and Group Information and Lists," page 62
- "Generating Reports," page 62
- "Managing Groups and Group Members," page 63
- "Updating and Saving Records," page 64
- "Exiting the Accounting Program," page 64

Setting Up Billing Rates

- "Multiple-rate Groups," this page
- "Weekday Rate," page 60
- "Weekend Rate," page 60
- "Holiday Rate," page 61

Single-Rate Users

To set up groups of single-rate users do the following:

1. Click **Edit** from the main menu and select **Add_Group**.
2. Type the name of the new accounting group (`Standard` in this example) in the **Group name** field in the window shown in Figure 8.

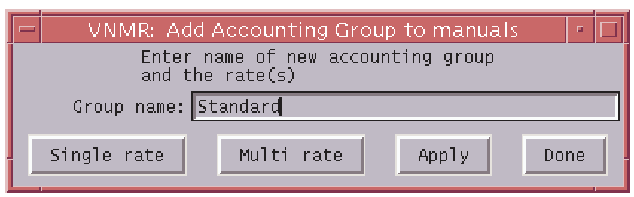


Figure 8. Add Accounting Group Window

3. Click the **Single rate** button to set a single billing rate for the group Standard.

   A window opens similar to Figure 9.

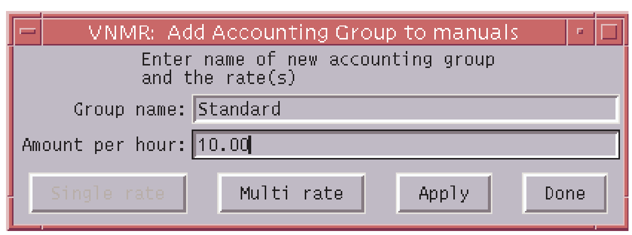


Figure 9. Add Group Window, Single Rate

4. Enter the hourly rate in the **Amount per hour** field and click the **Apply** button. The upper pane now lists the group Standard.
5. Repeats steps 2 and 3 to add additional single-rate groups. Each group is listed in the upper pane.
6. Click the **Done** button when all the groups are added.

Tip: To simplify accounting for the `root` user, set up a group named Maintenance with 0 as the charged rate and assign `root` to this group.

Multiple-rate Groups

Set up a multiple-rate group as follows for each group:

1. Click **Edit** in the main menu and select **Add_Group**.
2. Type the name of the new accounting group (`Special` in this example) in the **Group name** field.
3. Click the **Multi rate** button.

   A window opens similar to Figure 10.

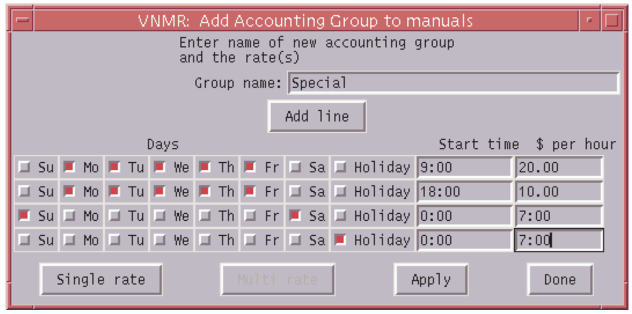


Figure 10. Add Group Window, Multi Rate

Set the days, times, and rates for the group, for example:

- From 9:00 a.m. to 5:59 p.m. on weekdays, time is billed at $20.00 per hour.
- Weekday evening time is billed at $10.00 per hour.
- Weekends (Saturday and Sunday) are billed at $7.00 per hour.
- Holidays are also billed at $7.00 per hour.

Weekday Rate

1. Set up weekday day time:
   a. Click the **Add line** button once.
   b. Click **Mo**, **Tu**, **We**, **Th**, and **Fr** in the top line.
   c. Enter a time (**9:00** for example) in the **Start time** field.
2. Set the weekday day time billing rate (**20.00** for example) in the **$ per hour** field.
3. Set up the weekday night time:
   a. Click **Mo**, **Tu**, **We**, **Th**, and **Fr** in the next line down.
   b. Enter a time (**18:00** for example) in the **Start time** field.
4. Set the weekday night time billing rate (**10.00** for example) in the **$ per hour** field.
5. Add as many rates as required by clicking the **Add line** button.
6. Click **Done** when all weekday rates are set.

Weekend Rate

1. Set up weekend time:
   a. Click the **Add line** button once.
   b. Click **Su** and **Sa** in the new line.
   c. Enter a time (**0:00** for example) in the **Start time** field.
2. Set the weekend time rate (**7.00** for example) in the **$ per hour** field.

   Note that the billing rate begins at the start time and runs until the next start time. Therefore, billing for Sunday night to Monday morning is at $7.00 per hour until 8:59 a.m. on Monday. Monday night billing (starting at 6:00 p.m. at $10.00 per hour) runs through to 8:59 a.m. Tuesday. It is not necessary to start an accounting day at 0:00; the preceding day continues until the first change.

Holiday Rate

1. Set up holiday time:
   a. Click the **Add line** button once.
   b. Click **Holiday** in the new line.
   c. Enter a time (**0:00** for example) in the **Start time** field.
2. Set the weekend time rate (**7.00** for example) in the **$ per hour** field.
3. Click the **Apply** button.
4. Set up any additional multiple rate groups by repeating each of the steps in "Multiple-rate Groups," page 60.
5. Click the **Done** button when all multiple rate groups are set up.

Designating Holidays

The multiple-rate group supports a holiday billing rate. Designate the days that are holidays as follows:

1. Click **Holidays** in the main menu and select **Add**.

   A monthly calendar similar to Figure 11 appears:

   The current day's date appears as a large, bold number. Use the arrows at the top of the window move the calendar forward and backward. Click the **Today** button and return to the current day's date.

2. Left mouse button click each day to designated the day as a holiday. Designated holiday dates change to red. There is no limit to the number of days that can be assign as a holiday.

Figure 11. Assign Holidays Window

3. Continue month by month as far ahead as needed.
4. Click the **Save** button and then the **Quit** button when done.

Calculating Billing Information

1. Click the **Recalc** button.

   Progress is displayed on the main screen. If there are many entries to be processed, this process can be time-consuming.

2. Click **Recalc** to update billing information —accounts are not automatically updated.

User and Group Information and Lists

- "Seeing a List of Users and Groups," next
- "Seeing Detailed User Information," next
- "Seeing a Chronological User Log," next

Seeing a List of Users and Groups

1. Click the **Console Users** button in the accounting window. A window, similar to Figure 16, appears with a list of established groups displayed in the top pane.
2. Double-click the name of the group to see more information about any group listed.

Seeing Detailed User Information

To see a list of console users and user information do the following:

1. Click the **Console Users** button in the accounting window. A window, similar to Figure 16.
2. Double-click the name of the group to open a window similar to Figure 12.

   User information includes login names, the day, month, and year that users were logged in; login and logout times, in hours and minutes; and a total of the time users were logged on to the console. This information is the most recent data since the last calculation of time and expenditure summaries for the known groups.

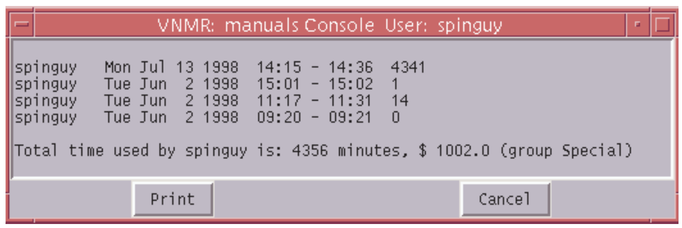


Figure 12. Console Users Window for a Selected User

Seeing a Chronological User Log

1. Click the **Console Log** button in the accounting window.
2. A chronological log of console use by each user similar to Figure 13, opens.

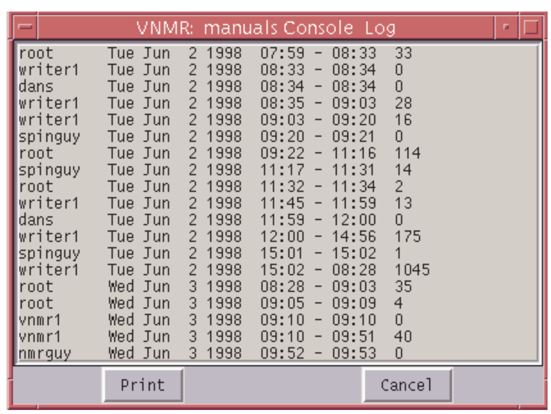


Figure 13. Console Log Window

Generating Reports

- "Seeing and Printing Reports," next
- "Selecting A Printer," next

Seeing and Printing Reports

1. Click the **Print all groups** button in the accounting window to see and print individual summaries for each group.

2. Click the **Print main window** button to print a summary of individual charges.

Selecting A Printer

To select a printer for reports do the following:

1. Click the **File** in the main menu and select **Printer** to open a Printer Selection window similar to Figure 14.
2. Enter the name of a printer known to his system in the **Printer** field. The default is `lp`.

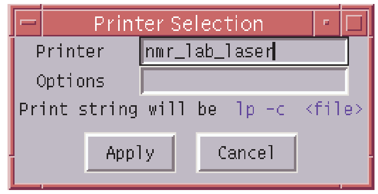


Figure 14. Printer Selection Window

3. Enters print options (if any) in the **Options** field.
4. Click **Apply** — printer selection remains current until the program quit.

Managing Groups and Group Members

- "Adding Users to Groups," next
- "Adding Users to an Existing Group," page 64
- "Deleting a User from a Group," page 64
- "Deleting a Group," page 64

Adding Users to Groups

Add users as either individuals or as members of a group. An easy way to define users as individuals is to create a group with the same name as the user and only assign that single user to the group (e.g., Bob Smith is the only member in the group Bob Smith). After a group is added, its name appears in the upper pane. Add users to the group as follows:

1. Click **Edit** in the main menu and select **Add_User**.

   A window, similar to Figure 15, opens.
2. Type **`Standard`** in the **Group name** field.
3. Enter the user name in the **User name** field and click the **Apply** button.

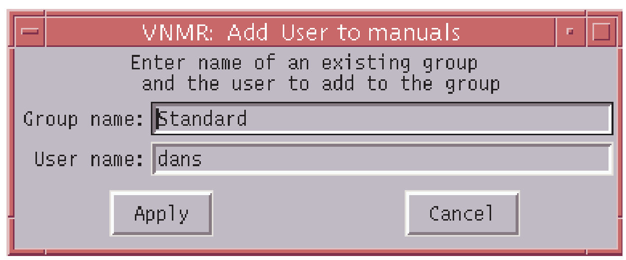
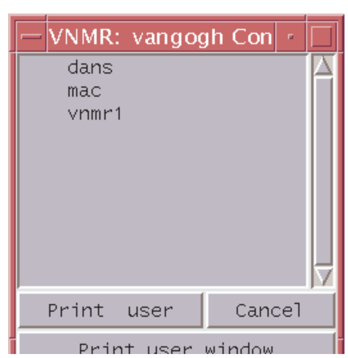


Figure 15. Add User Window

4. Repeat step 3 to add the next user.

Repeats steps 2 and 3 for each group until each user is in a group.



As users are assigned to a group, their names are removed from the Unaccounted Users list. If all users are assigned to a group, no names should appear in the Unaccounted Users pane. Assigning all users is recommended because it makes it easy to identify any unauthorized spectrometer access, because unauthorized users will appear in the Unaccounted User pane.

Adding Users to an Existing Group

To add one or more users to an existing group, do the following:

1. Click **Edit** in the main menu and select **Add_User** to open a window similar to Figure 15.
2. Type the name of the accounting group in the **Group name** field.
3. Type the name of the name of a user to add to the group in the **User name** field.

   To enter multiple users, separates each name with a space.
4. Click the **Apply** button to save his changes.

Deleting a User from a Group

To delete a user from an accounting group, do the following:

1. Click **Edit** in the main menu and select **Delete_User**.
2. Enter the name of the group from which the user is to be deleted in the **Group name** field.
3. Enter the name of the user to be deleted from the group in the **User name** field.
4. Click the **Apply** button.
5. If the group will be deleted, repeat this process until all the users in the group are removed.

Deleting a Group

To delete an empty accounting group, do the following:

1. Click **Edit** in the main menu and select **Delete_Group**.
2. Select the group to be deleted in the **Group name** field.

   Each member of the group must be deleted first before the group can be deleted.
3. Click the **Apply** button.

Updating and Saving Records

Updating and saving records is an administrative option available *only* to `root` users. This feature prevents users other than `root` from editing accounting records. To update and save records do the following:

1. Log in as **`root`**.
2. Click the **Update & Save** button.

   The information is saved in the `/var/adm` directory as the file `wtmp.mm.dd.yy` and the accounting logs are reset.

Exiting the Accounting Program

Click the **Exit** button OR select **File** from the main menu, then **Quit** to exit the program.

Chapter 7. VnmrJ User Account Administration

Sections in this chapter:

- 7.1 “Setting User Defined Templates,” page 65
- 7.2 “Setting Viewports,” page 67
- 7.3 “Setting up the Walkup Account,” page 68
- 7.4 “Setting Up the Imaging System,” page 72

This chapter covers the administration procedures executed within a user account to set up or customize the user account functions. These functions are set by the individual accounts and do not use the VnmrJ Admin interface.

7.1 Setting User Defined Templates

- “Opening the SaveData Setup Window,” page 66
- “Setting Up or Removing a Data Directory,” page 70
- “Setting Up or Removing a Study Name Template,” page 70

The directory and templates used with the Experimental interface to select where the data is saved and the file name) is set up using the Save Data Setup window shown in Figure 17.

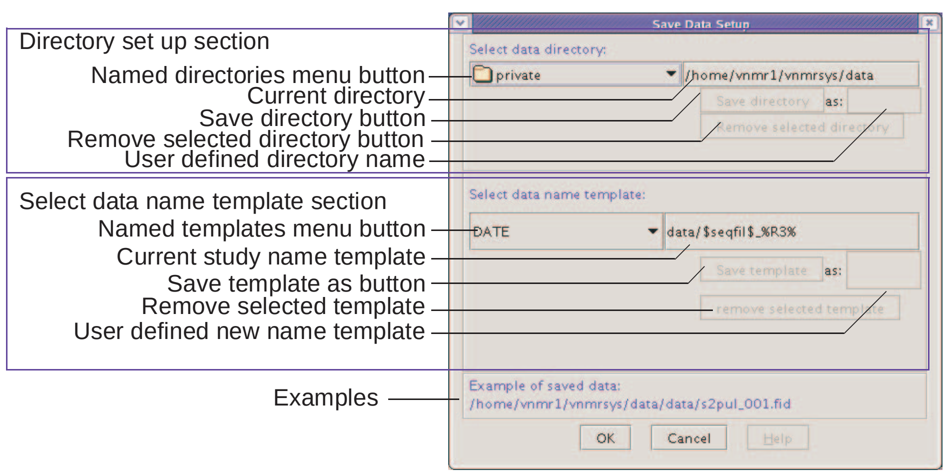


Figure 17. Save Data Setup Window, VnmrJ Administrator

Additional options are available to the walkup account for automation and automated sample handling. The full procedure for the walkup account is provided in *VnmrJ Walkup NMR* manual.

Opening the SaveData Setup Window

1. Click on **File**.
2. Select **Save data setup …**
3. Review the current directory and templates selections and do one of the following:
   - Click on the **Cancel** button to exit and make no changes.
   - Continue with "Setting Up or Removing a Data Directory," page 70.

Setting Up or Removing a Data Directory

VnmrJ default data saving templates includes DATE (producing filenames such as `20040921_01.fid`) and seqfil (e.g. `HMQC_01.fid`).

Specify data is saved using the controls in the Directory set up section of the Save Data Setup window, see Figure 18, using the following procedures as required:

Use an Existing Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Data Directory

1. Modify the existing directory path shown in **Current directory** field or enter a new full path in the **Current directory** field.
2. Press **Enter**.

   The *Current directory* field and *Save Directory* button are not active until the Enter key is pressed.
3. Enter a name for the new data directory path in the **User defined directory name** field.
4. Click on the **Save directory** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Data Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Click on the **Remove selected directory** button.

Setting Up or Removing a Name Template

The automation run data is named using the template set up section in the Name Template of the Save Data Setup window, see Figure 18. Define the template using one of the following procedures:

Use an Existing Name Template

1. Click on the **Named templates** menu button.

2. Select a named directory from the drop down menu of named directories:
   - DATE
   - data/$seqfil$_%R3%
   - date
   - seqfil
   - solvent
3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Name Template

1. Modify the existing directory path shown in **Current named template** field or enter a new study template in the **Current named template** field.
2. Press **Enter**.

   The *Current named template* field and *Save templates* button are not active until the Enter key is pressed.
3. Enter a name for the new data template in the **User defined new template name** field.
4. Click on the **Save template** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Name Template

1. Click on the **Named templates** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Click on the **Remove selected template** button.

7.2 Setting Viewports

1. Click the **VnmrJ** icon or enter **`vnmrj`** in the Terminal window if VnmrJ is not started.
2. Click on **Edit** on the main menu.
3. Select **Viewports…** to open the Viewports settings window.
4. Click on a **radio button** under **viewports** next to the number of viewports to create.

   A maximum of nine viewports can be created. Each viewport created is added to the vertical tool bar Viewport tab.
5. Check the box next to **Switch Layout for Viewport** to allow each viewport to have a different layout.
6. Options:
   - Keep the default workspace number or enter a custom name.
   - Keep the default label or enter custom label.

Suggested Viewport Settings

- **Liquids systems**

a. Select up to 9 viewports.

b. Select **Switch Layout for Viewports** to switch the layout of VnmrJ to the last viewed layout of a specific viewport.

c. Click **Close**.

- **Imaging systems** — set the initial viewports as follows.

a. Select **Viewports** from the **Edit** menu.

b. Click on **radio button 3** to set default viewports.

c. Click **Close**.

7.3 Setting up the Walkup Account

- "Walkup Interface Types," page 68
- "Location of Operator Data," page 68
- "Set Up Studies and Data Saving," page 69

Walkup Interface Types

Walkup Account owner – The walkup account owner is a user or users created in "Creating a Single New User Account," page 31 and "Creating Multiple New User Accounts," page 32, has an operating system login, and owns the account and any automation runs started while logged in. All default operations that occur during an automation run (shimming, locking, etc.) are set up by this user before the automation run is started. Refer to the manual *VnmrJ Walkup* for a full description of the Walkup interface the administrator account functions.

Walkup Operator – The walkup operator has VnmrJ access via a user name and password and is not a operating system login (the operator may have operating system level privileges for other accounts) and therefore does not own any of the files in the account. All default operations that occur during an automation run (shimming, locking, etc.) are first set up by the walkup administrator before the automation run is started. Refer to the manual *VnmrJ Walkup* for a full description of the Walkup interface the operator account functions.

Location of Operator Data

Operator data is saved as defined in the Save data setup window. Open the Save date setup window from the *Walkup account owner interface* by clicking **Edit** on the main menu bar and selecting **Save data setup**. The Save data setup window sets the following parameters:

Directory/Template	*Parameter*
Automation directory	`globalauto`
Study name template	`sqname`
File name template	`autoname`

The `walkup` macro runs and sets `autodir` from `globalauto`, plus the date (`autodir=globalauto +'/auto_' + $date`) when the Walkup account owner selects File -> New automation run. Parameters such as `$operator` are not substituted in the `walkup` macro.

After the user adds some protocols, the *Submit* buttons use `autodir+'/'sqname` to create the study name for each sample, which sets `sqdir` (full path to the study) and `stydyid` (a string parameter relative to autodir), then the value of `studyid` is not relative to `autodir`, and is the full path to the study.

Data is saved in automation using `autoname`, which is relative to `autodir`, unless it is an absolute path. The default values of `autoname` in the *Save data setup* window all start with `$studyid$`, which puts them within the `studyid` directory. This works whether studyid is a relative or absolute path.

Set Up Studies and Data Saving

The directory and templates used with automated sample handling systems (and for walkup operation where the operator does not have the option to select where the data is saved and the file name) is set up using the **Save Data Setup** window, **Study Data** tab, shown in Figure 18.

- "Opening the SaveData Setup Window," page 66
- "Setting Up or Removing a Data Directory," page 66
- "Setting Up or Removing a Name Template," page 66

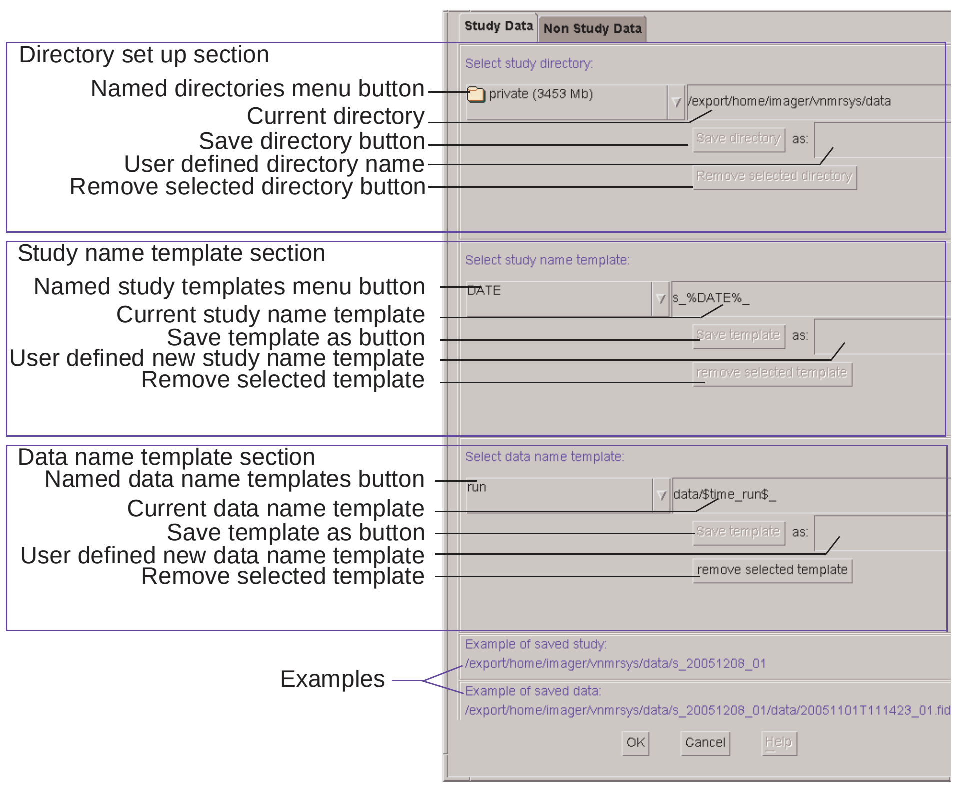


Figure 18. Save Data Setup Window, Walkup User

Open the Save Data Setup Window

1. Click on **File**.
2. Select **Save data setup …**
3. Review the current directory and templates selections and do one of the following:
   - Click on the **Cancel** button to exit and make no changes.
   - Continue with "Setting Up or Removing a Data Directory," page 70.

Setting Up or Removing a Data Directory

The automation run data is saved using the controls in the Directory set up section of the Save Data Setup window, see Figure 18, using any of the following procedures as required:

Use an Existing Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Data Directory

1. Modify the existing directory path shown in **Current directory** field or enter a new full path in the **Current directory** field.
2. Press **Enter**.

   The *Current directory* field and *Save Directory* button are not active until the Enter key is pressed.
3. Enter a name for the new data directory path in the **User defined directory name** field.
4. Click on the **Save directory** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Data Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the drop down menu of named directories.C
3. Click on the **Remove selected directory** button.

Setting Up or Removing a Study Name Template

The automation run data is named using the template set up section (no present on the **Non Study Data** tab) in the Study Name Template of the Save Data Setup window, see Figure 18, using any of the following procedures as required:

Use an Existing Study Name Template

1. Click on the **Named study templates** menu button.
2. Select a named directory from the drop down menu of named directories:
   - data/$seqfil$_%R3%
   - pslabel

- solvent
- time_run

3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Study Name Template

1. Modify the existing directory path shown in **Current named study template** field or enter a new study template in the **Current named study template** field. Refer to "Location of Operator Data," page 68 for a details about the parameter related to this template.
2. Press **Enter**.

   The *Current named study template* field and *Save templates* button are not active until the Enter key is pressed.
3. Enter a name for the new data template in the **User defined new study template name** field.
4. Click on the **Save template** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Study Name Template

1. Click on the **Named study templates** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Click on the **Remove selected template** button.

Setting Up or Removing a Data Name Template

The automation run data is named using the template set up in the Data name template section of the Save Data Setup window, see Figure 18, using any of the following procedures as required:

Use an Existing Study Name Template

1. Click on the **Named data name templates** menu button.
2. Select a named directory from the drop down menu of named directories.
   - comment
   - run
   - seqfil
3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Data Name Template

1. **Modify** the existing template shown in *User defined new data name template* field **or enter a new template** in the *User defined new data name template* field. Refer to "Location of Operator Data," page 68 for a details about the parameter related to this template.
2. Press **Enter**.

   The *User defined new data name template field* and *Save Directory* button are not active until the **Enter** key is pressed.

3. Enter a name for the new data directory path in the **User defined new data name template** field.
4. Click on the **Save template** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Data Name Template

1. Click on the **Named data name templates** menu button.
2. Select a named template from the drop down menu of named templates.
3. Click on the **Remove selected template** button.

The software is now configured for walkup.

7.4 Setting Up the Imaging System

1. Start VnmrJ as the system administrator (typically vnmr1).

   Enter **`vnmrj`** in the Terminal window or click on the VnmrJ icon.
2. Do each of the following:
   - "Set the Macro and Menu Path," page 72
   - "Set Up the Database," page 72
   - "Location of Investigator Data," page 73
   - "Setting Viewports," page 67

Set the Macro and Menu Path

Most of the imaging macros are located in the subdirectory `maclib.imaging` of `/vnmr/maclib`. The value of the parameter `appmode`, a global parameter that each user can set, sets the global parameters `sysmaclibpath` and `sysmenulibpath` to the following paths:

- `sysmaclibpath` is set to `'/vnmr/maclib/maclib.imaging'`
- `sysmenulibpath` set to `'/vnmr/menulib/menulib.imaging'`

Set the `appmode` parameter as follows:

1. Click on **Tools** on the main menu bar.
2. Select the **System Settings** window.
3. Select imaging from the **Application** mode drop down menu.
4. Click **OK.**

Set Up the Database

If the Locator shows **Error** under the column headings, or if the error message `DataBase contents version is not correct ...` appears on the bottom of the screen, exit VnmrJ, log in as the VnmrJ administrator (e.g., vnmr1) and run **`dbsetup`** in a terminal window.

Setting up the Studies and Data Saving Templates for Imaging

The directory and templates used with studies are set up using the **Save Data Setup** window, **Study Data** tab, shown in Figure 18.

- “Location of Investigator Data,” page 73
- “Open the Imaging Save Data Setup Window,” page 74
- “Setting Up or Removing an Imaging Data Directory,” page 74
- “Setting Up or Removing an Imaging Study Name Template,” page 74
- “Setting Up or Removing an Imaging Data Name Template,” page 75

Location of Investigator Data

Investigator data is saved as defined in the Save data setup window, which is opened by clicking **Edit** on the main menu bar and selecting **Save data setup**.

The Save data setup window sets the following parameters:

Directory/Template	*Parameter*
Base directory	`globalauto`
Study name template	`sqname`
File name template	`autoname`

A new study directory is created using `globalauto`, plus the file name template when the imaging user selects Study Options then selects Clear Study. The full path to the study is stored in `sqdir` and the relative path is stored in `studyid`. Data is saved using `autoname` and the path relative to `sqdir`.

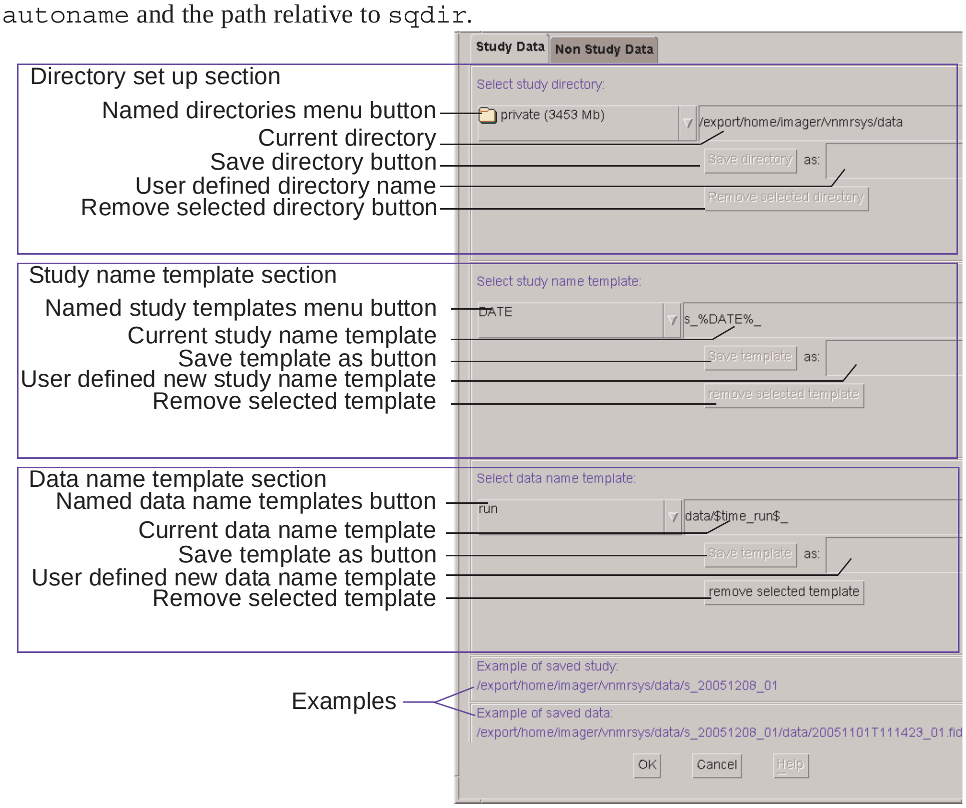


Figure 19. Save Data Setup Window, Imaging User

Open the Imaging Save Data Setup Window

1. Click on **File**.
2. Select **Save data setup …**
3. Review the current directory and templates selections and do one of the following:
   - Click on the **Cancel** button to exit and make no changes.
   - Continue with "Setting Up or Removing a Data Directory," page 70.

Setting Up or Removing an Imaging Data Directory

The data is saved using the controls in the Directory set up section of the Save Data Setup window, see Figure 18, using the following procedures as required:

Use an Existing Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Data Directory

1. Modify the existing directory path shown in **Current directory** field or enter a new full path in the **Current directory** field.
2. Press Enter.

   The *Current directory* field and *Save Directory* button are not active until the Enter key is pressed.
3. Enter a name for the new data directory path in the **User defined directory name** field.
4. Click on the **Save directory** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Data Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the drop down menu of named directories.C
3. Click on the **Remove selected directory** button.

Setting Up or Removing an Imaging Study Name Template

The automation run data is named using the template set up section (no present on the **Non Study Data** tab) in the Study Name Template of the Save Data Setup window, see Figure 18, using the following procedures as required:

Use an Existing Study Name Template

1. Click on the **Named study templates** menu button.
2. Select a named directory from the drop down menu of named directories:
   - DATE
   - ID
   - date

- name
- seqfil

3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Imaging Study Name Template

1. Modify the existing directory path shown in **Current named study template** field or enter a new study template in the **Current named study template** field. Refer to "Location of Operator Data," page 68 for a details about the parameter related to this template.
2. Press **Enter**.

   The *Current named study template* field and *Save templates* button are not active until the Enter key is pressed.
3. Enter a name for the new data template in the **User defined new study template name** field.
4. Click on the **Save template** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Imaging Study Name Template

1. Click on the **Named study templates** menu button.
2. Select a named directory from the drop down menu of named directories.
3. Click on the **Remove selected template** button.

Setting Up or Removing an Imaging Data Name Template

The automation run data is named using the template set up in the Data name template section of the Save Data Setup window, see Figure 18, using the following procedures as required:

Use an Existing Imaging Study Name Template

1. Click on the **Named data name templates** menu button.
2. Select a named directory from the drop down menu of named directories.
   - comment
   - run
   - seqfil
3. Continue with "Setting Up or Removing a Study Name Template," page 70.

Creating and Saving a New Imaging Data Name Template

1. **Modify** the existing template shown in *User defined new data name template* field **or enter a new template** in the *User defined new data name template* field. Refer to "Location of Operator Data," page 68 for a details about the parameter related to this template.
2. Press **Enter**.

   The *User defined new data name template field* and *Save Directory* button are not active until the **Enter** key is pressed.

3. Enter a name for the new data directory path in the **User defined new data name template** field.
4. Click on the **Save template** button.
5. Continue with "Setting Up or Removing a Study Name Template," page 70.

Removing a Saved Imaging Data Name Template

1. Click on the **Named data name templates** menu button.
2. Select a named template from the drop down menu of named templates.
3. Click on the **Remove selected template** button.

The software is now configured for imaging.

Chapter 8. System Calibrations

Sections in this chapter:

- 8.1 “System Calibration Procedure,” this page
- 8.2 “Calibrating ProTune,” page 78
- 8.3 “Calibrating a Probe,” page 84
- 8.4 “AutoCalibration Samples,” page 89
- 8.5 “AutoCalibration,” page 89
- 8.6 “Calibrating - Manual Methods,” page 90

This chapter describes the liquids NMR system calibration procedures for a newly installed Varian Inc. NMR spectrometer system. These calibrations and system test procedures can be used for routine system calibration maintenance. Procedures described here cover pulse width calibration, decoupler field strength, decoupler 90° pulse width, and decoupler pulse calibration. Additional calibration procedures are described in various probe installation and acceptance test procedure manuals, accessory test and installation manuals, and other test manuals.

8.1 System Calibration Procedure

These procedure require the following:

- Magnet is installed and ready for normal operation.
- System operating software is installed.
- All required network issues and connections are completed.
- VnmrJ software is installed, printers setup, and hardware configuration set.
- All accessories are installed and ready for calibration.

Referenced Manuals

The system calibration procedure here references the following manuals:

- Probe Installation and Acceptance Test manual(s).
- *AutoTest*
- *VnmrJ Liquids NMR User Guide*
- *VnmrJ Walkup*

Procedure

1. Install the primary system probe and complete all the acceptance test procedures.

   Typically this configuration consists of a conventional probe using 5 mm sample tubes, VT system, and gradient(s) (if present). Sample changers, flow systems and probes, cryogenic probe and system, and other specialized accessories are installed and calibrated last.

Refer to gradient shimming in the *VnmrJ Liquids NMR User Guide* manual

2. Run AutoTest.

   Refer to the *AutoTest* manual for instructions and the console acceptance test and installation procedures manual for specifications. This does not apply to Mercury systems, Imaging systems, or Infinity systems.

3. Calibrate the probe and create a calibration file.

   Choose all the calibration procedures that are appropriate for the probe. A new system or probe installation requires the creation of a system level probe calibration file. Refer to "Calibrating a Probe," page 84 for instructions – choose the calibration procedures that are compatible with the probe functions.

4. Install any additional probes - follow the instructions in the Probe Installation and Acceptance Test manual.

5. Calibrate and create a calibration file for each additional probe.

   Choose all the calibration procedures that are appropriate for the probe. A new system or probe installation requires the creation of a system level probe calibration file. Refer to "Calibrating a Probe," page 84 for instructions – choose the calibration procedures that are compatible with the probe functions.

6. Edit the probe calibration file for each probe as necessary and add any manually determined calibrations, e.g. add the N15 calibrations for an HCN probe.

   Refer to "Editing Probe Calibration Files to Add ^{15}N Calibrations," page 87.

7. Calibrate any installed accessories such as:

   - Cold Probe – refer to the *Cold Probe Installation* and *Cryogenic Systems Installation* manuals
   - Sample Changers – refer to the related manual
   - LC-NMR and LC-NMR/MS systems – refer to related manual
   - VAST – refer to related manual
   - ProTune – refer to "Calibrating ProTune," page 78.

8.2 Calibrating ProTune

This section applies only to systems equipped with ProTune.

- "Changing Probes," page 78
- "Connecting Protune Modules to the Probe," page 79
- "Indexing Motors," page 80
- "Calibrating Sweep Range," page 81

Changing Probes

1. Remove the current probe – do one of the following:

   Currently installed probe is an AutoX probe.

   a. Eject the sample if one is present.
   b. Turn OFF the master module

c. Disconnect flexible shafts from the probe
d. Remove rf cables and pneumatics lines.
e. Remove the probe from the magnet.

Currently installed probe is not an AutoX probe.

a. Eject the sample if one is present.
b. Remove rf cables and pneumatics lines.
c. Remove probe from the magnet.

2. Install the next probe in the magnet.
3. Set the system probe name to the currently installed probe.
4. Do one of the following:

Installed probe will use Protune

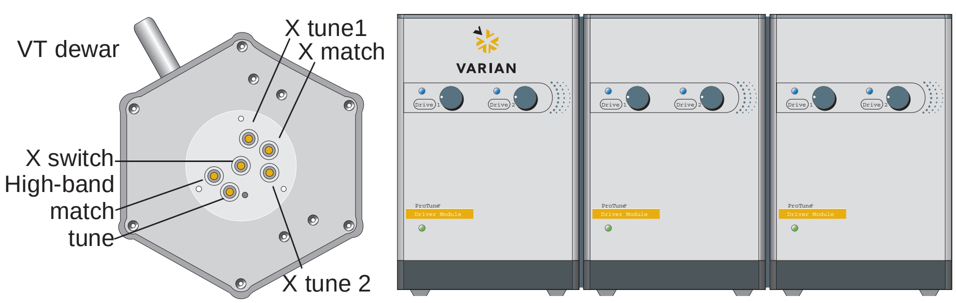
a. Connect flexible shafts — see "Connecting Protune Modules to the Probe," page 79
b. Connect the RF cables and turn the Master module ON
c. Set or verify that the system hardware option, Protune, is set to **present** — see "Spectrometer Configuration," page 22.
d. Start the ProTune interface.
e. Follow the procedure in "Indexing Motors," page 80.

Installed probe will not use Protune.

a. Set system hardware to Protune **not present** — see "Spectrometer Configuration," page 22.
b. Connect all cables and pneumatics lines to the probe.

Connecting Protune Modules to the Probe

1. Connect the cables from the Protune module to the probe in the order shown using the procedure in step 2



AutoX Probe Capacitor	*Master*	*Drive Module 1*	*Drive Module 2*
Switch	—	—	Drive 1
X Tune 1	—	—	Drive 2
X Match	—	Drive 1	
X Tune 2	—	Drive 2	
High-band Match	Drive 1		
High-band tune	Drive 2		

2. Connect each cable from the Protune modules to the probe as follows:

   a. Align the slot on the cable end with the pin on the knob of the probe.
   b. The slot (A) lines up with the set screw (B) on the flex shaft.
   c. Push the shaft on to the knob and compress the spring in the knob.
   d. Turn the capacitor knob approximately 90º clockwise to lock.
   e. Repeat this procedure for each capacitor and cable pair.

3. Continue with “Indexing Motors,” page 80.

Indexing Motors

The ProTune motors must be indexed after the following:

- The AutoX probe has changed to a different Auto X probe.
- The Master Driver Module has lost power, been power cycled, and during initial installation.

  The ProTune motor modules will automatically start indexing the motors associated with the current probe if the power to the master module was interrupted since the last time the `probtune` command was executed.

Procedure for Indexing all the ProTune Motors.

1. Log in as vnmr1.
2. Set the system probe name to the name of the currently installed probe.
3. Verify all ProTune connections are correct.
4. Turn the ProTune modules On and the system is Idle.
5. Enter **`protune('calibrate')`** on the VnmrJ command line.

   The ProTune Interface window appears.
6. Verify that the Motor and Sweep communication show **OK** in the top left corner of the ProTune Interface window.
7. Enter **index all** in the ProTune window Cmd field.

   Each motor will be indexed automatically.
8. Wait for the indexing process to complete.
9. Exit ProTune Interface.

Procedure for Indexing Individual ProTune Motors.

1. Log in as vnmr1.
2. Set the system probe name to the name of the currently installed probe.
3. Verify all ProTune connections are correct.
4. Turn the ProTune modules On and the system is Idle.
5. Enter **`protune('calibrate')`** on the VnmrJ command line.

   The ProTune Interface window appears.

6. Verify that the Motor and Sweep communication show **OK** in the top left corner of the ProTune Interface window.
7. Enter **index <motor number>** in the ProTune window Cmd field, refer to Table 5.

Table 5. Module and Motor Designations

	Master Module		*Dual Module 1*		*Dual Module 2*	
Alternate name	*Box 1*		*Box 2*		*Box 3*	
Motor number	1	0	3	2	5	motor
Drive number	1	2	1	2	1	2
Probe connection	HB Match	HB Tune	X Match	X Tune 2	X Switch	X Tune 1

The motor will be indexed automatically.

8. Wait for the indexing process to compleat.
9. Repeat step 7 and step 8 for next motor to be indexed.
10. Exit ProTune Interface.

Clearing Motor Stuck Message

The software displays the motor stuck warning if the indexing process does not reach and end or if the motor cannot turn the capacitor. The message will specify a box and drive number, see Table 5 for module and box number correlation. Clear the error message using the following procedures:

- Indexing does not reach an end.

1. Check and tighten all the screws on corresponding flexible shaft.

   Use the nonmagnetic tools provided with ProTune Tool Kit.
2. Re-index the motor.

- Tune knob is stuck.

1. Disconnect flexible shaft from the probe's tune knob

   Use the nonmagnetic tools provided with ProTune Tool Kit.
2. Use the tuning stick provided with the probe and turn the knob in the opposite direction as indexing to free the knob.
3. Reconnect flexible shaft and re-index the motor.

Calibrating Sweep Range

The sweep range must be calibrated if parts of the RF path such as; cables and filters, are changed. Sweep range calibration is probe independent.

Calibrate the ProTune sweep range by measuring the RF reflection using the following procedure:

1. Log in as the VnmrJ administrator (typically vnmr1) and start VnmrJ.
2. Enter **`protune('calibrate')`** on the VnmrJ command line.

   The ProTune Interface window is displayed.
3. Verify that for both Motor and Sweep communication **OK** is displayed (upper left corner of the window).

4. Set Raw Data to **On** in the ProTune window.

   The data displayed during the calibration is not corrected.

5. Set the sweep range for the Tune band to High.

Table 6. System and Frequency Ranges

System Frequency (MHz)	*Band*	*Min. (MHz)*	*Max (MHz)*
300	Low	27	140
	High	253	337
400	Low	30	185
	High	356	427
500	Low	45	220
	High	440	540
600	Low	56	256
	High	527	636

6. Calibrate the sweep range (sweep limits are set according to Table 6) as follows:

   a. Set up “Setting Up Open Circuit Reflection Calibration,” page 83.

   b. Click the **setCalSweep** button.

   c. Set up “Setting Up 50-Ohm Load Reflection Calibration,” page 83

   d. Click the **setCalSweep** button.

   e. Set up “Setting Up Short Circuit Reflection Calibration,” page 83

   f. Click the **setCalSweep** button.

7. Set the sweep range for the Tune band to Low and repeat step 6 for the low band channel.

8. Click on the **clearCal** button.

   The new calibrations are now ready.

9. Continue with “Calibration Verification,” page 82.

Calibration Verification

Now, test the calibration of this channel as follows:

1. Set the Raw Data Mode selector to Off.

   This tells the program to correct the raw data before displaying it.

2. Update the display by clicking the **Refresh** button.

   A flat line at reflection=1 is the ideal response

Exiting the Calibration Mode

1. Remove the shorting plug and reconnect the Probe.

2. Connect the proton and X channels to the probe.

3. Close the ProTune Interface window.

Setting Up Open Circuit Reflection Calibration

1. Disconnect the cable from the probe Proton (for High range sweep) or X channel (for Low range sweep) at the probe.
2. Click the **Refresh** button to update the display and confirm that the reflection signal looks correct. A typical sweep is shown in Figure 20.
3. Click **Refresh** again if data is not ready.
4. Click the button **Inf** next to the save CalData field.

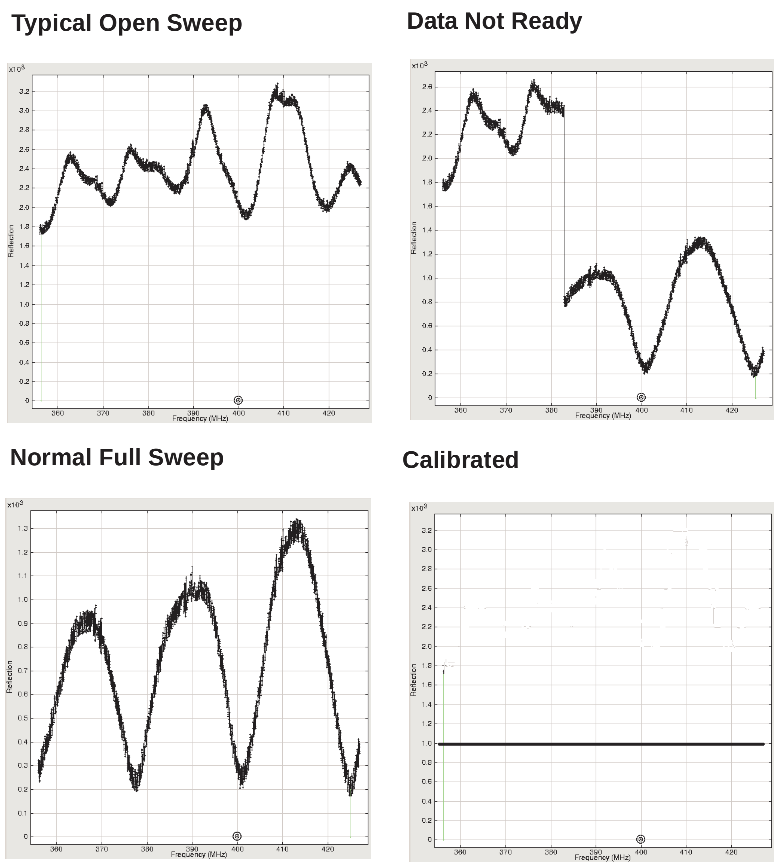


Figure 20. Sweep Images from Sweep Range Calibrations

Setting Up 50-Ohm Load Reflection Calibration

1. Connect a 50-Ohm load to the Proton (for High range sweep) or X channel (for Low range sweep) end of the cable in place of the probe.
2. Click the Refresh button to update the display and confirm that the reflection signal looks correct. Click Refresh again if data is not ready.
3. Click the button **50** next to the save CalData field.

Setting Up Short Circuit Reflection Calibration

1. Replace the 50-Ohm load on the Proton (for High range sweep) or X channel (for Low range sweep) with a shorting plug.

2. Click the **Refresh** button to update the display and confirm that the reflection signal looks correct.
3. Click **Refresh** again if data is not ready.
4. Click the button **0** next to the save CalData field.

8.3 Calibrating a Probe

This procedure uses the VnmrJ Experimental interface.

A complete list of samples and calibration tests are in "AutoCalibration," page 89.

- "Logging In and Installing the Probe," page 84
- "Setting Up the Initial Parameters," page 84
- "Setting Up the Probe Calibration File," page 85
- "Tuning Probes," page 86
- "Starting a Calibration," page 86
- "Editing Probe Calibration Files to Add ^{15}N Calibrations," page 87

Logging In and Installing the Probe

Completion of these steps is required for all the procedures that follow.

1. Log in to VnmrJ.

   Log in as the VnmrJ administrator (typically this is `vnmr1`) to create a system probe file (typical for initial installation). Write permission to `/vnmr/probes/probe_name` is required to create a system level probe file.

2. Install the probe to be calibrated.

   Probe installation instructions are provided in the *Installation and Operations* manual for the probe.

Setting Up the Initial Parameters

1. Click on **Tools** on the main menu.
2. Select **Locator**.
3. Click the locator **loop menu,** go to the category **Sort NMR Parameter Files**, and select **Test Files**.
4. Click the title above the right most column and select **Directory** from the lists that is displayed.
5. Scroll through the files and locate the parameter set **`shmd2o`**.
6. Click the parameter set **`shmd2o`** and drag it to the VnmrJ graphics canvas.
7. The parameter set is now ready for use.

Setting Up the Probe Calibration File

Set up the probe calibration file before calibrating a probe for the first time using the procedure described below.

1. Click the **Probe** button, see Figure 21, on the hardware bar in the VnmrJ interface or click **Tools** on the VnmrJ menu bar, select **Standard Calibration Experiments**, and select **Calibrate probe**.
2. The probe selection window will appear, see Figure 21.
3. Select the probe from the list of probes or create a new probe file.
4. Click the **Edit** check box -— editing options appear in the Probe window.
5. Do one of the following based upon the operating system login:
   - VnmrJ system administrator (typically vnmr1) or user with equivalent write permissions, select, from the **Level** drop down menu, either:

     System — writes the calibrations into: `/vnmr/probes/`*`probe_name`* and makes all calibration available to all users — typical for new system and probe installation.

     – OR –

     User — writes the calibrations into:`~/vnmrsys/probes/`*`probe_name`* and are available only to the logged in user creating the calibration file.

     The User level calibration file can be written to the system level directory, if the user has write permission to the system level directory, by clicking on the **Copy to system** button, see Figure 21.
   - Logged in a user (most users) without write permission to `/vnmr/probes` files.

     Continue with the next step - the Level option is not displayed and all calibrations will automatically be saved to: `~/vnmrsys/probes/`*`probe_name`*.

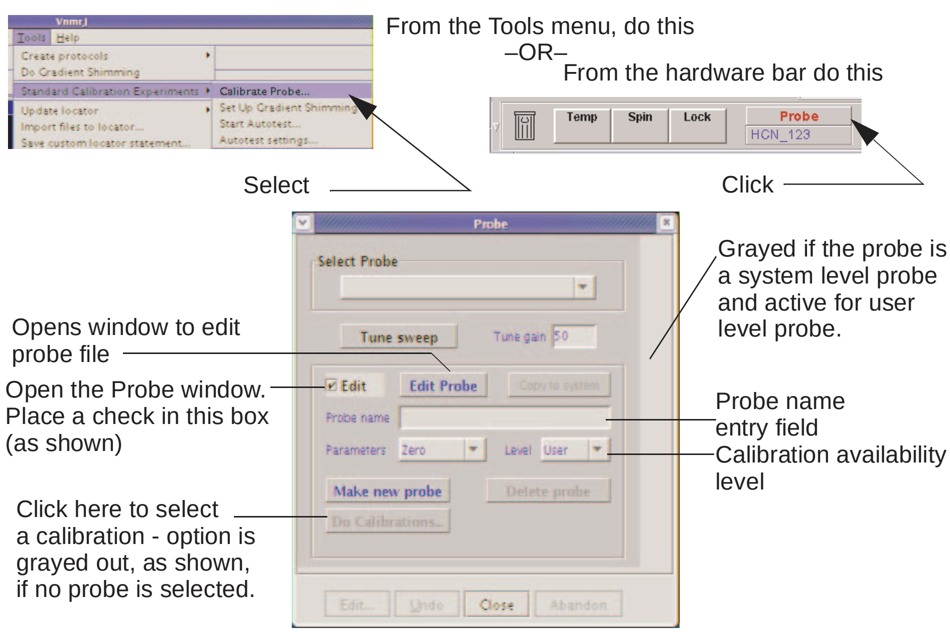


Figure 21. Calibrating a Probe

6. Do one of the following (refer to Figure 21 as needed):

   New probe

   a. Type the name of the probe in the **Probe name** field (letters first followed by numbers, e.g. abc456).
   b. Select system or user from the **Level** drop down menu.
   c. Press **Enter** (must press the enter key to add the new probe name).
   d. Click the **Add probe** button.
   e. Continue with "Starting a Calibration," page 86.

   Existing probe

   a. Click the Select Probes drop down menu.
   b. Select the probe.
   c. Continue with "Starting a Calibration," page 86.

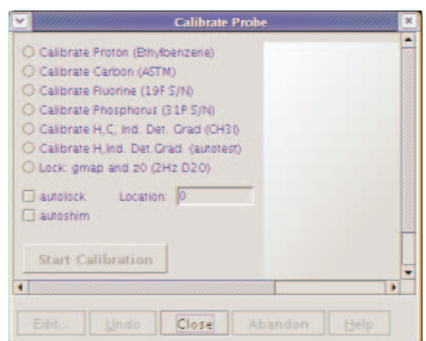
Tuning Probes

Probe tuning is covered in the *VnmrJ Liquids NMR* manual. Tuning operations and tuning ranges specific to each probe are covered in the manual provided with the probe.

Starting a Calibration

Refer to Figure 21 as needed.

1. Click the **Do Calibration** button in the probe calibration popup window.
2. Select calibrations from the calibration popup window

   a. Click a radio button in the calibrate probe window to select the calibration experiment.
   b. Enter the location of the calibration sample.

      No entry field appears if a sample changer is not attached to system.

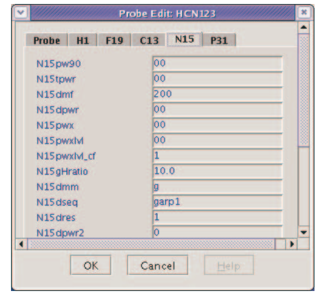
      Insert the sample into the magnet manually using the insert and eject button is located on the **Lock** page of the **Start** tab if a sample handler is not present or not used.
   c. Select **AutoLOCK YES** or **NO**.
   d. Click the **NO** button if the sample is already locked or to lock manually.
   e. Select **AutoSHIM YES** or **NO**.
   f. Click the **NO** button if the sample is already shimmed or to shim manually.

3. Follow the procedure in "AutoCalibration," page 89 for the autocalibration procedure that was selected in step 2a.
   - Verify the correct sample is present in the probe.
   - Probe calibration will begin.
   - The calibration files are created and written to the locations determined by the level that was selected in "Setting Up the Probe Calibration File," page 85.

Some probes, like the Autoswitchable and 4 nucleus probes, require additional calibrations not covered in this manual. For information on the calibration of these probes, see the installation, testing, and specifications manual for the probe.

Editing Probe Calibration Files to Add ^{15}N Calibrations

The calibrations for ^{15}N must be added to the probe calibration file following the manual calibration for probes with an X channel that can tune to ^{15}N or that have a pre-tuned ^{15}N channel.



Adding Calibrations for ^{15}N

1. Click the **Probe** button, see Figure 22 on the hardware bar in the VnmrJ interface or click **Tools** on the VnmrJ menu bar, select **Standard Calibration Experiments**, and select Calibrate probe.
2. Click to check the **Edit** check box — editing options appear in the Probe window.
3. Click the **Select Probes** drop down menu and select the probe.
4. Click on **Edit Probe**.

   A popup window appears with calibration names and fields to enter values.
5. Select the **N15** tab.
6. Add the calibration values in the fields provided – current calibration values are next to the parameter name e.g. pw90 (14).

   Leave the field blank if a calibration is not available — do not enter a zero.
7. Click **Save**.
8. Click **Exit**.

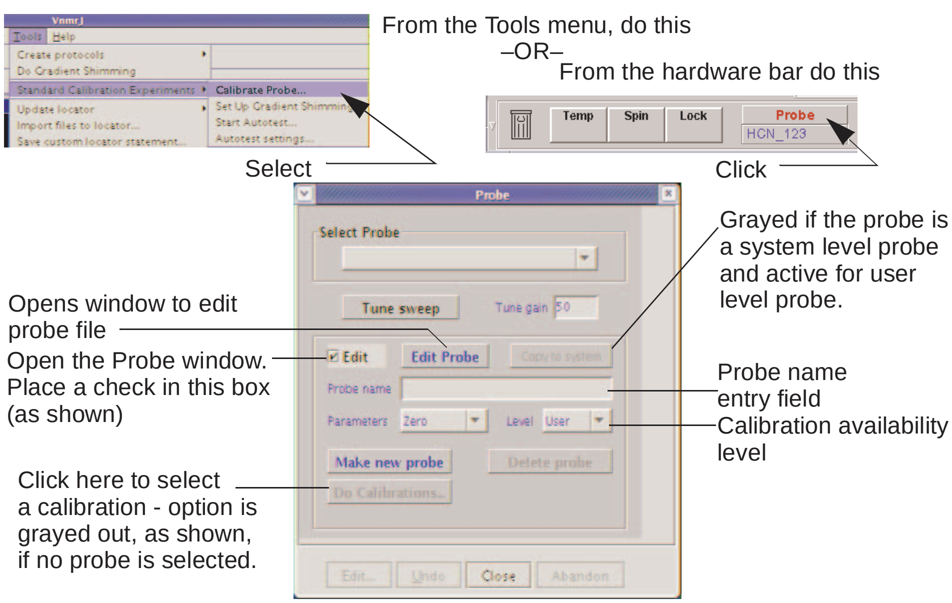


Figure 22. Calibrating a Probe

View or Edit Calibration Values

Each of the probe calibration files can be viewed and edited. Editing individual parameters is best done at the user level probe file and not at the system level. This is appropriate for specialized calibrations such as high salt concentrations, biological samples, low temperature calibrations etc. that are specific of an individual user but not appropriate for all users.

1. Click the **Probe** button in the VnmrJ interface.
2. Select a probe from the **Select Probe** drop down menu.
3. Place a **check** in the box next to Edit.
4. Click to check the **Edit** button — editing options appear in the Probe window see Figure 23.
5. Select the a tab to modify a probe calibration entry.
6. Change the calibration values in the fields provided.

   Leave the field blank if a calibration is not available — do not enter a zero.
7. Click **OK**.
8. Click **Exit**.

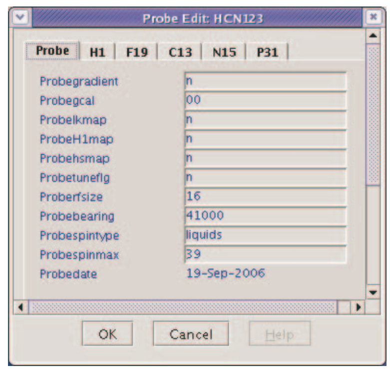


Figure 23. Probe File Edit Window

9. Repeat for each probe calibration file as required.
10. Click **Close** to exit the Probe calibration pop up window.

Optional – create a new version of the probe calibration file that will contain any special calibrations (typically a user level requirement):

1. Open a terminal window.
2. Do one of the following:
   - User level probe file:

     Enter **`cd ~/vnmrsys/probes`** – this is the probes directory of the current operating system log in user.
   - System level probe file:

     Enter **`cd /vnmr/probes`**.
3. Copy the directory for the probe of interest to a new directory name.
4. Change directories to the probe name directory.
5. Rename the probe file in the directory to exactly the same name as the directory.

8.4 AutoCalibration Samples

The samples listed in Table 7 can be used for auto calibration. Not all samples are provided with each system. The required samples for the acceptance test procedures during system installation will include one or more of these samples.

Table 7. AutoCalibration Samples

Sample	*Calibrate Option*	*Part Number*
0.1% ethylbenzene in $CDCl_3$ ^1H sensitivity	Proton	00-968120-70
40% dioxane in C_6D_6 ^{13}C sensitivity	Carbon	00-968120-69
0.485 M triphenylphosphate in $CDC1_3$ ^{31}P sensitivity	Phosphorus	00-968120-87
0.05% trifluorotoluene in benzene–d_6 ^{19}F sensitivity	Fluorine	00-968120-82
1% ^{13}C-enriched methyl iodide, 1% trimethyl phosphite, and 0.2% Cr(AcAc) in Chloroform-d	Proton, Carbon, ID, and Gradients (organic solvents)	00-968120-96
0.1% ^{13}C-enriched methanol with 0.30 mg/ml $GdCl_3$ in 1% H_2O/99% D_2O (AutoTest Sample)	Proton, Carbon, ID, and Gradients (aqueous solvents)	00-968120-68
2 Hz D_2O	LOCK, gmap and Z0	01-901855-01

8.5 AutoCalibration

1. Click on a Calibration radio button:
   - Calibrate Proton (Ethylbenzene)
   - Calibrate Carbon (ASTM)
   - Calibrate Fluorine (19F S/N)
   - Calibrate Phosphorus (31P S/N)
   - Calibrate H, C, Ind. Det. Grad (CH3I)
   - Calibrate H, C, Ind. Det. Grad (autotest)
   - Lock:gmap and z0 (2Hz D2O)
2. Follow the prompts, enter any required values, select options, and proceed according to the instructions presented in the Calibrate probe window, see Figure 24 for an example of the prompts presented:
3. Click on the **Start Calibration** button.

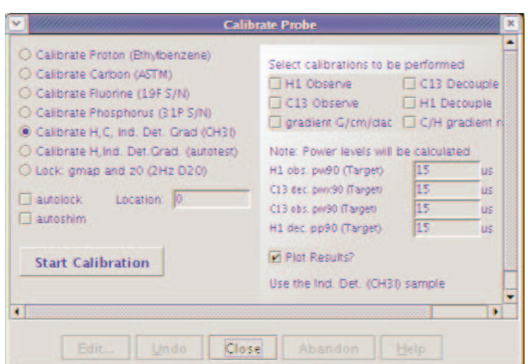


Figure 24. Prompts for Calibrate H, C, Ind. Det. Grad (CH3I)

8.6 Calibrating - Manual Methods

The manual calibrations are run from the command line. Parameter arrays are general examples and may need to be adjusted for individual probes and systems.

- "Calibrating Pulse Width," next
- "Calibrating Decoupler Field Strength," page 90
- "Calibrating Decoupler 90° Pulse Width with Polarization Transfer," page 92
- "Calibrating ^{1}H Decoupler Pulse Width with PPCAL," page 93
- "Calibrating ^{13}C (or X) Decoupler Pulse Width with PWXCAL," page 94

Calibrating Pulse Width

Sample	Any sample;
Parameter set	None.

1. Set up parameters to obtain a spectrum on the sample of interest.
2. Arrange the spectral window so that at least one resonance falls relatively near the center of the spectral window using either the macro `movetof` or the macro `movesw`.

   Estimate the relaxation time T_1 of the sample so that any experiments using intervals between pulses several times greater than that T_1 can be repeated.
3. Acquire one transient (`nt=1`) with no steady-state (`ss=0`) in absolute intensity mode (`ai`) using a transmitter power and pulse estimated at less than 90°.
4. Phase that spectrum properly.
5. Estimate the 90° pulse width, multiply by 4 to get the 360° pulse width, and enter an array around the 360° pulse width.
6. Make sure `d1` is greater than 3 times T_1, and acquire data using `ga`.

   The signals should be negative if the pulse is shorter than 360°, zero if the pulse is 360°, and positive if the pulse is longer than 360°.
7. Select a value of `pw` that gives the result nearest to zero, using rough mental interpolation if none of your results were exactly zero.

   Divide this value by 4 to give the 90° pulse width and enter this value in `pw90` as well as in your log book. To be sure you were not off by a factor of two, set `pw` equal to a 180° pulse and obtain a spectrum—the result should be near zero. Now set `pw` to a 90° pulse and the result should be a maximum.

The peak is rarely *exactly* zero but instead shows a dispersive signal with some signal positive and some negative. Do *not* readjust the phase in this case. This is normal behavior. Simply select the value of `pw` that gives "equally balanced" up and down resonances.

Calibrating Decoupler Field Strength

Sample	60% C_6D_6/40% dioxane (5-mm probe, Part No. 00-968120-69; 10-mm probe, Part No. 00-968123-69; 16-mm probe, Part No. 00-949134-69)
Parameter set	`/vnmr/tests/gamah2`

The strength of the *decoupler field*, known as γH_2, is important to know for a number of reasons:

- `dmm='f'` (swept fm or fm-fm modulation) decoupling, the decoupler field strength gives a rough measure of the range over which protons will be efficiently decoupled. Thus at 200 MHz, one might want a 10 ppm or 2 kHz decoupler field.; at 300 MHz, a 3 kHz decoupler field; etc.
- `dmm='w'` (WALTZ-16) decoupling, protons are efficiently decoupled over roughly twice that range; that is, efficient decoupling over a 2 kHz range can be achieved using only a 1 kHz decoupler field strength.
- For WALTZ-16 decoupling, the decoupler field strength must be known because the modulation frequency parameter `dmf` must be set to equal $4 \bullet \gamma H_2$.
- Various experiments that require the use of decoupler pulses will also require a knowledge of the decoupler field strength.

Decoupler field strength is a function of the decoupler power level (controlled by the parameters `dpwr` or `dhp`/`dlp`) and the probe. To a lesser extent, but especially when using highly ionic samples that can "detune" the probe, the decoupler field strength also depends on the sample. For "normal" organic solvents, it is usually sufficient to calibrate the decoupler field strength for each probe at a variety of settings and perhaps to repeat the calibration every few months. For polar solvents, and samples in water at high buffer concentrations, it may become necessary to calibrate the decoupler on the sample of interest, or at least on a comparable sample.

The standard method of calibrating the strength of the decoupler field is off-resonance decoupling. Two experiments are performed, one with the decoupler at a higher frequency than the proper decoupling frequency for a particular proton, and one with the decoupler at a lower frequency.

This technique produces two carbon spectra with "reduced" couplings—multiplets that have basically the same pattern as in a coupled spectrum (doublets, triplets, etc.) but in which the coupling constant is reduced. With these two spectra plus a knowledge of the full coupling constant, an appropriate equation can be used (see K.G.R. Pachler, *J. Magn. Reson.* **7**:442 (1972)) to determine the value of γH_2. The following procedure is recommended:

1. Insert the standard ^{13}C sensitivity sample (60% C_6D_6 and 40% dioxane).

   The dioxane produces a single resonance, a triplet with 1:2:1 amplitude, when coupled (from the CH_2 carbon in dioxane). This pattern will change when decoupling is used.
2. Retrieve an appropriate parameter set (assuming that `dpwr` or `dhp` is set correctly) by entering rtp('/vnmr/tests/gamah2')
3. Acquire two spectra by entering ga
4. Display the first spectrum with two cursors by entering `ds(1)`
5. Position the cursors on the outer lines of the triplet.
6. Read the value `delta` from the screen.

   Divide the result by 2 (because we really want just the value of a single splitting) and write down that number.
7. Display the second spectrum by entering `ds(2)`
8. Position the cursors in a similar fashion, and read the value of `delta`.
9. Write down half that difference.
10. Start the program to calculate the strength of the decoupler field by entering: `h2cal`.

When the system prompts for the low-field residual coupling value, enter the result from step 6.

When the system prompts for the high-field residual coupling, enter the result from step 8.

When the system prompts for the full coupling constant, enter `142`, the value for dioxane.

The system displays the calculated value of the decoupler field strength γH_2, the predicted coalescence point (the frequency at which single-frequency decoupling would collapse the dioxane to a singlet), and the pulse width for decoupler pulses if this decoupler level is to be used for pulsed decoupling.

Calibrating Decoupler 90° Pulse Width with Polarization Transfer

Sample	30% menthol in $CDCl_3$ (Part No. 00-968120-94)
Parameter set	`/vnmr/stdpar/C13`

The decoupler 90° pulse width value (parameter `pp`) from the test above should be appropriate for polarization transfer experiments. It is also possible to calibrate `pp` separately by using a polarization transfer pulse sequence directly, on the sample of interest. As an example of this procedure, a sample such as menthol having CH, CH_2 and CH_3 carbons is useful. If menthol is unavailable, use any small molecule organic compound that is highly soluble.

1. Enter **`jexp2 setup('C13','CDCl3') nt=4 ga`**.
2. Phase the spectrum and place the two cursors around the aliphatic region.
3. Enter **`movesw ga`** to narrow the spectral window. Phase the new, narrowed spectrum.
4. Enter **`jexp1 setup('H1','CDCl3') nt=4 ga`**.
5. Place the cursor in the center of the aliphatic region and enter **`sd`**. Note the value of `dof` (decoupler offset) after entering `sd`.
6. Enter **`jexp2`** and set **`dof`** to the value just found by `sd`.

   The follow is an alternative to this step:

   a. Set the decoupler offset `dof` to –2.5 times the spectrometer frequency of the system (e.g., on a 200-MHz system.
   b. Set `dof=-500`; on a 400-MHz, set `dof=-1000`).
7. Enter **`Dept`**.
8. Enter an estimate of the decoupler 90° pulse width that was obtained previously, or some other conservative estimate, after the help file is displayed.
9. Enter **`mult=0.5 d1=1 ss=2 nt=16 ga`**.
10. Phase the data when finished. All resonances should be positive.
11. Enter **`pp=10,20,30,40,50,60,70`** and rerun the experiment.
12. Enter **`dssh`** after the data are transformed.
13. Select the value of **`pp`** that gives the maximum peak heights (use `da` to check the array).

14. Enter a new array of **pp** values, bracketing the value determined in step 12 by ±20%, using about six smoothly-spaced values. Rerun the experiment and determine the `pp` value for maximum intensity, the same as step 12. This value is a reasonable estimate of the decoupler 90° pulse width.

Very accurate value of the decoupler 90° pulse width is required for spectral editing with the `adept` program or MAGICAL macros such as `cdept`, `hcdept`, or `dept`. Determine the decoupler 90° pulse Obtain this by observing `pp` dependence of CH_3 and CH_2 carbons for `mult=1.0` (CH selection).

1. Enter **mult=1**.
2. Make an array of **pp** in steps of 1 µs, from –5 to +5 µs around the `pp` value determined above.
3. Enter **ga** and when finished, enter **dssh**.
4. Phase the CH carbons vertically.

   The CH_2 carbons go from positive to negative with increasing `pp`. The CH_3 carbons decrease to zero and then increase. The `pp` value corresponding to a decoupler 90° pulse is the value that nulls the CH_2s. Use the J value in the parameter set is correct for the type of CH_2 in the molecule: 125 Hz for menthol. Reset the `pp` range to cover a smaller span with smaller steps in `pp` if a more precise 90° pulse is required.
5. Update the system log book and probe file.

Calibrating ^{1}H Decoupler Pulse Width with PPCAL

The PPCAL pulse sequence is used to calibrate the proton decoupler pulse width for experiments such as DEPT, INEPT, and HETCOR. Figure 25 shows the sequence.

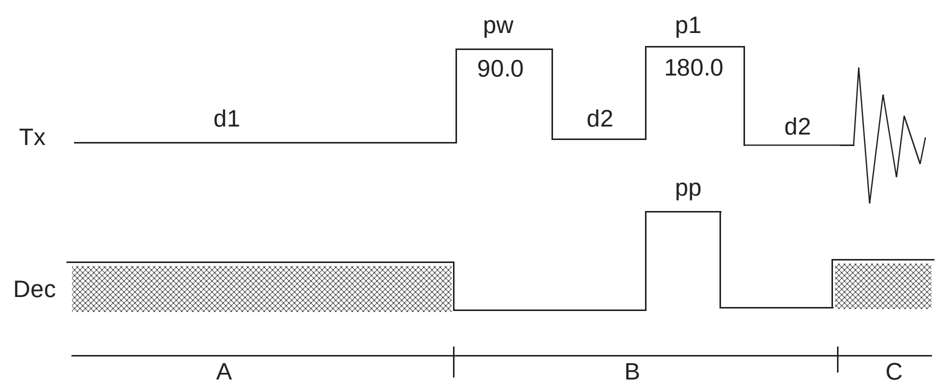


Figure 25. PPCAL Pulse Sequence

Parameters

The `ppcal` macro sets up the parameters for PPCAL as follows:

`pp` is a proton 90° decoupler pulse (in µs).

`d2` is a delay that should equal $1/(2*J_{CH})$ (in sec).

`pw` is a 90° pulse on ^{13}C (in µs).

`p1` is a 180° pulse on ^{13}C (in µs).

dm is the decoupler mode. The value should be 'yny'.

dmm is the decoupler modulation mode. Its value should be 'wcw' or 'fcf'.

pplvl is the power level for the proton decoupler pulse. dpwr is the power level for broadband proton decoupling if the decoupler channel uses a linear amplifier. If the decoupler channel uses a class C amplifier, maximum power is used for the proton decoupler pulse and dhp is the power level for broadband proton decoupling.

Technique

The following technique is recommended:

1. Array parameter pp, starting at 0.
   Make sure that delay d1 is reasonably long compared to the ^{13}C relaxation times.
2. Phase the first spectrum (pp=0). CH and CH_3 carbons should go from positive to negative, and CH_2 from positive to zero and again positive.
   All peaks should null when pp is a 90° pulse. The CH carbons are the most sensitive.

Calibrating ^{13}C (or X) Decoupler Pulse Width with PWXCAL

The PWXCAL pulse sequence is used to calibrate the pulse width characteristics of the probe's decoupler channel(s) in indirect detection or triple resonance experiments. PWXCAL can also be used to determine the rf field homogeneity of the decoupler. This calibration is a more sensitive measure of the decoupler X pulse widths than the first increment of HMQC. PWXCAL is designed for dual-broadband systems only and does not support "reverse mode" acquisition.

Parameters

The pwxcal macro sets up the parameters for PWXCAL as follows:

pw is a proton pulse width (in µs)

pwx1 is a 90° pulse on X (in µs) for the first decoupler.

pwx2 is a 90° pulse on X (in µs) for the second decoupler.

pwx3 is a 90° pulse on X (in µs) for the third decoupler.

jC13, jN15, or jP31 should be set to the appropriate coupling constant.

jname is set by the pwxcal macro to indicate which nucleus has been selected.

dm is the decoupler modulation and must be 'nnn'.

dmm is the decoupler modulation mode and should be 'ccc'.

dof is the X-nucleus resonance location (note: CH_3I dof is –14800 for a 500-MHz system at 11.4 T).

dpwr (or dpwr2) is the power level of the "X" decoupler pulse, and tpwr is the power level for proton observe if the decoupler channel uses a linear amplifier.

Technique

The following technique is recommended:

1. Starting from a 1D proton parameter set, type `pwxcal` and answer the questions "use decoupler 1, 2, or 3 [1]" and "calibrate C^{13}, N^{15}, or P^{31} [C^{13}]". Pressing the Return key to either of the questions selects the default response enclosed in square brackets.
2. Array parameter `pwx1`, starting at 0, making sure that delay `d1` is reasonably long compared to the ^{1}H relaxation times.
3. Phase the first spectrum (`pwx1=0`). All peaks null when `pwx1` is a 90° pulse.
4. If a second decoupler is present, the parameter `pwx2` is arrayed to calibrate the 90° pulse width on that decoupler. If a third decoupler is present, the parameter `pwx3` is arrayed to calibrate the 90° pulse width on that decoupler.

Chapter 9. Magnet and Spectrometer Maintenance

Sections in this chapter:

- "30-Day System Maintenance," page 97
- "Preventative Maintenance," page 97
- "Handling Liquid Helium," page 98
- "Continuing Dewar Service," page 103
- "Troubleshooting," page 108

30-Day System Maintenance

The following procedures must be performed while logged in as `vnmr1`.

1. Updating Solvent Shims

   Reshim lineshape and then save shims to `/vnmr/shims/acetone`.

2. Check Calibration of `pw90` and `tpwr`, as described in the "Calibrating a Probe" section of the *Installation and Acceptance* manual.

3. Perform hard drive maintenance: delete unused files, directories, old FIDs, macros, shims, or users.

4. Check magnet drift, as described in the "Magnet Drift" section of the *Installation and Acceptance* manual. If necessary (when Z0 is high or close to maximum 32767, reset Z0 by adjusting the `lockfreq` parameter as follows:

   a. Load **`H1sn.par`**.

   b. Set **`pw=1`**, **`gain=2`**, **`d1=0`**, **`in='n'`**, **`at=1`**, **`sw=500`**.

   c. Set Z0 to 0.

   d. Insert a pure water sample and acquire a spectrum.

   e. Enter **`f full aph0`**.

   f. Place a cursor on the water peak and enter **`nl movetof setlockfreq`**.

Preventative Maintenance

Performing preventative maintenance on a schedule can go a long way toward trouble-free operation of the spectrometer system. If problems do occur, we suggest you review the troubleshooting section in this chapter before calling your Varian service person. The following scheduled preventative maintenance and documentation is suggested.

- "Scheduled Maintenance," next
- "Maintenance Documentation," page 98

Scheduled Maintenance

A maintenance schedule such as the following is recommended.

Weekly

1. Check air line traps for dirt or condensed water.
2. Record the following readings (note that the flow rates of nitrogen and helium depends on a variety of factors such as atmospheric pressure and a high reading is not necessarily an indication of a problem, but it is worth investigating):
   - Pressure at the air valve for the magnet.
   - Liquid nitrogen level.
   - Readings on the nitrogen and helium flow meters.

Twice Each Month

- Check liquid helium level.

Monthly or Bimonthly

- Check signal-to-noise and lineshape using the standard proton sample, the ^{13}C 90° pulse width, and the decoupler field strength. keep the resulting spectra and parameters in a secure place for future reference and update the probe file.

Periodically

Back up data to tape using programs such as `dump` and `tar`.

Maintenance Documentation

It is a good idea to maintain three notebooks to document your system:

- *System Log* – For entering cryogen check and fills, service calls, problems, etc.
- *Operations Log* – For recording what you do every day—what samples were run, what new procedures were tried, what macros were written, what problems were encountered, etc.
- *Procedures Log* –For documenting new procedures, for example, a successful DEPT run (listing all parameters), a standard parameter set for ^{11}B, the procedure for determining 90° pulse widths, etc.

Each of these notebooks should set aside space for a table of contents on the first page and contain as much detail as possible.

Handling Liquid Helium

Safe and economical use of liquid helium (LHe) requires close attention to details. This section examines the physical properties of helium to show the relationship of these properties to problems in transferring helium.

- "Handling Liquid Helium Safely," next
- "Measuring Liquid Helium," page 101
- "Transferring Liquid Helium," page 102
- "Liquid Helium Service," page 103
- "Helium Refilling on Oxford 200- and 300-MHz Magnets," page 107
- "Determining Stinger Lengths for Storage Containers," page 107

WARNING: **To prevent possible personal injury, observe all warnings posted on equipment and stated in this manual. Before operating or servicing**

any part of the system, read the "Safety Precautions" section in the front of this manual.

Physical Properties of Helium

Table 8 compares the physical properties of helium to nitrogen. When establishing general procedures for handling LHe, consider the special properties of helium described in the following sections.

Table 8. Physical Properties of Helium and Nitrogen

Property	*Helium*	*Nitrogen*
Molecular weight	4.0026	28.01
Boiling point (1 atm)	4.2 K	77.4 K
Melting point	1.1 K (25 atm)	63.2 K (1 atm)
Critical temperature	5.2 K	126.0 K
Critical pressure	2.26 atm	33.5 atm
Density of liquid at boiling point	0.125 gm/cm^3	0.807 gm/cm^3
Density of gas at boiling point	0.0176 gm/cm^3	0.00462 gm/cm^3
Density of gas at 27°C	0.163 kg/m^3	1.138 kg/m^3
Heat of vaporization	2.58 J/cm^3	161.0 J/cm^3
Δ H=H300-H boiling point	192.0 J/cm^3 liq.	186.0 J/cm^3 liq.

Sources: R. B. Scott, 1959, *Cryogen Engineering*, D. Van Nostraud Co., Inc.
R. Barron, 1966, *Cryogenic Systems*, McGraw Hill Book Co.
A Wexler, 1951, *Journal of Applied Physic*s, 22:1463.

Low Boiling Point

Because LHe at atmospheric pressure boils at 4.2 K (kelvin), efficient insulation is required to minimize heat input to the cryogenic fluid (4.2 K is equivalent to –269.0°C). Care must be taken to prevent frozen air plugs from blocking pressure-relief valves and to keep other gases from entering the LHe container. Storage at a pressure slightly above atmospheric is essential to exclude air from storage containers and magnet dewars containing LHe.

Low Latent Heat of Vaporization

Of all cryogens, helium has the lowest heat of vaporization, on either a weight or volume basis. On a volume basis, the latent heat of helium is about one-sixtieth the latent heat of nitrogen and one-half the latent heat of liquid hydrogen. Therefore, the slightest heat input from any source (pressurizing gas or poor insulation) causes loss of LHe.

High Specific Heat of Vapor

To vaporize one liter of LHe requires 2580 joules. The same heat input will raise the temperature of the resultant vapor less than 4 K. To heat the vapor to room temperature requires 1.9×10^5 joules. Liquid losses can be substantially reduced, including loses from initial system cooldown, by using this vaporization property. Disregard of the property can lead to high losses during operations, such as topping-off a partially filled container.

Low Liquid Density

The density of LHe, 125 grams per liter, is about one-sixth the density of liquid nitrogen (LN). Because of the low density, the LHe content of a nitrogen-shielded container is difficult to gauge by weight.

High Vapor Density

Although helium is a very light gas at normal pressure and temperature, its vapor density at the normal boiling point is higher than that of any of the atmospheric gases. Helium vapor expands greatly upon warming to ambient temperatures, and if confined to a fixed volume, the pressure increase is correspondingly large. As a result, "empty" containers, filled only with very cold vapor, must be treated the same as containers containing liquid. Adequate venting must be maintained, and precautions must be taken to prevent formation of frozen air plugs in the container neck tubes.

Small Difference Between Vapor and Liquid Densities

The small difference between the densities of LHe and cold helium vapor may lead to high entrainment losses under flow or boiling conditions.

Handling Liquid Helium Safely

WARNING: **The extremely low temperature of liquefied helium and nitrogen can cause skin damage similar to high-temperature burns. Contact with the cold gas evolving from the liquid may produce the same effect. Delicate body tissues, such as the eyes, are easily damaged by exposure to cold gas or liquid. Skin can stick to metal that is refrigerated by liquid helium and can tear when pulled away. Immediately flood with large quantities of unheated water any area of the body that is "burned" by liquid or cold gas, and then apply cold compresses. If the skin is blistered or there is any chance the eyes are affected, immediately seek medical treatment.**

Before any transfer of LHe is attempted, know the safety precautions and operating instructions for the hardware used, especially the following:

- Avoid contact of gaseous helium with any part of the body. Wear safety coverings, including a complete face mask and thermo-insulated gloves. The gloves should be clean and dry, and should be loose-fitting so that you can throw them off quickly if frozen by contact with the gas.
- Handle and store helium containers in adequately ventilated areas. Helium and nitrogen gases are not toxic or flammable. However, gas evolving from the liquid in an enclosed space can reduce the oxygen content of the surrounding air and cause a potential asphyxiation hazard. Because nitrogen and helium gases are odorless, colorless, and tasteless, their presence is undetectable by the human senses.
- Be sure pressure-relief valves are adequately sized. LHe vaporizes rapidly when heat is introduced. Therefore, the pressure-relief valve for LHe containers and equipment must have sufficient capacity to safely release the rapidly expanding helium gas.
- Prevent pressure-relief valves from freezing open. An open valve allows the container to blow down, and eventually air backflows into the container and freezes.

- Neck tubes may still be unobstructed even if pressure inside the helium container is above atmospheric. Check containers when received and periodically recheck each container to be sure the vents are unobstructed.
- Very cold helium gas vents upon removal of the top fitting of a container. Cap or seal the container rapidly because the top fillings and valves will become cold and frosted, making sealing more difficult.

Most LHe storage containers are designed with an inner assembly within the vacuum jacket. Because the innermost neck is made of a thin material, the container is vulnerable to rough handling, and especially to a sudden shock. Take the following precautions to prevent damaging containers:

- Never try to pour liquid out of the container; use a vacuum-insulated transfer tube.
- Keep the container vertical at all times.
- Never roll, tip or slide the container. Use a dolly when moving it.
- Do not drop the container.
- When transporting the container, fasten it securely to prevent it from moving or falling over.

Measuring Liquid Helium

The thermal acoustical liquid level indicator, or flutter tube, is used to locate the surface of LHe inside a container. The device depends upon the thermal-acoustic oscillations generated in tubes that have one end at room temperature and the other at LHe temperature.

The flutter tube consists of a length of 1/8 in. thin-wall stainless steel tubing with a small cup, or funnel, shape at the warm end, flared to a diameter of about 1/2 in. When the tubing end is inserted into a dewar of LHe, acoustical oscillations occur that abruptly change in intensity and frequency as the end of the tube passes through the liquid zone into the dense gas zone.

Using the Flutter Tube

Take the following steps to measure LHe with a flutter tube:

1. Slowly insert the tube into the LHe container until the tube touches bottom, then place an alligator clamp on the tube, level with the top of the container.
2. While slowly raising the tube, observe vibrations by closing off the top end of the tube with your thumb. When the end of the probe passes from the liquid zone to the dense gas zone, the vibrations intensify and the frequency changes. Place another clamp on the tube, level with the top of the container.
3. Measure the distance between centers of the two clamps; this is the LHe depth.

Air and Moisture Ice Hazard

A hazard is created when air and moisture are pulled into the nitrogen shield and the inner chamber of LHe containers. Sudden barometric pressure changes can cause the air diffusion to increase. Once into the LHe neck tube, the heavier gases in the air diffuse to the bottom and condense, and then solidify near the LHe end of the tubes. The moisture in the air also forms ice in the LN tubes. The plugs formed by the ice can cause damage to equipment.

CAUTION: Air and moisture condensation can result in a solid ice plug in the LHe chamber pressure vents. This obstruction can result in damaged equipment. Keep all vents capped or sealed when possible.

Transferring Liquid Helium

The following sections summarize transferring LHe from a storage container to the LHe chamber in a superconducting magnet. The actual procedure used to transfer LHe when installing and maintaining Varian NMR superconducting magnets is given later in this chapter.

Helium Movement through the Transfer Line

When a cryogenic liquid is started through a typical transfer line that is initially at room temperature, the liquid at first is quickly evaporated and nearly the entire line contains only gas. As more liquid enters, part of the cryogenic source end of the line becomes cooled below the saturation temperature, and this part contains a pure liquid phase. Toward the destination end of the transfer line is a region in which both liquid and vapor are present. In the remainder of the transfer line, only gas is flowing. A very light gas plume appears at the exit end of the tube.

As the line is further cooled by the evaporating liquid and by the resulting cold vapor, the liquid phase travels farther along the line until finally liquid approaches the exit end. The vaporized liquid appears as a very dense white fog blown out from the end of the tube.

If the warm vapor that precedes the liquid is discharged into the LHe chamber of the magnet, it evaporates some of the liquid already present. This evaporation can be largely avoided by making sure the transfer tube is precooled before inserting it into the equipment, which already contains LHe.

If the warm line is permitted to deliver excessive warm gaseous helium to the LHe chamber of the magnet, a serious evaporation of liquid can result. The turbulence caused by the discharge of warm (nonliquid) helium can result in a quench of the magnet field present.

Preparations for Transfer

The transfer tube must have a good vacuum (50 microns warm, maximum pressure). The appearance of condensed moisture or frost on the tube during transfer shows that the vacuum is poor, reducing the insulation properties created by the vacuum and possibly preventing the transfer. A small spot of frost indicates a thermal “short” caused by contact of metal surfaces. Stop the transfer immediately because LHe is vaporizing in the tube, due to the heat conducted through this thermal short.

Make sure that the vacuum-jacketed portion of the transfer tube extends below the bottom of the neck tubes on the supply and receiving containers.

Typical Transfer Procedure

1. Verify the amount of LHe needed and make sure that amount is available for transfer.
2. Set or verify that helium gas pressure is 4 to 5 psig.
3. Precool the transfer tube, as follows:
   a. Vent the storage dewar.
   b. Insert the transfer tube in the storage dewar only.
   c. Reduce the boiloff pressure by venting.

d. Close the low-pressure safety vent valve on the storage dewar.

e. Pressurize the dewar. Set flow to 4 on the flowmeter (pressure will slowly rise). Wait for the dense, white, “flame-like” exit gas from the deflector nozzle (while waiting, release the internal pressure from the magnet slowly). Vent the storage dewar pressure (leave dewar vent open to prevent pressure buildup).

4. Insert the transfer tube and repressurize the storage dewar, as follows:

   a. Wipe to clear any ice build up at the deflector nozzle.

   b. Open the magnet entry port.

   c. Lift up and insert the transfer tube into both dewar and magnet (lower to the insertion stop located on the transfer tube magnet side).

   d. Close the dewar vent (the flowmeter should still be set to 5). Pressure should slowly rise.

5. Start the fill. While filling, pressure in the dewar should slowly rise.

6. When the exit cloud is accelerated and shows increased density, filling is complete. Complete the transfer as follows:

   a. Vent the storage dewar pressure.

   b. Remove the transfer tube from both the dewar and the magnet.

   c. Close and cap the storage dewar and the magnet.

   d. Open the low-pressure safety valve on the storage dewar.

   e. Close off the helium gas source.

Continuing Dewar Service

This section describes servicing a dewar with liquid helium after the liquids have dropped to the point where refilling (topping off) is necessary. Because of its very low latent heat of vaporization, LHe must be transferred through a well-insulated vacuum jacketed tube.

- “Liquid Helium Service,” next
- “Helium Refilling on Oxford 200- and 300-MHz Magnets,” page 107
- “Determining Stinger Lengths for Storage Containers,” page 107
- “Sample Scoring Problems,” page 108

WARNING: **Before attempting any transfer of liquid helium or liquid nitrogen, know the safety precautions and operating instructions for the hardware in use. Serious injury can occur in the handling of very cold gases and liquids.**

Liquid Helium Service

Before the transfer occurs, *the transfer tube must be precooled*. Precooling takes from 10 to 40 seconds. Immediately after precooling, the transfer tube is inserted into the magnet dewar and the transfer of LHe initiated. Difficulties in filling occur if unnecessary delays occur between precooling and insertion of the transfer tube.

CAUTION: **When servicing with helium, do not bend or twist the transfer tube when inside the magnet neck tube because the tube is thin-wall**

stainless steel and is easily punctured with sharp objects. When clearing ice plugs, use the supplied clean-out tube.

1. Position the LHe storage container with the discharge port about 26.5 in. (68 cm) horizontally from the HELIUM SERVICE port, so that the transfer tube can be inserted into the storage container and the magnet HELIUM SERVICE port simultaneously. (This distance applies only to the LHe transfer tube available from Varian.)

2. Make sure that the helium gas storage cylinder is equipped with a pressure regulator having a range of 2 to 10 psig.

3. *Measure the amount of LHe in the storage container and in the magnet dewar* to be sure of a sufficient supply to top off the magnet. Attempting to top off the dewar with a minimal supply could result in a quench. The available liquid helium in the storage container is not the capacity of the storage dewar or the amount of liquid helium in the dewar upon its delivery. *The available liquid helium is the amount of liquid helium accessible to the transfer tube with a stinger.*

4. Make sure, by measurement, that the tip of the transfer tube (that is, the end of the stinger if used) on the storage container side reaches to within 2 cm of the bottom of the dewar when the stop tab on the magnet side of the transfer tube is resting on the lip of the magnet HELIUM SERVICE port. Check that the deflector nozzle is attached to the magnet end of the transfer tube.

5. Depressurize the storage container. During shipment and non-use time, the storage dewar may build up internal pressure.

6. Place the pressurizing collar on the storage container side of the transfer tube.

7. *Precool the helium transfer tube* by slowly inserting one end into the storage dewar with the other end open to the room (see Figure 26). Do not close the storage dewar exhaust port during insertion. The heat of the transfer tube (room temperature) will cause increased liquid helium boiloff while being inserted. This helium boiloff should *not* be allowed to build up inside the storage dewar causing pressure.

   Once the transfer tube is fully inserted, pressurize the storage dewar by closing the exhaust port. Adjust the flowmeter valve so that the flow rate is about 5 on the scale. The pressure will rise slowly. After 10 to 40 seconds, a plume of LHe (in the form of a very dense, milk-like white, flamed-shaped fog) emerges from the deflector nozzle, indicating that the precooling has been accomplished.

8. After observing the exhaust for 5 to 15 seconds, depressurize the storage dewar by opening the exhaust port.

   If the transfer tube frosts over or condenses moisture from the room air (in areas not directly exposed to cold exhaust), it is likely that there is a poor or faulty vacuum within the transfer tube jacket. The transfer tube should be removed from use, warmed, and pumped down to 5 microns (5 millitorr) or better.

9. Pull the transfer tube up enough to clear the magnet dewar. Remove the HELIUM SERVICE filling port cap. Swing the transfer tube over the magnet and immediately insert it slowly into the magnet LHe access port and the storage container simultaneously (see Figure 27). As a guide, use 10 to 15 seconds for insertion up to the stop tab.

   If you observe excessive turbulence or a sudden increase in the exhaust rate, the transfer tube insertion is too rapid and hot gas is reaching the LHe in the magnet dewar. This can cause a quench when the LHe level is below the top of the solenoid. The insertion rate should be slowed down.

10. Once the transfer tube is fully inserted so that the stop disk rests on the lip of the magnet access port, start to pressurize the storage dewar by closing the storage container exhaust port. The flow rate of approximately 5 on the scale is still present and will now pressurize the dewar.

CAUTION: **Watch the pressure gauge on the gauge head assembly. Any rapid pressure buildup may indicate a frozen air or water blockage in the transfer tube or the fill tube. If ice blockage occurs, halt the LHe transfer, remove the LHe transfer line, and again purge the line with gaseous helium. After the line is cleared, restart the transfer from the beginning. Be sure to plug the storage container and the HELIUM SERVICE port as soon as the LHe transfer tube is removed from them in order to prevent air and moisture from entering the dewars.**

Open the vent port of the magnet on the filling side only.

The pressure will rise slowly toward 1 psig. During the 15 seconds to 1 minute, a collapsing exhaust plume is usually observed. The collapsing exhaust indicates that the liquid helium is reaching the magnet end of the transfer tube and is filling the magnet.

If the pressure is not increasing toward 1 psig when the flowrate is set to 5 on the scale, there may be a leak of the pressurizing gas that is preventing the storage dewar from being pressurized.

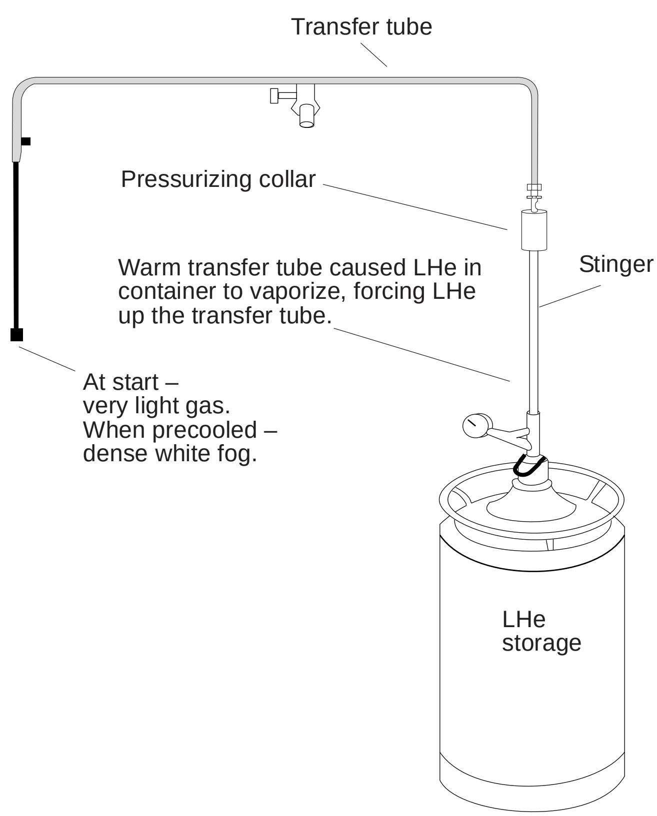


Figure 26. Precooling the Liquid Helium Transfer Tube

If the pressure exceeds 2 psig when the flowrate is set to 5, it is likely a blockage has occurred in the transfer tube. It will be necessary to remove the transfer tube, cap the magnet, warm the transfer tube, and start over again at the precooling step.

If a frost spot occurs in any section of the transfer tube that is not directly exposed to cold exhaust, there is probably a metal to metal touch across the vacuum jacket. The transfer tube should be replaced. A defective transfer tube can cause a magnet quench. Varian recommends that you observe the transfer tube for normal operation at each use. The transfer tube can be routinely pumped down once or twice a year as preventive maintenance.

11. The filling continues at this pressure and rate until the magnet dewar is full, which is indicated by a marked increase in the rate of exhaust from the magnet access port. This increased exhaust is accompanied by an increase in the density of the exhaust

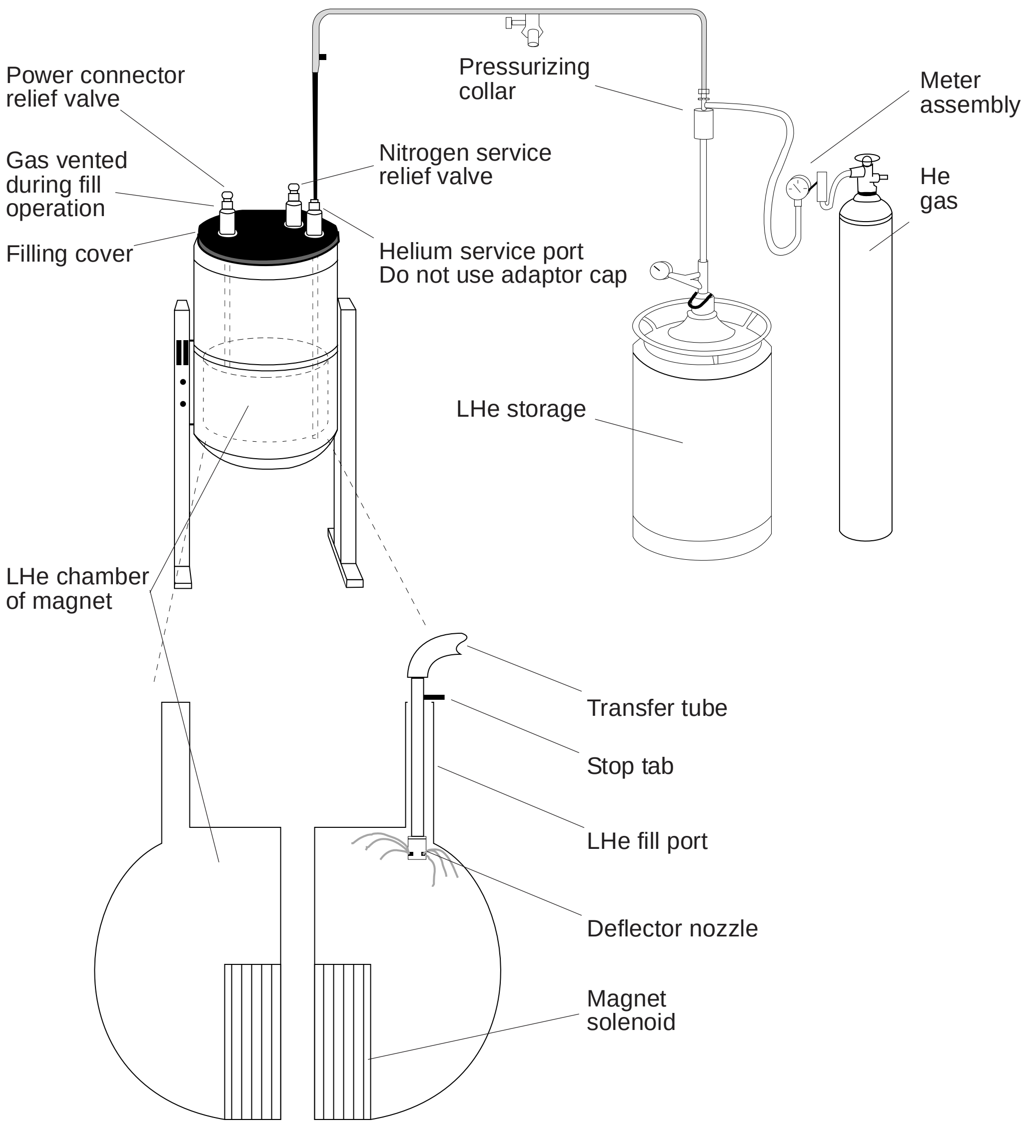


Figure 27. Routine Filling of the Magnet Dewar

cloud. If there is any doubt about the dewar contents level, use a flutter tube measurement to verify.

12. Depressurize the storage dewar. Remove the transfer tube from both containers. (Removal is much less risky than insertion.) Cap the magnet access port. Close the appropriate storage dewar valves.

Helium Refilling on Oxford 200- and 300-MHz Magnets

To maintain optimum refill safety and minimize the risk of accidental quenches, follow these special recommendations when refilling Oxford 200- and 300-MHz magnets:

- When you start filling the magnet (particularly if the helium level is low), open *only* the vent port on the side on which the transfer tube is inserted. Although this procedure should fill most magnets completely, some magnets are only partially filled.
- If a magnet is only partially filled with the vent port open, wait several minutes until the transfer has stabilized (indicated by the collapsing of the initial plume), and then open the port on the demountable lead side. If the second port is opened too soon after filling with the vent port open, warm gases could be sent across the solenoid.
- Under no circumstances should LHe be transferred with the port on the transfer tube side closed and the port on the demountable lead side open.

Determining Stinger Lengths for Storage Containers

A stinger may be necessary to extend the transfer tube into the LHe storage container. Refer to Figure 28 for the measurements needed to determine the stinger length for a storage container. Take the following steps for each container:

1. Measure distance A, the top of the storage container storage port to the bottom of the liquid helium chamber (a flutter tube can be used for this purpose).
2. Measure distance B, the top of the storage container service port to the top of the liquid helium chamber (a stiff wire with a crimp on the bottom to catch at the top of the chamber works well).

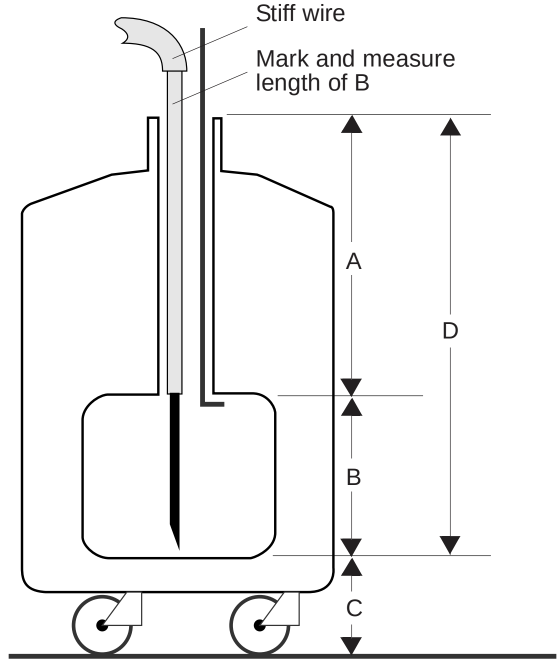


Figure 28. Stinger Configuration Measurements on the Storage Container

3. Subtract B from A to obtain the depth of the liquid helium chamber. This is measurement C, *the maximum length of a stinger for this containe*r.

CAUTION: **The stinger on the storage container side of the transfer tube must not be longer than the height of the LHe chamber (distance C). Exceeding this maximum will cause filling difficulties and can cause a quench.**

The following steps identify whether an elevating platform is needed below the storage dewar. Because the stinger has a limit to its maximum length, and the transfer tube cannot be lowered further than the stop disk allows (on the magnet side), an elevating platform for the storage dewar may be required to enable the stinger entry tip to reach the LHe to be transferred.

1. Measure distance D, the bottom of the liquid helium chamber to the floor.
2. Add C to D to give the distance from the top of the LHe chamber to the floor.

- If this distance is 26 inches or greater, then you will be able to fill from this container without an additional platform to elevate the storage dewar (this distance applies only to the LHe transfer tube available from Varian.).
- If this distance is less than 26 inches, constructing a platform under the storage container is necessary before proceeding. The platform must be designed to elevate the container so that the storage chamber top (C + D in Figure 28) is level with or higher than 26 inches above floor level. The design of the platform must also allow the storage container to be positioned with its service port 68 cm (26 3/4 in.) from the HELIUM SERVICE port on the magnet, as measured on a horizontal line that simulates the transfer tube.

Troubleshooting

- "Sample Scoring Problems," next
- "Sample Changer Troubleshooting," next
- "Other Troubleshooting Solutions," next

Sample Scoring Problems

Sample scoring and spinning instabilities are often caused by improper mating between the upper barrel and the probe. The following spin test checks for this problem.

1. Cover the sample tube using a felt-tipped ink marker pen (blue or black ink is best).
2. Let the sample spin for 1 to 3 hours in the magnet.

Any scoring should show up clearly in the inked sample tube. If scoring is evident, perform the following:

1. Loosen the probe flange thumbscrews one full turn and retighten them without twisting the probe body.
2. Spin test the sample again.

If scoring is still present, follow this procedure:

1. Loosen the upper barrel thumbscrews one full turn.
2. Loosen the probe flange thumbscrews one full turn.
3. Semi-loosen the probe flange set screws.
4. Push up on the probe body until the upper barrel moves approximately 1 inch.
5. Push down on the upper barrel until it hits the stops.
6. Tighten the probe flange set screws and thumbscrews.

7. Tighten the upper barrel thumbscrews.
8. Insert the sample and spin test for scoring.

If scoring is still evident, perform steps 1 to 8 again. If the scoring continues, contact you field service engineer.

Sample Changer Troubleshooting

Some problems that can be dealt with by the user are the following:

Sample Changer Not Responding

On the SMS sample changer, first check that the emergency stop button is off, then check the power switches on the back of the System V control and the robot. Also check the cable from System V control to the NMR console.

On the ASM-100 sample changer, check the power switch on lower rear of sample changer, check that RS-232 cable to sample changer is connected, and check whether any fuses in the sample changer are blown.

Gripper Drops Sample Back into Magnet when Sample is Ejected

On the SMS sample changer, check for bent fingers.

On the ASM-100 sample changer, gripper is not grasping enough of spinner— raise air pressure to sample changer by 1 to 2 pounds, or adjust the height of the gripper retrieval (bottom) position.

Other Troubleshooting Solutions

Spinner does not rotate.

Remove, disassemble, and clean upper barrel with ethanol.

Magnet has high boil off.

Check for ice in the power connector.

Appendix A. Printers and Plotters Troubleshooting

This appendix contains troubleshooting and setup information for printers and plotters.

Configuring Printer and Plotter Hardware

This section describes a number of printers and plotters tested as compatible with VnmrJ. Check the Varian website for new printers that work with VnmrJ. Refer to the original system manuals supplied with the printer or refer to the on-line manuals for printers supplied with older spectrometers. The following printers and plotters are covered in this manual:

- "Hewlett-Packard LaserJet 840C Printer," next
- "Hewlett-Packard DeskJet 5550 Printer," page 113
- "Hewlett-Packard DeskJet 970Cxi Printer," page 113
- "Hewlett-Packard LaserJet 2300 Printer," page 114
- "Hewlett-Packard LaserJet 2100 Printer," page 114
- "Hewlett-Packard Color LaserJet 4550 Printer," page 115
- "Hewlett-Packard Color Inkjet CP1700 Printer," page 116

Hewlett-Packard LaserJet 840C Printer

Printer I/O	HP IEEE-1284-B Parallel Universal serial bus 1284-B receptacle
Printer Language	HP PCL 3.
Printer Memory	2 MB standard memory
Cartridges	black and color
Resolution	Black – 600 x 600 dpi with black pigmented ink Color – HP color layering technology
Pages per Minute	Black – 4 ppm Black and color – 0.8 ppm
Configuration Control	Software controlled.

There are two buttons and three lights on the front of the printer. The lights indicate when the printer is operating correctly or when it needs attention from you and the buttons are used to control the printer.

Self-Test Procedure

1. Turn the HP DeskJet 810C and 830C series printer off and remove the cable that connects the printer to the computer.
2. Turn the printer back on.

3. Press and hold the **Power** (top) button. Press the **Resume** button 4 times and then release the **Power** button.
4. The self-test page will print with a report containing the printer model name, serial number and a diagonal self-test pattern. The test pattern verifies that all nozzles on the print cartridge are firing. If a gap appears along the diagonal self-test pattern, one or more nozzles are not firing.

Operation

1. Turn off the power.
2. Connect the interface and power cables.
3. Press **go** to turn the power on. The ready light should come on.
4. Open a terminal window, log in as `root`, and activate `LaserJet_150`, `LaserJet_150R`, `LaserJet_300`, `LaserJet_300R, LaserJet_600, and LaserJet_600R` using the procedures in the beginning of this chapter.
5. Set the parameter `printer`, from within VnmrJ, to the name you entered in the previous step, for example, `printer='LaserJet_300'` or `printer='lj'`. Enter `printon dg printoff` to produce a test print.

   To use as a plotter, set the parameter `plotter` to the name you entered in the previous step, for example, `plotter='lj 300'` (If you activated more than one resolution, there will be different names corresponding to the different resolutions). To test, enter `pl page`.

Lexmark Optra Color 45 Inkjet Printer

Printer I/O	IEEE 1284 ECp compliant,1284-B receptacle, Internal Solutions Port (6 options).
Printer Language	PostScript Level and PCL 5c emulation.
Printer Memory	8 MB.
Cartridges	Dual head thermal inkjet
Resolution	600 x 600 dpi
Pages per Minute	Black - 8 ppm Color - 4 ppm
Configuration Control	Software controlled.

The Varian supplied customized Optra Color 45 printer/plotter includes special software and is HPGL, PS, and PCL compatible. This custom printer is not available from other sources. The optional tri-port serial port board is installed in the Varian Optra Color 45 allowing either serial or parallel port mode. The Optra Color 45 replaces the Lexmark 4079, HP 7475, and the HP 7550A plotters.

Self-Test Procedure

1. Follow the set up instructions in the printer manual and then plug into ac power.
2. The print display should show **Ready** and the green light is **on**.
3. Press the **Menu** button until **TESTS MENU** is displayed and push **Select**.
4. Press the **Menu** button until **Print Demo** is displayed and push **Select** twice.

5. A multi-color page should be printed and the Menu returns to **Ready**.

Hewlett-Packard DeskJet 5550 Printer

Printer I/O	Centronics Parallel Universal serial bus
Printer Language	HP PCL 3, PostScript
Printer Memory	512 Kbyte standard memory sufficient for full page graphics at 600 dpi.
Cartridges	black and color
Resolution	Black – 600 x 600 dpi Color – depends on paper type
Pages per Minute	Black – 12 ppm Black and color – 10 ppm
Configuration Control	Software controlled.

The Hewlett-Packard 5550 features 600 dpi color printing and is software controlled. It has a color cartridge and a black cartridge. The control panel has two switches. Refer to the Hewlett-Packard manual for operating procedures.

There are three buttons. The power button and light should always be used to turn the printer on and off. Using a power strip, surge protector, or a wall-mounted switch to turn on the printer may cause premature printer failure.

The cancel button stops the print task.

The resume button and light is used when the light above the resume button is flashing. Press the button to continue printing.

Varian software does not support two sided printing.

Hewlett-Packard DeskJet 970Cxi Printer

Printer I/O	Centronics Parallel Universal serial bus 1284-B receptacle
Printer Language	HP PCL 3.
Printer Memory	512 Kbyte standard memory sufficient for full page graphics at 600 dpi.
Cartridges	black and color
Resolution	Black – 600 x 600 dpi Color – depends on paper type
Pages per Minute	Black – 12 ppm Black and color – 10 ppm
Configuration Control	Software controlled.

The Hewlett-Packard 970CXI features 600 dpi color printing and is software controlled. It has a color cartridge and a black cartridge. The control panel has two switches. Refer to the Hewlett-Packard manual for operating procedures.

There are three buttons. The power button and light should always be used to turn the printer on and off. Using a power strip, surge protector, or a wall-mounted switch to turn on the printer may cause premature printer failure.

The cancel button stops the print task.

The resume button and light is used when the light above the resume button is flashing. Press the button to continue printing.

Varian software does not support two sided printing.

Hewlett-Packard LaserJet 2300 Printer

Printer I/O	Centronics Parallel, USB port
Printer Language	HP PCL 6
Printer Memory	4 MB standard memory (expandable to 52 MB
Cartridges	black
Resolution	1200 x 1200 dpi
Pages per Minute	10 ppm
Configuration Control	Software controlled.
Devicetable entry	LaserJet_600 and LaserJet_600R

The Hewlett-Packard LaserJet 2100 features 1200 dpi printing and is software controlled. The control panel has two switches and two lights. Refer to the Hewlett-Packard manual for operating procedures.

Self-Test Procedure

To print the configuration page, press and release the **go** (large button at bottom of control panel) and **job cancel** (button at top of control panel with upside down triangle) buttons simultaneously when the printer is in the ready mode.

Hewlett-Packard LaserJet 2100 Printer

Printer I/O	Centronics Parallel, 1284-B receptacle LocalTalk port
Printer Language	HP PCL 6
Printer Memory	4 MB standard memory (expandable to 52 MB
Cartridges	black
Resolution	1200 x 1200 dpi
Pages per Minute	10 ppm
Configuration Control	Software controlled.

The Hewlett-Packard LaserJet 2100 features 1200 dpi printing and is software controlled. The control panel has two switches and two lights. Refer to the Hewlett-Packard manual for operating procedures.

Self-Test Procedure

To print the configuration page, press and release the **go** (large button at bottom of control panel) and **job cancel** (button at top of control panel with upside down triangle) buttons simultaneously when the printer is in the ready mode.

Hewlett-Packard Color LaserJet 4550 Printer

Printer I/O	Bidirectional parallel port (requires a “C” connector), Two Enhanced Input/Output (EIO) slots; paper handling accessory port; infrared receiver port. IEEE compliant, 1 open EIO slot, HP JetDirect EIO print server for fast Ethernet 10/100Base-TX in second EIO slot. (optional) HP JetDirect 600N and 610N (EIO) internal print servers, external print servers, connectivity card
Printer Language	HP PCL 5C, PostScript Level 3 Emulation, HP PCL 6
Printer Memory	64 MB standard memory (expandable to 192 MB)
Resolution	600 dpi
Pages per Minute	16 ppm (black); 4 ppm (color)
Configuration Switches	Expanded Control Panel

Operation

Set up the printer as described in the Hewlett-Packard manual. Specify the printer as a PostScript printer. On the `Name` and `Type` lines in the file `/vnmr/devicenames`, enter `PS` for a printer and `PS_AR` for a plotter. In the user’s `global` file, set `maxpen=8`.

Hewlett-Packard LaserJet 5000 Series Printers

Printer I/O	IEEE 1284-compliant bidirectional parallel, RS-232 9-pin serial, 2 PCI-based EIO slots
Printer Language	HP PCL 5e, HP PCL 6, and Postscript Level 2 emulation
Printer Memory	4 MB standard memory (expandable to 100 MB)
Resolution	1200 dpi
Pages per Minute	16 ppm
Configuration Switches	Control Panel

Overview

The Hewlett-Packard 5000 provides large format (11 x 17") printing at 16 pages per minute.

The control panel has an LCD display, three LEDs and six buttons.

The LaserJet 5000 features 1200 dpi resolution, but for NMR typical applications the plot lines are too fine. You may even fail to plot a full page at this resolution without expanding the printer memory since a full 11 x 17" page takes up to 32 MBytes of pixel information. Also even in parallel interface applications transferring data is unacceptably slow. For good plot resolution, 600 dpi is a good choice; for publication quality spectra and reproduction 300 dpi is a better option since the plot looks darker.

Switching between large and standard formats requires changing the paper size in the printer configuration menu on the LaserJet 5000.

Self-Test Procedure

1. Load paper and toner cartridge. Press the **Go** button to turn printer on. Wait until the printer warms up.
2. The `READY` message should be displayed.
3. Press **Menu** until the display reads **INFORMATION MENU**.
4. Press **Item** until the display reads **PRINT CONFIGURATION**.
5. Press **Select** to print the configuration page.
6. The configuration page shows the printer's current configuration.

Operation

Set up as described in the Hewlett-Packard printer manual.

Hewlett-Packard Color Inkjet CP1700 Printer

Printer I/O	Bidirectional parallel port (requires a "C" connector) Two Enhanced Input/Output (EIO) slots Paper handling accessory port Infrared receiver port. USB, IEEE-1284 (parallel), Infrared, and network LIO. (optional) HP JetDirect 600N and 610N (EIO) internal print servers, external print servers, connectivity card
Printer Language	HP color Inkjet cp1700: HP PCL 3 enhanced HP color Inkjet cp1700d: HP PCL 3 enhanced HP color Inkjet cp1700ps: HP PCL 3 enhanced
Printer Memory	16 megabyte (MB) built-in random access memory (RAM), cannot be upgraded. 4 megabytes (MB) built-in read only memory (ROM), cannot be upgraded
Resolution	1200 x 1200 dpi (black); 2400 x 1200 dpi (color)
Pages per Minute	16 ppm (black); 14.5 ppm (color)

Overview

The control panel has an LCD display representing ink levels and printer status. There are also three push buttons to control power on/off, resume, and cancel. The resume and power switches have a LED associated with them.

The CP1700D features 1200 dpi resolution for black and white printing and 2400 dpi for color, but for NMR typical applications the plot lines are too fine. It might not be possible to plot a full page at this resolution without expanding the printer memory because a full 11 x 17 page takes up to 32 MBytes of pixel information. Also, even in parallel interface applications transferring data is unacceptably slow. For good plot resolution, 600 dpi is a good choice; for publication quality spectra and reproduction 300 dpi is a better option since the plot looks darker.

Self-Test Procedure

1. Load paper, ink tanks, and print heads.

2. Press the power button to turn printer on. Wait until the printer initializes and reports `Ready`.
3. Press and hold the **resume** button on the control panel for three seconds until the LCD display reports `processing Job`.
4. Release the button. A test page is automatically printed.

Operation

Set up as described in the Hewlett-Packard printer manual.

Appendix B. Locator Administration

Sections in this appendix:

- "Restricting User's Data Viewing Privileges in Locator," page 119
- "Configuration Files," page 120
- "Large Database Recommendations," page 120
- "Network Database," page 121
- "Database Hints," page 122

Restricting User's Data Viewing Privileges in Locator

The system administrator can restrict how files appear in the Locator for each user. An access list controls which users can see which data.

Show the Access List

Use these steps to show the Access field in the User Information panel on the right side of the VnmrJ Admin interface.

1. Open the **VnmrJ Administration** interface if is not already open.
2. Click the button with the user's name to select the user.
3. Open the **Users Defaults** window, select **Configure** -> **Users** -> **Defaults**).
4. Check the **show** column of access.
5. Click **OK**.

   An **Access** line appears in the User Information panel on the right side of the VnmrJ Admin interface.

Access List

The following steps describe how to set up an access list for a user.

1. Select a user account by clicking the user name button.
2. Enter a space-separated list of user whose files the selected user can access.

   For example, if user1 will be allowed to view files for user2, user3, and user99, enter: `user2 user3 user99`
3. Click **Save User**.
4. Repeat for each user.

Configuration Files

Configuration files for the Locator are contained in the following directories for the different appmode types:

Interface	*Directory*
Standard (experimental)	`/vnmr/shuffler`
Imaging	`/vnmr/imaging/shuffler`
Walkup	`/vnmr/walkup/shuffler`
Individual users	`$vnmruser/shuffler`

Large Database Recommendations

The maximum number of items to display in the Locator can be controlled by setting its value in Systems Settings window.

Do one of the following depending upon the VnmrJ interface:

- **Imager Interface**:
  a. Select **Tools**.
  b. Select **System settings**.
  c. Click the **Display/Plot** tab.
  d. Enter a value for **Max # of items to show in Locator**.
- **Liquids Interface** (Walkup or experimental):
  a. Select **Edit**.
  b. Select **System settings**.
  c. Click the **Display/Plot** tab.
  d. Enter a value for **Max # of items to show in Locator**.

Setting **Max # of items to show in Locator** higher than 2000 slows down the response of the Locator by filling Locator table with a large number of rows. A value between 1000 to 2000 gives optimal performance. A row is shown with the word *Truncated* if the database returns more items than the limit. The message indicates that more items returned but are not shown in the Locator to save time.,

Use the following guidelines if the database contains more than 10000 items:

- Set the Locator to show only items that match the criteria of the statement as follows:
  - **Imager Interface**:
  a. Select **Tools**.
  b. Select **System settings**.
  c. Click the **Display/Plot** tab.
  d. Check the box next to **Display only matching items in locator**.
  - **Liquids Interface** (Walkup or experimental):
  a. Select **Edit**.
  b. Select **System settings**.
  c. Click the **Display/Plot** tab.
  d. Check the box next to **Display only matching items in locator**.

- Set values in the Locator statement to match 1000 or 2000 items.Do not values in the Locator statement of *all*, etc.
- Use the File Browser to limit the directory scope. The Locator only matches items that are in and under the directory the browser defines if the File Browser is displayed.
- Set **Max # of items to show in Locator** to between **1000** to **2000**.

Network Database

Several computers running VnmrJ can access the same Postgres database server. This way, all of the VnmrJ users will have immediate access to data saved on other machines (if the user has access to that data of course).

This access requires that all computers running in network database mode be mounted to any directories of other computers containing data that is intended to be accessed. The mounts can be hard mounts listed in the `vfstab` file or automount, but somehow they must be mounted to gain access.

Set the environment variable `PGHOST` to the host name of the machine to use for the DB server in every user account. The default is the local host. Different users can use different DB servers or some computers can use their own database server. A computer which is to be a DB server will need the Postgres postmaster daemon running on it. Even if it is running, if `PGHOST` is set to a remote computer, the remote computer will be used.

Non DB server computers default to network mode DB access by comparing `PGHOST` with the local host name. Specifying a remote host sets the non DB server computer in network mode. The DB server computer has itself as `PGHOST` and the VnmrJ administrator on the server computer must create an empty file

`/usr/varian/config/NMR_NETWORK_DB`

to force it into network mode. Data access from other computers will not work correctly if this is not done. Setting this variable on non server computer will force it into network mode.

The file `/usr/varian/config/NMR_NETWORK_DB`, if it is used, must to be in place before `dbsetup` is run during installation or the DB will not be set up correctly.

The attribute `'hostdest'` in the database contains the host name where the file actually resides (destination) when a computer is set up for network mode. The attribute `'host_fullpath'` contains `hostdest:`*`fullpath`* where *`fullpath`* is the path as it looks on the machine, `hostdest`. It does show the mounted path from the current machine.

Pushing `automount` relations from a server makes the following necessary:

VnmrJ must be able to translate between the mounted path and the actual path on the destination computer. It will first look for a file

`'/usr/varian/mount_name_table'`

It only uses this file if it is found. An example of this file is as follows:

```
# Table of remote system mount names and paths
# One line per entry, Syntax:|
#     host:direct_path  mount_path
mongoose:/export/home     /mongoose_home
voyager:/export/home      /home
```

If `'mount_name_table'` is not found, it looks in `'/etc/mnttab'` and in `'/etc/auto_direct'` and gets relationships out of these. If automount relations are pushed from a server, they will not always be available in these files and will need to be put into a 'mount_name_table file'. Mounts from the vfstab file and from the local auto_direct file, should work properly without a 'mount_name_table' file.

Changing the UNIX port number should not normally be necessary, but might be done if more than one Postgres daemon is to run on the system at one time. The port will default to 5432 unless specified otherwise in every users .login file with the environment variable, PGPORT. It should be possible for different users (and thus different groups) to use entirely different database daemons and databases on the same computer. If PGPORT is set to something other than 5432, then every user on every computer using that DB server, will need PGPORT set in their accounts.

Database Hints

If the Locator shows **Error** under the column headings, or if the error message DataBase contents version is not correct… appears on the bottom of the screen, exit VnmrJ and run **dbsetup** in a terminal window.

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